The Laboratory of Theoretical Bases of Microelectronics: 30 years

(Book of Abstracts)

(1998-2018)

Ioffe Institute

St. Petersburg

2018

The Laboratory of Theoretical Bases of Microelectronics: 30 years
(Book of Abstracts: 1998-2018)

Editor:
V. S. Kharlamov

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http://www.ioffe.ru/Dep_TM/abst30.html

The 10th Jubilee of the Laboratory Abstract Collection (1988 – 1998) is available at:
http://www.ioffe.ru/Dep_TM/abst10.html

Table of Contents

Foreword

30 years ago, the Laboratory of the Theoretical Bases of the Microelectronics was founded at Ioffe Institute. During these years, we had to wage a continuous struggle against the underwater currents and squally winds which been knocking down us from the right course. We are proud that we managed to keep the right directions of research, which, we hope, are still at the forefront. Now-days and former members of our Lab became leading scientists in Russia and around the world.

You can find below the Foreword to the Abstract Collection issued to 10th Jubilee of the Lab. Of course, the collaboration of the Lab with experimental and theoretical groups at Ioffe Institute, in Russia, and around the world became much wider. It is why the list of our partners is too long to be presented in this brief Foreword. However, it is easy to get a picture of the collaboration by looking at the list of the coauthors of the abstracts presented.

The members of our Lab are very active as lecturers in number of Universities. The list of the Universities of the Foreword presented below, should be expanded by the St.-Petersburg Academic University and the ITMO University.

The Lab members were awarded a number of Russian and International scientific awards including the special awards and grants for students and young scientist. Two members of the Lab were awarded in 2001 the State Prize of the Russian Federation.

Foreword to the 10th Jubilee Abstract Collection

It is 10 years since the Laboratory of Theoretical Bases of Microelectronics headed by Prof. R.A. Suris was founded in summer of 1988.

The main fields of research at the Laboratory include:

- Electronic and optical properties of low-dimensional semiconductor heterostructures
- Theory of epitaxial growth of semiconductor compounds

- Physics of bulk, quantum well, and quantum dot semiconductor heterostructure lasers
- Physics of carbon nanoclusters (fullerens and nanotubes)
- Physics of radiation properties in semiconductor alloys and multilayered structures
- Properties of HTSC films and devices

The Solid State Physics Sub-Faculty of the St. Petersburg State Technical University was also founded in 1988. Graduate and post-graduate students of this sub-faculty have been actively participating in the research carried out by the laboratory staff. The laboratory and sub-faculty form the bases of the center for theoretical investigation and mathematical simulation of nanostructures and related devices. In these scientific streams, the laboratory members participate in the intensive co-operative research together with experimentalists and technologists at Ioffe Institute working at laboratories and groups headed by Profs. S. A. Gurevich, V. I. Ivanov-Omskii, P. S. Kop'ev, A. Ya. Shik, A. N. Titkov, Yu. P. Yakovlev, Drs. B. Ya. Ber, V. P. Evtihiev, S. V. Ivanov, V. P. Kochereshko, T. L. Makarova, I. S. Tarasov, as well as at the St.-Petersburg State Electro-Technical University: Prof. L. E. Vorobiev, Prof. V. F. Masterov; Dr. A. V. Bobyl'; and at the State Optical Institute: Dr. I. A. Khrebtov.

The staff is also strongly involved in the international scientific collaboration with several groups headed by:

- Prof. F. Beltram, Scuole Normale Superiore, Pisa, Italy
- Prof. Yu. M. Galperin, University of Oslo, Norway
- Prof. P. Lavallard, Groupe de Physique des Solides, Universités Paris 6 et Paris 7, France
- Prof. M. Militzer, Centrte for Metallurgical Process Engineering, The University of British Columbia, Canada, Vancouver
- Prof. W. Ossau, Physicalisches Institut der Universitaet Wuerzburg, Germany
- Dr. J. Pezoldt, Technische Universitaet Ilmenau, Instutut fuer Festkoerperelektronik, Germany, Ilmenau
- Prof. W. Pompe, Technische Universitaet Dresden, Instutut fuer Werkstoffwissenschaft, Germany, Dresden

- Dr. W. Scorupa, Forschungszentrum Rossendorf, Instutut fuer Ionenstrahlphysik und Materialforschung, Germany, Rossendorf
- Prof. N. V. Tkach, Chernovtsy State University, Ukraine
- Prof. H. W. Weber, Atominstitut der Oesterreichischen Universitaeten, Austria, Wien

Among the sector members there are three professors and assistant professors that give lectures and conduct exercises at the State Technical and State Electro-Technical Universities. The courses currently read are:

- R. A. Suris, Tunnel Phenomena in Solids and Wave Function Engineering
- Yu. V. Trushin, Material Science
- G. G. Zegrya, Physics
- V. V. Rotkin, Bases of Quantum-Field Theory of Solid State

During this 10-year period the Laboratory members have participated in 12 works awarded with the prizes of Ioffe Institut and Solid State Electronics Department and with Rank Prize in optoelectronics (see appendix).
The Laboratory members have been strongly involved in the organization of a number of international and national scientific conferences and symposiums as the members of Program and Organizing Committees (see appendix).

Staff

Current Staff

Robert A. Suris	Scientific Advisor of the Laboratory	Full member of the Russian Academy of Sciences, Prof., Dr. Sci.
Georgy G. Zegrya	Head of the Laboratory	Professor, Dr. Sci.
Yuri V. Trushin	Chief Researcher	Professor, Dr. Sci.
Vladimir S. Kharlamov	Senior Researcher	Dr. (Ph. D.)
Alexey G. Petrov	Senior Researcher	Dr. (Ph. D.)
Andrew A. Greshnov	Senior Researcher	Dr. (Ph. D.)
Marina A. Semina	Senior Researcher	Dr. (Ph. D.)
Andrey M. Boiko	Researcher	Dr. (Ph. D.)
Ivan A. Dmitriev	Researcher	Dr. (Ph. D.)
Andrey A. Bogdanov	Researcher	Dr. (Ph. D.)
Dmitri M. Samosvat	Researcher	Dr. (Ph. D.)
Leonid V. Danilov	Researcher	
Nikolay V. Pavlov	Junior Researcher	
Alexander N. Afanasiev	Junior Researcher	
Vitali M. Freiman	Engineer-researcher	
Vasili B. Korsakov	Leading Engineer	
Margarita F. Bryzhina	Leading Engineer	
Natalia D. Koblinetz	Senior Engineer	
Anastasia A. Karpova	Laboratory Assistant	

Former members of the Laboratory in 1998-2018

Levon V. Asryan	Virginia Polytechnic Institute and State University, USA
Slava V. Rotkin	Lehigh University, USA
Daniel V. Shantsev	University of Oslo, Norway
Dmitri V. Kulikov	St.Petersburg Academic University, Russia
Anatoli S. Polkovnikov	Boston University, USA
Rinat A. Sergeev	Harvard University, USA
Maxim N. Lubov	St.Petersburg Academic University, Russia
Andrey Yu. Serov	University of Illinois, USA

Appendix

Awards of the Laboratory members:

- A. A. Bogdanov, 2013 Laureate of competition of business ideas, scientific and technical developments and research projects under the motto "Young. Cheeky. Perspective." For work: "Development of a tunable metamaterial based on a semiconductor superlattice for the control of terahertz radiation"

- R. A. Suris, A.F. 2008 Ioffe Prize by Government of St. Petersburg and St. Petersburg Scientific Center of the Russian Academy of Sciences for the series of works "Theoretical study of low-dimensional surface phenomena in semiconductors"

- R. A. Suris, M. P. Petrov, V. V. Bryskin, 2006 A.F. Ioffe Prize by Ioffe Institute of the Russian Academy of Sciences for the series of works "Waves of charge exchange in semiconductors"

- R. A. Suris, 2005 A.F. Ioffe Prize by Ioffe Institute of the Russian Academy of Sciences for a series of works "Investigation of semiconductor superlattices based on quantum wells and quantum dots"

- I. A. Dmitriev, 2004 AIXTRON Young Scientist Award at 12 International Symposium “Nanostructures: Physics and Technology”

- I. A. Dmitriev, R. A. Suris, 2003 Prize for the best series of works of the International Academic Publishing Company “Nauka”

- I. A. Dmitriev, 2003 INTEL Young Scientist Award at VI National Russian Conference on Semiconductor Physics

- I. A. Dmitriev, 2002 Best Research Award at Workshop “Frontiers in Electronics” WOFE-02, St. Croix (2002)

- Zh. I. Alferov, L. V. Asryan, D. Bimberg, P. S. Kop'ev, N. N. Ledentsov, V. A. Shchukin, R. A. Suris, and V. M. Ustinov. Highest Award (State Prize) of the Russian Federation in Science and Technology for the year 2001 with the citation: “For fundamental investigations of heterostructures with quantum dots and development of quantum dot lasers”

- M. V. Maximov, L. V. Asryan, Yu. M. Shernyakov, A. F. Tsatsul'nikov, I. N. Kaiander, V. V. Nikolaev, A. R. Kovsh, S. S. Mikhrin, V. M. Ustinov, A. E. Zhukov, Zh. I. Alferov, N. N. Ledentsov, and D. Bimberg. First Best Paper Award of the IEEE Journal of Quantum Electronics for the paper *“Gain and threshold characteristics of long wavelength lasers based on InAs/GaAs quantum dots formed by activated alloy phase separation,” IEEE J. Quantum Electron.*, vol. 37, no. 5, pp. 676-683, May 2001.

- I. A. Dmitriev, 2001 Ioffe Institute Prize for Junior Scientists for the Best Research

- I. A. Dmitriev, 1999 Prize for the Best Research at the Russian National Conference on Physics of Semiconductors and Semiconductor Opto- and Nanoelectronics for Junior Scientists.

Heterostructures and superlattices

J. Phys.: Conf. Ser.
vol. 1038, no. 1, pp. 012056, 2018

Study of Strained Superlattices Grown by MOCVD Method

I. V. Fedorov, R. V. Levin, L. A. Sokura, L. V. Danilov

This study is dedicated to the development of the technology of InAs/GaSb superlattice by MOCVD. There was obtained an InAs/GaSb superlattice consisting of 10 pairs of alternating layers of InAs and GaSb grown at the temperature of 500°C. The obtained structures were studied by transmission electron microscopy (TEM) and photoluminescence (PL). Also, a light-emitting structure with quantum well was obtained to substantiate the developed technology.

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Semiconductors
vol. 50, no. 3, pp. 314-319, 2016

Role of acoustoelectric interaction in the formation of nanoscale periodic structures of adsorbed atoms

R. M. Peleshchak, I. I. Lazurchak, O. V. Kuzyk,
O. O. Dan'kiv, G. G. Zegrya

The role of acoustoelectric effects in the formation of nanoscale structures of adatoms, resulting from the self-consistent interaction of adatoms with a surface acoustic wave and the electronic subsystem, is studied for the case of charged and uncharged adatoms. It is shown that an increase in the doping level of a semiconductor with donor impurities at a fixed average adatom concentration results in an increase in the critical temperature below which self-organization processes occur.

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Semiconductors
vol. 47, no. 4, pp. 514-524, 2013

Theory of space-charge-limited ballistic currents in nanostructures of different dimensionalities

M. V. Beznogov, R. A. Suris

A new unified approach to the description of ballistic unipolar-injection currents is proposed for nanostructures of different dimensionalities. It is shown that in the case of three-dimensional (3D), two-dimensional (2D), and one-dimensional (1D) structures the problem can be reduced to a nonlinear integral equation with a dimensionless parameter determining the coefficient of the universal current-voltage characteristic. The existence of a maximum for this parameter, which is analogous to the Bursian limit for a vacuum diode, is proven for each dimensionality. The current-voltage characteristics and the potential and charge distributions are calculated for 3D, 2D, and 1D structures.

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Phys. Solid State
vol. 55, no. 10, pp. 2182-2189, 2013

Quasi-stationary electron states in a multilayered structure in longitudinal electric and transverse magnetic fields

G. G. Zegrya, N. V. Tkach, I. V. Boiko, Yu. A. Seti

A theory of spectral parameters, dynamic conductivity, and relative integrated emission intensity has been proposed in the model of the open resonant-tunneling structure as a separate cascade of a quantum cascade laser in a transverse magnetic field. It has been shown that, according to the experiment by Blaser and colleagues, as the magnetic field strength increases to 8 T, the emission peak shifts to higher energies, while its relative integrated intensity in the strength range of 0–14 T decreases abruptly

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Rom. J. Phys.
vol. 57, no. 3-4, pp. 620-629, 2012

Conductivity of three-barrier resonance tunnel structure

M. V. Tkach, Y. O. Seti, O. M. Voitsekhivska, G. G. Zegrya

Within the model of rectangular potentials and different effective electron masses it is developed a theory and performed a quantum-mechanical calculation of dynamical conductivity for the electrons interacting with electromagnetic field in open three-barrier resonance tunnel structure with arbitrary outer barriers. For the experimentally investigated structure with $In_{0.53}Ga_{0.47}As$-wells and $In_{0.52}Al_{0.48}As$-barriers, it is shown that there exist the optimal geometrical configurations determined by the position of the inner barrier respectively the outer ones, providing the optimal operation of nano-device as a separate detector or an active element of such a detector in desired frequency range.

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JETP Lett.
vol. 76, no. 4, pp. 222-226, 2002

Cyclotron resonance in the InAs/GaSb heterostructure in an inclined magnetic field

A. A. Greshnov, G. G. Zegrya, Yu. B. Vasil'ev, S. D. Suchalkin, B. Ya. Mel'tser, S. V. Ivanov, P. S. Kop'ev

The mechanism of cyclotron resonance line splitting in the InAs/GaSb heterostructure in an inclined magnetic field has been studied experimentally and theoretically. It is shown that the admixing of electron and hole states leads to anticrossing of the Landau levels and, hence, to splitting of the cyclotron resonance line. In the case of an inclined magnetic field, the splitting is not observed, which is explained by the suppression of the admixing of electron and hole states due to the occurrence of an additional barrier for electrons and holes given a longitudinal magnetic field component.

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Semiconductors
vol. 34, no. 10, pp. 1172-1176, 2000

Influence of an electric field on the strained state of a heterostructure

R. M. Peleshchak, B. A. Lukiyanets, G. G. Zegrya

In the framework of an electron–deformation model, a mechanism of electron–deformation dipole formation at a strained heterointerface was considered. For a ZnSe/ZnS heterostructure, an external electric field ~120 kV/cm normal to the heterointerface brought about an additional compression strain of ~4% (~3%) in the ZnSe (ZnS) lattice. For an opposite field direction, a tensile strain of ~5% (~5%) was observed.

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Phys. Low-Dim. Struct
vol. 1998, no. 9-10, pp. 43-54, 1998

Nonlinear electron transport in semiconductor superlattices in transverse magnetic field

B. Shchamkhalova, R. A. Suris

Magnetotransport phenomena in semiconductor superlattices (SL) are shown to depend nonlinearly on the electric field in a transverse magnetic field. The magnetoresistivity along the SL layers changes its sign with increasing electric field. The Hall voltage depends nonlinearly on both the magnetic field strength and the current density in the structure.

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Quantum wells

J. Phys.: Conf. Ser.
vol. 1038, no. 1, 012122, 2018

Intraband light absorption by holes in InGaAsP/InP quantum wells

N. V Pavlov, G. G. Zegrya

A microscopic analysis of the radiation intraband absorption mechanism by holes with their transition to a spin-split band for quantum wells based on InGaAsP/InP solid solutions is performed within the framework of the four-band Kane model. The calculation is made for two polarizations of the incident radiation: along the crystal growth axis and in the plane of the quantum well. It is shown that this process can be the main mechanism of internal radiation losses for quantum well lasers. It is also shown that the dependence of the absorption coefficient on the width of the quantum well has a maximum at a well width from 40 to 60 A.

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Semiconductors
vol. 52, no. 8, pp. 1037-1042, 2018

Photoconductivity amplification in a type-II n-GaSb/InAs/p-GaSb heterostructure with a single QW

M. P. Mikhailova, I. A. Andreev, G. G. Konovalov, L. V. Danilov, E. V. Ivanov, E. V. Kunitsyna, N. D. Il'inskaya, R. V. Levin, B. V. Pushnyi, Yu. P. Yakovlev

Significant photocurrent/photoconductivity amplification is observed at low reverse biases in a type-II n-GaSb/InAs/p-GaSb heterostructure with a single quantum well (QW), grown by metal-organic vapor phase epitaxy. A sharp increase in the photocurrent by more than two orders of magnitude occurs under exposure of the heterostructure to monochromatic light with a wavelength of 1.2–1.6 μm (at 77 K) and the application of a reverse bias in the range 5–200 mV. The optical gain depends on the applied voltage and increases to 2.5 × 102 at a reverse bias of 800 mV. Theoretical analysis demonstrated that the main role in the phenomenon is played by the screening of the external electric field

by electrons accumulated in the deep InAs QW and by the mechanism of the tunneling transport of carriers with a small effective mass. It is shown that the effect under study is common to both isotype and anisotype type-II heterojunctions, including structures with QWs and superlattices.

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Semiconductors
vol. 52, no. 4, pp. 493-496, 2018

Enhancement of photoconductivity by carrier screening effect in n-GaSb/InAs/p-GaSb heterostructure with single deep quantum well

L. V. Danilov, M. P. Mikhailova, R. V. Levin, G. G. Konovalov, E. V. Ivanov, I. A. Andreev, B. V. Pushnyi, G. G. Zegrya

n-GaSb/n-InAs/p-GaSb heterostructure with a single InAs QW was grown for the first time by MOVPE. Photocurrent spectra were obtained at reverse bias in the range from 0 to 0.8 V. It was shown that the photocurrent increases nonlinearly. The maximum of differential photoconductivity is archived at low applied voltage up to 0.2 V. This effect was explained by electrostatic screening of electrons localized in QW.

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Semiconductors
vol. 52, no. 2, pp. 195-208, 2018

Intraband radiation absorption by holes in InAsSb/AlSb and InGaAsP/InP quantum wells

N. V. Pavlov, G. G. Zegrya, A. G. Zegrya, V. E. Bugrov

Microscopic analysis of intraband radiation absorption by holes with their transition to the spin-split band for InAsSb/AlSb and InGaAsP/InP semiconductor quantum wells is performed in the context of the four-band Kane model. The calculation is performed for two incident-

radiation polarizations: along the crystal-growth axis and in the quantum-well plane. It is demonstrated that absorption with transition to the discrete spectrum of spin-split holes has a higher intensity than absorption with transitions to the continuous spectrum. The dependences of the intraband absorption coefficient on temperature, hole density, and quantum- well width are thoroughly analyzed. It is shown that intraband radiation absorption can be the main mechanism of internal radiation losses in lasers based on quantum wells.

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Semiconductors
vol. 51, no. 10, pp. 1343-1349, 2017

Vertical transport in type-II heterojunctions with InAs/GaSb/AlSb composite quantum wells in a high magnetic field

M. P. Mikhailova, V. A. Berezovets, R. V. Parfeniev, L. V. Danilov, M. O. Safonchik, A. Hospodková, J. Pangrác, E. Hulicius

Vertical transport in type-II heterojunctions with a two-barrier AlSb/InAs/GaSb/AlSb quantum well (QW) grown by MOVPE on an *n*-InAs (100) substrate is investigated in quantizing magnetic fields up to $B = 14$ T at low temperatures $T = 1.5$ and 4.2 K. The width of the QWs is selected from the formation condition of the inverted band structure. Shubnikov–de Haas oscillations are measured at two orientations of the magnetic field (perpendicular and parallel) relative to the structure plane. It is established that conduction in the structure under study is occurs via both three-dimensional (3D) substrate electrons and two-dimensional 2D QW electrons under quantum limit conditions for bulk electrons ($B > 5$ T). The electron concentrations in the substrate and InAs QW are determined. The g-factor for 3D carriers is determined by spin splitting of the zero Landau level. It is shown that the conductance maxima in a magnetic field perpendicular to the structure plane and parallel to the current across the structure in fields $B > 9$ T correspond to the resonant tunneling of 3D electrons from the emitter substrate into the InAs QW through the 2D electron states of the Landau levels.

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Semiconductors
vol. 51, no. 9, pp. 1148-1152, 2017

Effect of electrostatic shielding on the photoelectric properties of heterostructures with deep QWs

L. V. Danilov, M. P. Mikhailova, I. A. Andreev, G. G. Zegrya

The effect of the electrostatic potential induced by charge carriers of the same sign, localized in a deep quantum well, on the current–voltage characteristics of photodetector heterostructures is theoretically analyzed. It is shown for the example of a *p–i–n* structure with a single deep quantum well in the i-type region that the shielding of an external electric field makes the differential photoconductivity of the heterostructure higher than that in a *p–i–n* structure without an intermediate 2D layer.

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J. Phys.: Conf. Ser.
vol. 769, no. 1, 012076, 2016

Intersubband light absorption by holes in InAsSb/AlSb quantum well heterostructures

N. V. Pavlov, G. G. Zegrya

The absorption coefficients of intersubband optical transitions in the valence band of the AlSb/$InAs_{0.84}Sb_{0.16}$/AlSb quantum wells in framework of the four-band Kane model. It is established that the light absorption by holes may lead to the laser generation breakdown. It is shown that we need to decrease the quantum well width to range a<6 nm to neutralize the negative influence of this effect.

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J. Phys.: Conf. Ser.
vol. 661, no. 1, 012052, 2015

Effect of subband nonparabolicity on optical properties of InSbAs/AlSb deep quantum well heterostructures

N. V. Pavlov, G. G. Zegrya

Optical properties of heterostructures with deep quantum wells have been studied in the framework of four-band Kane mode permitting a nonparabolic energy spectrum of charge carriers to be taken into account. The system $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ was used as an example. It is established that the nonparabolicity weakly influences the overlap integral between *s*- and *p*-states, but notably increase the state density and optical absorption coefficient in the conduction band.

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Proc. SPIE
vol. 9450, 94500J, 2015

Superlinearity and temperature dependence of electroluminescence in heterostructures with deep AlSb/InAs1-xSbx/AlSb quantum well

M. Mikhailova, E. Ivanov, L. Danilov, A. Petukhov, K. Kalinina, N. Stoyanov, Yu. Yakovlev, A. Hospodková, J. Pangrác, J, Oswald, M. Ziková, E. Hulicius

We report on superlinear electroluminescent structures based on $AlSb/InAs_{1-x}Sb_x/AlSb$ deep quantum well grown by MOVPE on n-GaSb:Te substrate. Dependence of the electroluminescence (EL) spectra and optical power on the drive current in nanoheterostructures with $AlSb/InAs_{1-x}Sb_x/AlSb$ quantum well at 77 – 300 K temperature range was studied. Intensive two-band superlinear EL in the 0.5 - 0.8 eV photon energy range was observed. Optical power enhancement with the increasing drive current at room temperature is caused by the contribution of the additional electron-hole pairs due to the impact ionization by the electrons heated at the high band offset between AlSb and the first electron level E_{e1} in the InAsSb QW. Study of the EL

temperature dependence at 90 – 300 K range enabled us to define the role of the first and second heavy hole levels in the radiative recombination process. It was shown that with the temperature decrease, the relation between the energies of the valence band offset and the second heavy hole energy level changes due to the temperature transformation of the energy band diagram. That is why the EL spectrum revealed radiative transitions from the first electron level E_{e1} to the first hole level E_{h1} in the whole temperature range (90 – 300 K) while the emission band related with the transitions to the second hole level occurred only at T < 200 K.

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Semiconductors
vol. 49, no. 5, pp. 604-614, 2015

Effect of nonparabolicity of the electron and light-hole energy spectrum on the optical properties of heterostructures with deep AlSb/$InAs_{0.86}Sb_{0.14}$/AlSb quantum wells

N. V. Pavlov, G. G. Zegrya

The optical characteristics of heterostructures with deep quantum wells are studied using the AlSb/$InAs_{0.86}Sb_{0.14}$/AlSb structure within the framework of the four-band Kane model with regard to the nonparabolicity of the carrier energy spectrum. It is demonstrated that consideration of the nonparabolicity increases the number of size-quantization levels in the conduction band. At a quantum-well width of 100 Å, the investigated heterostructure contains three size-quantization levels within the parabolic model and six levels within the Kane model. This is due to the fact that the effective mass of high-energy electrons is found to be larger than the mass of electrons at the bottom of the conduction band by a factor of four. It is shown that account for the nonparabolicity only slightly affects the overlap integral for the *s* and *p* states, but significantly increases the density of states in the conduction band, which causes considerable growth in the radiation-absorption coefficient.

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Semiconductors
vol. 48, no. 9, pp 1185-1195, 2014

Optical properties of heterostructures with deep $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ quantum wells

N. V. Pavlov, G. G. Zegrya

Using the Kane model, the energy of the dimensional quantization levels, absorption coefficient, and radiative-recombination rate are calculated for interband optical transitions between different dimensional quantization subbands in a heterostructure with a deep $AlSb/InAs_{0.86}Sb_{0.14}/AlSb$ quantum well with regard to and without regard for the spin–orbit interaction. It is shown that the corrections introduced by the spin–orbit interaction in calculating these quantities are no larger than a few tens of percent even at spin–orbit interaction constants exceeding the band gap and account for the nonparabolicity in the calculation of the energy of dimensional quantization levels and absorption coefficient is much more important than account for the spin–orbit interaction. In calculation of the radiativere-combination rate, both these effects should be taken into account.

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Tech. Phys. Lett.
vol. 40, no. 10, pp. 883-886, 2014

The influence of the nonparabolic energy spectrum of charge carriers on the optical characteristics of $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ heterostructures with deep quantum wells

N. V. Pavlov, G. G. Zegrya

The optical characteristics of heterostructures with deep quantum wells have been studied by the example of the $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ system with allowance for a non-parabolic energy spectrum of charge carriers in the framework of the four-band Kane model. It is established that the

nonparabolicity weakly influences the overlap integral between *s* and *p* states, but leads to a significant increase in the density of states in the conduction band and, in turn, to a considerable growth in the optical absorption coefficient.

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Proc. SPIE
vol. 8781, 87810K, 2013

Enhancement of the optical power stimulated by impact ionization in GaSb-based heterostructures with deep quantum wells

M. Mikhailova, G. Zegrya, L. Danilov, E. Ivanov, K. Kalinina, N. Stoyanov, Kh. Salikhov, Yu. Yakovlev, E. Hulicius, A. Hospodkova, J. Pangrac, M. Zikova

We report on the observation of superlinear electroluminescence in nanoheterostructures based on GaSb with a deep narrow Al(As)Sb/InAsSb/Al(As)Sb quantum well in the active region, grown by metal organic vapor phase epitaxy. Electroluminescence spectra for different driving currents were measured at temperatures of 77 and 300 K. It is shown that such structure exhibits superlinear dependence of optical power on the drive current and its increase of 2-3 times in the current range 50-200 mA. This occurs due to impact ionization in the Al(As)Sb/InAsSb quantum well in which a large band offset at the interface ΔE_C = 1.27 eV exceeds ionization threshold energy for electrons in the narrow-gap well. Theoretical calculation of the size quantization energy levels is presented, and possible cases of impact ionization, depending on the band offset ΔE_C at the interface and on the quantum well width, are considered. This effect can be used to increase quantum efficiency and optical power of light emitting devices (LEDs, lasers) operating in mid-infrared spectral range, as well as for photovoltaic elements.

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Tech. Phys. Lett.
vol. 39, no. 3, pp. 255-257, 2013

Resonance Coulomb trapping of electrons in a deep quantum well

L. V. Danilov, G. G. Zegrya

The role of the Coulomb interaction in trapping of electrons in a deep quantum well is investigated. By an example of a three-level quantum well, the fundamental mechanisms of trapping of electrons are considered: upon interaction with optical phonons and Coulomb interaction of electrons with one another. The corresponding trapping probabilities and lifetimes of electrons are calculated. With regard to the effect of Auger recombination on the charge-carrier distribution in a quantum well, the system of rate equations for the nonstationary regime is solved and the time dependences of electron concentrations at the ground energy level in the quantum well are determined. The contribution of each recombination process is shown.

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Semiconductors
vol. 47, no. 10, pp 1347-1355, 2013

The role of electron-electron interaction in the process of charge-carrier capture in deep quantum wells

L. V. Danilov, G. G. Zegrya

The role of electron-electron interaction in the process of electron capture to a deep quantum well is investigated. Using two-level and three-level quantum wells as examples, the basic electron-capture mechanisms, i.e., the interaction with optical phonons and the Coulomb electron-electron interaction, are considered, and the corresponding capture probabilities and electron lifetimes are calculated. The effect of Auger recombination on the charge-carrier distribution in a quantum well is also taken into account. With this taken into consideration, a set of rate

equations is solved for a nonsteady-state mode, and the time dependences of the electron concentration at the ground energy level in the quantum well are found. The contributions of each of the recombination processes under consideration are shown.

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JETP Lett.
vol. 97, no. 2, pp. 102-106, 2013

Manifestation of a semimetallic state in cyclotron resonance in low-symmetry HgTe-based quantum wells

A. A. Greshnov, Yu. B. Vasil'ev, N. N. Mikhailov, G. Yu. Vasil'eva, D. Smirnov

Cyclotron-resonance measurements in 21-nm-thick HgTe/CdHgTe quantum wells of different crystallographic orientations have been performed. It has been found that, in contrast to the structures with the (001) orientation of the quantum-well plane, (013)-oriented quantum wells are semimetallic and their absorption spectra exhibit both electron and hole cyclotron-resonance lines. The simultaneous presence of the two types of charge carriers originates from an overlap between the upper heavy-hole quantum-confinement subbands *hh1* and *hh2*. This overlap is caused by the strong interaction of these subbands with the Dyakonov–Khaetskii interface state. Calculations carried out using the eight-band *kp*-Hamiltonian indicate that, for known values of the band-structure parameters, the overlap between *hh2* and *hh1* subbands does not occur; this result is in agreement with the cyclotron-resonance data for (001)-oriented structures. The enhanced interaction between heavy-hole and interface states owing to the existence of steps at low-symmetry heterointerfaces may be the mechanism responsible for the appearance of an overlap between subbands in HgTe quantum wells with orientation different from (001).

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AIP Conf. Proc.
vol. 1566, pp. 99-100, 2013

Magneto-infrared study of electron-hole system in strained semimetallic HgTe quantum wells

Yu. B. Vasilyev, N. N. Mikhailov, A. A. Greshnov, S. D. Suchalkin, L.-C. Tung, D. Smirnov, F. Gouider, G. Nachtwei

Magneto infrared absorption measurements have been performed on HgTe/CdHgTe quantum wells with different thicknesses grown on (013) GaAs substrate. Cyclotron resonance effective masses, inter-Landau-level transition energies and their dependence on magnetic field are measured. The measured intersubband energies are in good agreement with the theoretically calculated values [1]. Strong spin-orbit interaction is responsible for cyclotron resonance splitting in asymmetric quantum wells. We demonstrate that the increase of the quantum well thickness leads to a semimetallic state, allowing for simultaneous observation of holes and electron transitions.

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Semiconductors
vol. 46, no. 6, pp. 773-778, 2012

Optical transitions in $Cd_xHg_{1-x}Te$-based quantum wells and their analysis with account for the actual band structure of the material

N. L. Bazhenov, A. V. Shilyaev, K. D. Mynbaev, G. G. Zegrya

Quantum-confinement levels in a Cd_xHg_{1-x}Tebased rectangular quantum well are calculated in the framework of the four-band Kane model taking into account mixing between the states of electrons and three types of holes (heavy, light, and spin-split holes). Comparison of the calculation results with experimental data on the photoluminescence of $Cd_xHg_{1-x}Te$-based quantum wells suggests that optical transitions involving the conduction and light-hole bands are possibly observed in the spectra.

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JETP Lett.
vol. 92, no. 1, pp. 33-35, 2010

Pure spin currents generation under quantum wells photoionization

O. I. Utesov, G. G. Zegrya, A. A. Greshnov

A theory describing the generation of pure spin currents has been developed for the case of the photoionization of *n*-type quantum wells with spin–orbit splitting induced by the built-in electric field. It is shown that the optical transitions of electrons from the size-quantization level to the continuum give rise to two competing components of the pure spin current. An important feature of the process under study is an additional degree of freedom acquired by the charge carriers, which could be promising for spintronic applications.

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Semiconductors
vol. 42, no. 8, pp. 980-983, 2008

Effects of self-consistent electrostatic potential in quantum wells with several quantum confinement levels in high magnetic fields

A. A. Greshnov, G. G. Zegrya

The effect of self-consistent electrostatic potential on the spectrum of two-dimensional electron states in high magnetic fields is studied under the conditions where more than one quantum confinement subband is filled. The cases of magnetic field directed perpendicular to the quantum well plane and tilted magnetic field are considered. In the case of perpendicular magnetic field it is shown that two or more Landau levels that belong to different quantum confinement subbands can be degenerate in some ranges of concentrations (magnetic fields). The inclination of the magnetic field with respect to the growth direction produces opening of the energy gap between these levels; however, the gap as a function of concentration (magnetic field) remains almost constant in the same range of parameters.

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Semiconductors
vol. 42, no. 5, pp. 557-562, 2008

Threshold characteristics of an IR laser based on deep InAsSb/AlSb quantum well

L. V. Danilov, G. G. Zegrya

The basic threshold characteristics of a semiconductor IR laser based on a heterostructure with deep $InAs_{0.84}Sb_{0.16}$/AlSb quantum wells (QWs) have been studied. The threshold carrier densities and threshold current densities of radiative and Auger recombination (AR) were found. It is shown that at certain QW parameters the AR rate is strongly (by several orders of magnitude) suppressed. In this case, the emission wavelength falls within the interval 2–3.5 *μ*m, which corresponds to the mid-IR spectral range. The internal quantum efficiency of emission at the lasing threshold was calculated and its dependence on the QW width within the AR suppression range was demonstrated. The laser structure was optimized with respect to the number of QWs.

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AIP Conf. Proc.
vol. 893, pp. 493-494, 2007

Terahertz photovoltaic effect in bilayer two dimensional systems

Yu. B. Vasilyev, R. A. Suris, C. Stellmach, G. Nachtwei

We report the observation of THz photovoltage in double quantum wells in tilted magnetic field. The signal appears at the normal component of the magnetic field corresponding to the electron cyclotron resonance conditions and directly related to electron CR absorption. The phenomenon is accounted for by a photovoltaic effect in both electron-electron and electron-hole bilayer systems.

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Phys. Stat. Sol. B
vol. 243, no. 7, pp. 1625-1629, 2006

Analytical model for the quantum-confined Stark effect including electric field screening by non-equilibrium carriers

K. A. Bulashevich, S. Yu. Karpov, R. A. Suris

We have derived an analytical approximation for the energy levels in a symmetric quantum well applicable in a wide range of the electric field variation. Suppression of the quantum-confined Stark effect due to the electric field screening by non-equilibrium carriers is considered self-consistently within the perturbation theory. Theoretical predictions are compared with available observations. Specific features of the quantum-confined Stark effect in light-emitting diode heterostructures are discussed.

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JETP
vol. 99, no. 1, pp. 147-156, 2004

Resonant tunneling through a double-barrier quantum well in a transverse magnetic field

A. Yu. Serov, G. G. Zegrya

We theoretically analyze the tunneling of electrons through a heterostructure with two barriers and a quantum well between them in a magnetic field perpendicular to the current. We take into account the contribution from electrons with various positions of the magnetic oscillator center to the current. The region of the *Z*-shaped current–voltage characteristic for the heterostructure is shown to narrow as the magnetic field strengthens. Our analysis reveals a critical magnetic field strength at which the *Z*-shaped current–voltage characteristic transforms into an N-shaped one. We compare our results with experimental data.

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Semiconductors
vol. 38, no. 9, pp. 1053-1060, 2004

Effect of electron-electron and electron-hole collisions on intraband population inversion of electrons in stepped quantum wells

V. L. Zerova, G. G. Zegrya, L. E. Vorob'ev

The effect of intersubband electron–electron (*e*−*e*) and electron–hole (*e*−*h*) scattering on intraband population inversion of electrons in a stepped InGaAs/AlGaAs quantum well is investigated. The characteristic times of the most probable e−e and e−h processes, which affect the electron densities on the excited levels, are calculated for the temperature range 80–300 K. Dependences of these times on the electron and hole density on the ground levels are studied. Temperature dependences of the intraband inversion of population for two nonequilibrium densities are calculated by solving a system of rate equations. It is shown that the intersubband e−e and e−h scattering only slightly affects the population inversion for electron densities below 1×10^{12} cm^{-2}.

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Semiconductors
vol. 38, no. 6, pp. 689-695, 2004

Electron-electron scattering in stepped quantum wells

V. L. Zerova, L. E. Vorob'ev, G. G. Zegrya

A method for calculating the probability of intersubband electron–electron scattering in quantum wells of complex shape is suggested. Numerical data for stepped InGaAs/AlGaAs quantum wells are obtained. The principal mechanisms of electron–electron scattering that exert the strongest effect on the intersubband inversion of population in laser structures are determined.

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Proc. SPIE
vol. 5126, pp. 129-140, 2003

Quantum well and quantum dot infrared photodetectors: Physics of operation and modeling

V .Ryzhii, M .Ryzhii I. Khmyrova, R. Suris, V. Mitin, M. Shur

We review recent studies of physical phenomena in quantum well infrared photodetectors (QWIPs), and some other QW and QD infrared devices and discuss their features. We show that the optimization of QWIPs, improvement of QDIPs, and creation of novel QWIP- and QDIP-based devices still requires an in-depth understanding of underlying physical effects.

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Int. J. Nanoscience
vol. 2, no. 6, pp. 401-409, 2003

Spectrum of carriers and optical properties of 2D heterostructures in tilted magnetic field

A. A. Greshnov, E. N. Kolesnikova, G.G. Zegrya

The structure and features of spatially-confined states in the presence of a tilted magnetic field are theoretically investigated. The electron states in single- and double-quantum wells are described using the variational method. It is shown that the finite ratio of magnetic length to the width of heterostructure could not be neglected in the strong tilted magnetic field. The electronic structure of broken-gap heterostructures is considered similar to the case of usual double-quantum-well with the high narrow barrier. It is shown that tilted magnetic field can eliminate the strong coupling between two degenerated electron states or those of the electron and hole. The existence of such an effect is in accordance with cyclotron resonance studies of InAs/GaSb heterostructures.

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Proc. SPIE
vol. 5023, no. 1, pp. 306-309, 2003

Current-induced cooling of nanostructures

E. B. Dogonkin, G. G. Zegrya

A mechanism of electric current-induced cooling of nanostructures is proposed and analyzed. The conditions are studied of electric current flow through a heterostructure with two quantum wells, with electrons from one quantum well passing into the other via phonon-assisted indirect tunneling. As a result, the system is cooled by the flowing current, with the temperature of the system depending on the current nonmonotonically. A universal law for the maximal cooling temperature is derived.

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NATO Science series II
vol.119 (Optical Properties of 2D Systems
with Interacting Electrons)
pp. 125-136, 2003

Combined exciton-electron optical processes in optical spectra of modulation doped QWs

V. P. Kochereshko, D. R. Yakovlev, R. A. Suris, G. V. Astakhov, W. Faschinger, W. Ossau, G. Landwehr, T. Wojtowicz, G. Karczewski, J. Kossut

We present a detailed study of combined exciton-electron processes in modulation doped quantum well structures contain a 2DEG of low density. We observed resonance exciton-electron processes in magnetic fields reveal in a separate narrow spectral lines, as well as nonresonant processes reveal in the exciton line broadening. Combine processes with participate of the excitons have been observed as well as with participate of trions (negatively charged exciton-electron complexes).

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Proc. SPIE
vol. 5023, pp. 82-85, 2003

Filling-factor dependence of magneto-luminescence in II-VI QWs with 2DEG

A. S. Gurevich, G. V. Astakhov, R. A. Suris, V. P. Kochereshko, D. R. Yakovlev, W. Ossau, S. A. Crooker, G. Karczewski

Photoluminescence spectra of modulation-doped quantum well structures based on II-VI semiconductors (CdTe/CdMgTe and ZnSe/ZnBeMgSe) were studied in high magnetic fields it the range of 2D electron concentrations of (1-5)x10^{11} cm^{-2}. The following peculiarities were found at low mangetic fields: (1) linear increase of the photoluminescence energy with increasing magnetic fields, (2) jumps in this dependence at integer filling-factors, (3) periodical changing of Zeeman splitting. The observed behavior are interpreted in a frame of a model which takes into account combined exciton electron recombination processes in the presence of magnetic fields.

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Jpn. J. Appl. Phys.
vol. 40, part 1, no. 2A, pp. 513-517, 2001

Nonlocal hot-electron transport and capture model for multiple quantum well structures excited by infrared radiation

V. Ryzhii, R. Suris

In this paper, a model for hot-electron transport and capture phenomena in semiconductor heterostructures with multiple uncoupled quantum wells (QW) excited by infrared radiation is presented. The model takes into account the nonlocal character of the electron transport and capture of mobile electrons propagating over the barriers. It includes the Poisson equation and balance equations for electrons and their energy. The model is used for the calculation of steady-state spatial distributions of the electric-field and the average electron energy in multiple QW

structures. The conditions of the formation of periodic electric-field domains revealed recently in ensemble Monte Carlo particle simulations are found. The obtained results are compared with the previous analytical calculations based on a simplified model. The relationships between phenomenological parameters of the latter and QW structure parameters are obtained. The developed analytical model highlights the origin of periodic electric-field domains in multiple QW structures and explains some features of such domain behavior.

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Semicond. Sci. Technol.
vol. 16, no. 4, pp. 202-208, 2001

Self-organization in multiple quantum well infrared photodetectors

M. Ryzhii, V. Ryzhii, R. Suris, C. Hamaguchi

We investigate the spatio-temporal electric-field distributions in multiple quantum well infrared photodetectors (QWIPs) excited by infrared radiation using ensemble Monte Carlo particle modelling. It is shown that self-organized stable periodic electric-field structures can occur in QWIPs excited by infrared radiation. These electric-field distributions have a period equal to twice the period of the QWIP structure. The periodic distributions are superimposed by relatively weak spatio-temporal oscillations. The transition between two stable periodic structures in response to step-like variation of the applied voltage is demonstrated. The periodicity of the electric-field structures is conserved after the cessation of illumination for a long time. This time is determined by relatively slow thermoexcitation processes. The occurrence of the electric-field distributions can pronouncedly affect the QWIP steady-state and noise characteristics.

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Phys. Status Solidi B
vol. 227, no. 2 pp. 343-352, 2001

Excitons and trions modified by interaction with a two-dimensional electron gas

R. A. Suris, V. P. Kochereshko, G. V. Astakhov, D. R. Yakovlev, W. Ossau, J. Nurnberger, W. Faschinger, G. Landwehr, T. Wojtowicz, G. Karczewski, J. Kossut

A concept of mixed exciton-trion states is formulated theoretically and proved experimentally for II–VI semiconductor quantum wells with a two-dimensional electron gas. The concept considers the resonances of neutral excitons and charged excitons (trions) as mixed (with each other) via their interaction with free electrons. Reflectivity spectra of modulation-doped ZnSe/(Zn,Mg)(S,Se) and CdTe/(Cd,Mg)Te quantum wells are analyzed. A good qualitative agreement of the experimental results with model calculations is achieved.

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Phys. Rev. B
vol. 62, no. 11, pp. 7268-7274, 2000

Phenomenological theory of electric-field domains induced by infrared radiation in multiple quantum well structures

V. Ryzhii, I. Khmyrova, M. Ryzhii, R. Suris, C. Hamaguchi

We review the occurrence of periodic or near periodic electric-field domains stimulated by bound-to-continuum transitions under the influence of infrared radiation in multiple uncoupled quantum wells. The conditions of formation of such domains and their stability are studied theoretically using the proposed phe-nomenological model.

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Proc. of the 8th Int. Symposium
Nanostructures: Physics and Technology,
St.Petersburg, Russia, 2000
pp. 194-197, 2000

Theoretical investigation of intraband absorption of electromagnetic radiation by holes in quantum wells

N. A. Nezlobin, A.S. Polkovnikov, G.G. Zegrya

Using four-band Kane model we calculate intraband absorption coefficient of light by holes followed by their transition to the spin-orbital split-off band for A(III)B(V) semiconductor quantum wells. It is shown that such an absorption mechanism is possible without any participation of a third particle like a phonon or an impurity and this mechanism can give the major contribution to the absorption of light in semiconductor quantum well lasers.

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Phys. Rev. B
vol. 61, no. 4, pp. 2742-2748, 2000

Periodic electric-field domains in optically excited multiple-quantum-well structures

M. Ryzhii, V. Ryzhii, R. Suris, C. Hamaguchi

We demonstrate using an ensemble Monte Carlo particle modeling that periodic electric-field domains can arise in optically excited multiple quantum well structures under applied voltage. In particular, the formation of the electric-field distributions with the period equal to twice the structure period is possible. This effect is attributed to the excitation of the recharging waves due to decreasing energy dependence of the capture rate of hot electron capture into quantum wells and nonlocal heating of electrons by electric field.

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NATO science series 3
vol. 81 (Optical Properties
of Semiconductor Nanostructures)
pp. 299-308, 2000

Combined exciton-electron processes in modulation doped quantum well structures.

V. P. Kochereshko, D. R. Yakovlev, G. V. Astakhov, R. A. Suris, J. Nurnberger, W. Faschinger, W. Ossau, G. Landwehr, T. Wojtowicz, G. Karczewski, J. Kossut

Combined exciton-electron processes were studied in modulation doped quantum well structures in magnetic fields. In the case of such combined processes an incident photon creates an exciton and induces a transition of an additional electron between two Landau levels. In the present work we found the combined process in which the incident photon creates a trion (negatively charged exciton-electron complex) and also promotes the inter-Landau level transition of an additional electron. Such combined processes are found and studied in CdTe/CdMgTe and ZnSe/ZnMgSSe modulation-doped quantum wells containing two dimensional electron gas of low and moderate density.

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Phys. Solid State
vol. 41, no. 5, pp. 751-756, 1999

Exciton-electron interaction in quantum wells with a two dimensional electron gas of low density

W. Ossau, D. R. Yakovlev, C. Y. Hu, V. P. Kochereshko, G. V. Astakhov, R. A. Suris, P. C. M. Christianen, J. C. Maan

II–VI quantum-well structures containing a 2DEG of low density have been investigated by means of polarized photoluminescence, photoluminescence excitation and reflectivity in external magnetic fields up to 20 T. The spin splittings of the exciton X and the negatively charged exciton X^{-} are measured as a function of the magnetic field

strength. The behavior of the magnetic-field-induced polarization degree of the luminescence line related to X^{-} demonstrates the formation process of negatively charged excitons from excitons and free carriers polarized by the external magnetic field. We have determined the binding energies of the trion formed either with the heavy-hole or the light-hole exciton. The optically detected magnetic resonance (ODMR) technique was applied for the first time to study the optical transition processes in a nanosecond timescale. The electron ODMR was observed with the detection on either the direct exciton or the negatively charged exciton *X*. Further evidence for the interaction of excitons with the electrons of the two-dimensional gas are demonstrated by a combined exciton-cyclotron resonance line observed in reflectivity and luminescence excitation, shake-up processes observed in photoluminescence, as well as inelastic and spin-dependent scattering processes.

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Jpn. J. Appl. Phys.
vol. 39, pp. 6654-6658, 1999

Theoretical study of recharging instability in quantum well infrared photodetectors

I. Khmyrova, M. Ryzhii, V. Ryzhii, R. Suris, C. Hamaguchi

We study the response of the electron system in quantum well infrared photodetectors under illumination by infrared radiation to small electric-field and charge fluctuations using the proposed analytical model. It is shown that uniform electric-field distributions corresponding to quasi-neutral quantum wells can be unstable with regard to the excitation of the recharging waves in a wide range of infrared radiation intensities

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Jpn. J. Appl. Phys.
vol. 38, part 2, no. 12A, pp. L1388-L1390, 1999

Recharging instability and periodic domain structures in multiple quantum well infrared photodetectors

M. Ryzhii, V. Ryzhii, R. Suris, C. Hamaguchi

Using ensemble Monte Carlo particle modeling we demonstrate that monotonic electric-field distributions in multiple quantum well infrared photodetectors (QWIPs) can be unstable. This instability can lead to oscillatory electric-field and charge domains with a period equal to twice the QW structure period. This effect is due to the heating of the electron gas in continuum states resulting in a nonlocal dependence of the capture rate on the electric field.

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JETP Lett.
vol. 68, no. 10, pp. 792-798, 1998

On the nature of the oscillations of cyclotron absorption in InAs/GaSb quantum wells

S. D. Suchalkin, Yu. B. Vasil'ev, K. von Klitzing, V. N. Golovach, G. G. Zegrya, S. V. Ivanov, P. S. Kop'ev, B. Ya. Mel'tser

The mechanism of oscillations of the half-width and intensity of the cyclotron resonance (CR) line of electrons in a semimetal quantum well based on an InAs/AlSb/GaSb heterostructure is investigated experimentally and theoretically. It is shown that the oscillations of the CR spectrum are due to mixing of states of the spatially separated two-dimensional electrons and holes.

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J. Cryst. Growth
vol. 184, pp. 826-830, 1998

Exciton-electron interactions in CdTe/CdMgTe modulation-doped QW structures

V. P. Kochereshko, D. R. Yakovlev, R. A. Suris, W. Ossau, G. Landwehr, T. Wojtowicz, M. Kutrowski, G. Karczewski, J. Kossut

Reflectance, photoluminescence and photoluminescence excitation spectra have been studied in modulation-doped CdTe/(Cd,Mg)Te quantum well structures containing a 2DEG of low density. Optical transitions related to the creation of excitons, bound exciton-electron complexes (trions) and exciton-cyclotron resonance (ExCR) states have been found in these spectra. A modification of the high-energy tail on the exciton absorption line into several discrete ExCR lines was observed when a magnetic field was applied. The polarization of the exciton and ExCR reflectance lines has been analyzed.

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Phys. Low-Dim. Struct
vol. 1998, no. 1-2, pp. 205-211, 1998

Exciton-electron interactions in modulation-doped QW structures

W. Ossau, D. R. Yakovlev, G. Landwehr, V. P. Kochereshko, R. A. Suris, D. Turchinovich, T. Wojtowicz, G. Karczewski, J. Kossut

Reflectivity spectra of modulation-doped quantum well structures have been studied in external magnetic fields. Resonance reflectivity lines of excitons, trions and combined exciton-cyclotron resonances have been observed. Parameters of these resonances have been analyzed as a function of magnetic field. We have found that in doped structures the resonance contribution to the dielectric function from the trion and combined exciton-cyclotron resonance exceeds the exciton contribution.

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Quantum dots

Nano Lett.,
vol. 18, no. 1, pp 373–380, 2018

Electron and hole g factors and spin dynamics of negatively charged excitons in CdSe/CdS colloidal nanoplatelets with thick shells

E. V. Shornikova, L. Biadala, D. R. Yakovlev, D. Feng, V. F. Sapega, N. Flipo, A. A. Golovatenko, M. A. Semina, A. V. Rodina, A. A. Mitioglu, M. V. Ballottin, P. C. M. Christianen, Y. G. Kusrayev, M. Nasilowski, B. Dubertret, M. Bayer

We address spin properties and spin dynamics of carriers and charged excitons in CdSe/CdS colloidal nanoplatelets with thick shells. Magneto-optical studies are performed by time-resolved and polarization-resolved photoluminescence, spin-flip Raman scattering and picosecond pump–probe Faraday rotation in magnetic fields up to 30 T. We show that at low temperatures the nanoplatelets are negatively charged so that their photoluminescence is dominated by radiative recombination of negatively charged excitons (trions). Electron g-factor of 1.68 is measured, and heavy-hole g-factor varying with increasing magnetic field from −0.4 to −0.7 is evaluated. Hole g-factors for two-dimensional structures are calculated for various hole confining potentials for cubic- and wurtzite lattice in CdSe core. These calculations are extended for various quantum dots and nanoplatelets based on II–VI semiconductors. We developed a magneto-optical technique for the quantitative evaluation of the nanoplatelets orientation in ensemble.

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Superlattices Microstruct.
vol. 111, pp. 166-172, 2017

Resonant electronic excitation energy transfer by exchange mechanism in the quantum dot system

O. P. Chikalova-Luzina, D. M, Samosvat, V. M. Vyatkin, G. G. Zegrya

A microscopic theory of nonradiative resonance energy transfer between spherical A_3B_5 semiconductor quantum dots by the exchange

mechanism is suggested. The interdot Coulomb interaction is taken into consideration. It is assumed that the quantum dot-donor and the quantum dot-acceptor are made from the same A_3B_5 compound and are embedded in the matrix of another material that produces potential barriers for electrons and holes. The dependences of the energy transfer rate on the quantum-dot system parameters are found in the frame of the Kane model that provides the most adequate description of the real spectra of A_3B_5 semiconductors. The analytical treatment is carried out with using the density matrix method, which enabled us to perform an energy transfer analysis both in the weak-interaction approximation and in the strong-interaction approximation. The numerical calculations showed the saturation of the energy transfer rate at the distances between the donor and the acceptor approaching the contact one. The contributions of the exchange and direct Coulomb intractions can be of the same order at the small distances and can have the same value in the saturation range.

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J. Electron. Mater.
vol. 46, 3922, 2017

Förster Resonance Energy Transfer and Harvesting in II–VI Fractional Monolayer Structures

T. V. Shubina, M. A. Semina, K. G. Belyaev, A. V. Rodina, A. A. Toropov, S. V. Ivanov

We report on Förster resonance energy transfer in the dense arrays of epitaxial quantum dots (QDs), formed by fractional monolayer CdSe insertions within a ZnSe matrix. In such arrays comprising the QDs of different sizes, the energy transfer can take place between the ground levels of small QDs and the excited levels of large radiating QDs, when these states are in resonance. This mechanism provides directional excitation of a limited number of the large QDs possessing the excited levels. It reveals itself by the shrinkage of photoluminescence (PL) bands and the appearance of the narrow single excitonic lines in micro-PL spectra. The strong shortening of characteristic PL decay times in the energy-donating QDs is observed when the distance between them and the energy-accepting QDs decreases. Photoluminescence excitation spectroscopy demonstrates the switching of the dominant energy transfer mechanism at the energy predicted by theoretical modeling of the excitonic levels in the QD arrays. Our results pave the way for engineering of the architecture of excitonic levels in the QD arrays to realize efficient nano-emitters.

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J. Phys.: Conf. Ser.
vol. 769, no. 1, 012078, 2016

Resonant electronic excitation energy transfer by Dexter mechanism in the quantum dot system

D. M. Samosvat, O. P. Chikalova-Luzina, V. M. Vyatkin, G. G. Zegrya

In present work the energy transfer between quantum dots by the exchange (Dexter) mechanism is analysed. The interdot Coulomb interaction is taken into consideration. It is assumed that the quantum dot-donor and the quantum dot-acceptor are made from the same compound A3B5 and embedded in the matrix of other material creating potential barriers for electron and holes. The dependences of the energy transfer rate on the quantum-dot system parameters are found using the Kane model that provides the most adequate description spectra of semiconductors A_3B_5. Numerical calculations show that the rate of the energy transfer by Dexter mechanism is comparable to the rate of the energy transfer by electrostatic mechanism at the distances approaching to the contact ones.

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J. Phys.: Conf. Ser.
vol. 741, no. 1, 012155, 2016

Switching of resonance energy transfer mechanism in a dense array of II-VI quantum dots

K. G. Belyaev, T. V. Shubina, M. A. Semina, A. V. Rodina, A. A. Toropov, S. V. Ivanov

We report on Förster resonance energy transfer (FRET) in a dense array of II-VI epitaxial quantum dots (QDs). Besides FRET between the ground states of QDs of different sizes, we observe the energy transfer via the excited levels of large QDs which are in resonance with the ground levels of small QDs. The switching of dominant energy transfer mechanism, revealed by photoluminescence excitation spectroscopy, takes place at the energy controlled by the architecture of quantum levels in these arrays.

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JETP
vol. 121, no. 1, pp. 76-95, 2015

Nonradiative resonance energy transfer between semiconductor quantum dots

D. M. Samosvat, O. P. Chikalova-Luzina, G. G. Zegrya

A microscopic analysis of the mechanisms of nonradiative energy transfer in a system of two semiconductor QDs caused by Coulomb interaction of donor and acceptor electrons is performed. The energy transfer rate is calculated for QDs based on III–V compounds using the Kane model. Conditions are analyzed under which energy transfer from a donor to an acceptor is possible. The mixing in of the p states of the valence band to the s states of the conduction band is found to give rise to additional contributions to the matrix element of energy transfer. It is shown that these additional contributions play a considerable role in the energy transfer process at distances between QDs close to contact distances or much greater. The influence of the exchange interaction on

the energy transfer mechanism is analyzed, and it is shown that this inter action should be taken into account for a quantitative description of the energy transfer when QDs are separated by a distance close to the contact distance.

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Phys. Rev. B
vol. 90, 155431, 2014

Anharmonicity-assisted multiphonon transitions between distant levels in semiconductor quantum dots

I. A. Dmitriev, R. A. Suris

We calculate the multiphonon transition rate from the excited state of a single-occupied two-level quantum dot. The electron interacts with certain optical phonon modes which in turn transfer the transition energy to the bath of other phonon modes decoupled from the electron states. Our theory covers the previously unexplored range of transition energies several times larger than the optical phonon energy and systematically studies the role of quantum interference of the processes involving different virtual polaron states.

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Tech. Phys. Lett.
vol. 40, no. 4, pp. 350-352, 2014

The role of exchange interaction in nonradiative energy transfer between semiconductor quantum dots

O. P. Chikalova-Luzina, D. M. Samosvat, G. G. Zegrya

The contribution of exchange interaction to the probability of nonradiative energy transfer between two (donor and acceptor) semiconductor quantum dots based on A_3B_5 compounds has been analyzed using the Kane model of energy-band structure. It is established that the dependence of the exchange contribution on the distance between donor and acceptor centers has a power character for nearly contact distances and acquires an exponential character when the distance increases. Numerical calculations showed that the exchange contribution is comparable with that of the dipole-quadrupole interaction of quantum dots and is one to two orders of magnitude lower than the contribution of the dipole–dipole interaction at shorter distances.

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Semiconductors
vol. 47, no. 1, pp 22-27, 2013

On the lifetime of charge carriers in quantum dots at low temperatures

D. M. Samosvat, V. P. Evtikhiev, A. S. Shkol'nik, G. G. Zegrya

The nonequilibrium lifetime of charge carriers in a quantum dot has been experimentally and theoretically investigated. It has been shown that, at low temperatures when the ground state is fully occupied, the lifetime is almost independent of the excitation density and determined only by radiative recombination. Such behavior is theoretically explained and it is shown that, under the condition of the fully occupied ground state, the Auger recombination process can be suppressed by spin effects. The suppression of Auger recombination in such a system is microscopically described.

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J. Phys.: Conf. Ser.
vol. 461, no. 1, 012001, 2013

Nonradiative resonance energy transfer between quantum dots

A. S. Stepashkina, D. M. Samosvat,
O. P. Chikalova-Luzina, G. G. Zegrya

In the work we examined the mechanism of nonradiactive resonant energy transfer between quantum dots (QD), the probability of this process was calculated. The valence band has difficult structure due to the additional matrix element connected with another polarization of

heavy holes. Dependences of transfer probability on distance between quantum dots and barrier heights for electrons were studied.

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Tech. Phys. Lett.
vol. 39, no. 1, pp. 74-77, 2013

Nonradiative resonance energy transfer between two semiconductor quantum dots

D. M. Samosvat, O. P. Chikalova-Luzina,
A. S. Stepashkina, G. G. Zegrya

We consider the nonradiative resonance energy transfer between two semiconductor quantum dots (donor and acceptor), taking into account the nonparabolicity of the electron dispersion law, and the energy transfer due to the Coulomb interaction between charge carriers of the donor and acceptor. We show that, when nonparabolicity of the dispersion law is taken into account, a new term enters the matrix element of the energy transfer, which enhances the probability of the resonance energy transfer.

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Tech. Phys. Lett.
vol. 36, no. 12, pp. 1118-1120, 2010

Calculating potential and electron density for strained semiconductor quantum dots

R. M. Peleshchak, I. Ya. Bachynsky, G. G. Zegrya

Distributions of the electrostatic potential, electric field strength, and electron concentration for a strained semiconductor quantum dot (QD) have been calculated within the nonlinear Poisson model with allowance for the deformation potential that arises due to a lattice misfit between the QD and matrix.

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JETP
vol. 108, no. 6, pp. 907-916, 2009

Carrier energy spectrum and lifetime in quantum dots in electric field

G. G. Zegrya, D. M. Samosvat

The *S*-matrix formalism is used to perform analytical calculations of the spectrum of quasi stationary states of charge carriers in a core-shell quantum dot. Analytical expressions are obtained for the second-order perturbative corrections to the position and half-width of a quasi-stationary energy level, and level shifts are calculated numerically for a core-shell quantum dot in the presence of an electrostatic field. The corrections to level half-width due to Stark effect are analyzed as functions of level energy and barrier thickness. It is shown that there exists a level position E_{cr} such that the correction $\delta\Gamma$ to the level half-width changes sign. An analytical expression for the quadratic Stark shift in a dc-biased quantum well is found in semiclassical approximation. It is shown that the corresponding correction $\delta\Gamma$ to half-width also changes sign as energy passes through E_{cr}. As an example, the Stark shift is calculated for a core-shell quantum dot in the electrostatic field of an adjacent protein molecule.

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Semiconductors
vol. 42, no. 9, pp. 1076-1083, 2008

Baric properties of InAs quantum dots

B. V. Novikov, G. G. Zegrya, R. M. Peleshchak, O. O. Dan'kiv, V. A. Gaisin, V. G. Talalaeva, I. V. Shtrom, G. E. Cirlin

In the context of the deformation potential model, baric dependences of the energy structure of InAs quantum dots in a GaAs matrix are calculated. Under the assumption of the absence of interaction between the spherical quantum dots of identical sizes, the energy dependence of the baric coefficient of energy of the radiative transition in the quantum

dot is determined. A similar dependence is also found experimentally in the photoluminescence spectra under uniform compression of the InAs/GaAs structures. Qualitative agreement between the theory and experiment as well as possible causes for their quantitative difference are discussed. It is concluded that such factors as the size dispersion, Coulomb interaction of charge carriers, and tunnel interaction of quantum dots contribute to this difference.

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Semiconductors
vol. 42, no. 6, pp. 714-719, 2008

Generation of superradiation in quantum dot nanoheterostructures

A. V. Savelyev, L. Ya. Karachinsky, I. I. Novikov, N. Yu. Gordeev,
R. P. Seisyan, G. G. Zegrya

Conditions for the generation of Dicke supperradiation are studied for two types of quantum dot nanoheterostructures: a planar waveguide and a microdisk. The domain model for the generation of superradiation suggested earlier for quantum wells is generalized to inhomogeneous quantum dot arrays. Different scenarios of the generation of superradiation in a semiconductor microdisk are classified.

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Semiconductors
vol. 42, no. 3, pp. 291-297, 2008

The role of transport processes of nonequilibrium charge carriers in radiative properties of arrays of InAs/GaAs quantum dots

A. S. Shkolnika, A. V. Savelyev, L. Ya. Karachinsky, N. Yu. Gordeev,
R. P. Seisyan, G. G. Zegrya, S. Pellegrini, G. S. Buller, V. P. Evtikhiev

The results of time-resolved photoluminescence studies of heterostructures containing monolayer arrays of InAs/GaAs quantum

dots are presented. A two-component time dependence of intensity of photoluminescence from the ground state of quantum dots, with characteristic times of the slow component up to hundreds of nanoseconds and those of rapid one several nanoseconds, is studied. It is shown that the slow component is determined by the transport of nonequilibrium charge carriers between the quantum dots. At low temperatures, the time of the slow component is determined by tunneling, and at high temperatures by thermal escape of nonequilibrium charge carriers. The ratio of the contributions of tunneling and thermal escape is determined by the degree of isolation of quantum dots. A theoretical model is constructed that describes the effect of the dynamics of carrier transport on the emergence and decay of the slow component of photoluminescence.

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AIP Conf. Proc.
vol. 893, no. 1, pp. 987-988, 2007

Bipolar charging in quantum dots array

A. V. Savelyev, L. Ya. Karachinsky, A. S. Shkolnik, S. Pellegrini, N. Yu. Gordeev, A. I. Tartakovskii, V. P. Evtikhiev, G. G. Zegrya, M. V. Maximov, V. M. Ustinov, R. P. Seisyan, G. S. Buller, M. S. Skolnick

New type of carrier distribution among quantum dots - a spatially separated bipolar-charging state - has been studied experimentally and theoretically. Experimental methods such as pump-probe spectroscopy of electrically pumped samples and time-resolved photoluminescence were used. Theoretical approach based on a detailed statistics of carrier distribution was developed and proposed for interpretation of the experimental results.

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Tech. Phys. Lett.
vol. 33, no. 1, pp. 35-39, 2007

Electron properties of open semiconductor quantum dots

N. V. Tkach, Yu. A. Seti, G. G. Zegrya

The energy spectrum and lifetimes of electron states in an open semiconductor quantum dot (QD) have been studied using the scattering S-matrix method. It is established that the lifetime of electron states in the QD is highly sensitive to changes in the QD radius and the thickness of an external coating layer. As the coating layer thickness increases from one to five monolayers, the electron lifetime grows by a factor of 20–60.

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Semiconductors
vol. 41, no. 5, pp. 575-589, 2007

Nonequilibrium population of charge carriers in structures with InGaN deep quantum dots

D. S. Sizov, E. E. Zavarin, N. N. Ledentsov, V. V. Lundin,
Yu. G. Musikhin, V. S. Sizov, R. A. Suris, A. F. Tsatsul'nikov

Electronic and optical properties of ensembles of quantum dots with various energies of activation from the ground-state level to the continuous-spectrum region were studied theoretically and experimentally with the InGaN quantum dots as an example. It is shown that, depending on the activation energy, both the quasi-equilibrium statistic of charge carriers at the levels of quantum dots and nonequilibrium statistic at room temperature are possible. In the latter case, the position of the maximum in the emission spectrum is governed by the value of the demarcation transition: the quantum dots with the transition energy higher than this value feature the quasi-equilibrium

population of charge carriers, while the quantum dots with the transition energy lower than the demarcation-transition energy feature the nonequilibrium population. A model based on kinetic equations was used in the theoretical analysis. The key parameters determining the statistic are the parameters of thermal ejection of charge carriers; these parameters depend exponentially on the activation energy. It is shown experimentally that the use of stimulated phase decomposition makes it possible to appreciably increase the activation energy. In this case, the thermal-activation time is found to be much longer than the recombination time for an electron-hole pair, which suppresses the redistribution of charge carriers between the quantum dots and gives rise to the nonequilibrium population. The effect of nonequilibrium population on the luminescent properties of the structures with quantum dots is studied in detail.

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Tech. Phys. Lett.
vol. 32, no. 2, pp. 174-176, 2006

A new method for amino acid diagnostics using semiconductor quantum dots

G. G. Zegrya

Advantages offered by the use of quantum dots (QDs) for the investigation and diagnostics of biological systems are considered. A new method for the QD diagnostics of amino acid is proposed. The interaction of isolated QDs with charged amino acid residues is analyzed. It is shown that this interaction can shift the luminescence spectrum of QDs by several tens of millielectronvolts, which opens broad possibilities for the identification of biological objects with the aid of QDs.

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Appl. Phys. Lett.
vol. 86, no. 21, 211112, 2005

Observation of the biexponential ground-state decay time behavior in InAs self-assembled quantum dots grown on misoriented substrates

A. S. Shkolnik, L. Ya. Karachinsky, N. Yu. Gordeev, G. G. Zegrya, V. P. Evtikhiev, S. Pellegrini, G. S. Buller

Biexponential behavior of the time-resolved photoluminescence decay from the ground state has been studied over a temperature range of 77–300 K on samples with varying sized self-assembled InAs/GaAs quantum dot ensembles controlled by substrate misorientation alone. The slower second decay component is considerably longer than the first one, and has been measured to be as long as 300 ns. This slow component is attributed to carrier recapturing and indirect radiative recombination processes.

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CAS 2005 Proc. (2005 International
Semiconductor conference, Sinaia, Romania)
vol. 1, pp. 73-76, 2005

Application of semiconductor quantum dots for a study of biological systems

G. G. Zegrya, N. L. Bazhenov, K. D. Mynbaev, S. I. Pokutnyi

Advantages of semiconductor quantum dots (QDs) for study and diagnostics of biological systems are discussed A new method for amino acid diagnostics using semiconductor QDs is proposed. Interaction of isolated QDs with charged amino acids is studied in detail. It is shown that such interaction results in a shift of the QD luminescence spectra by several dozens of meV. This effect provides new possibilities for identification of biological objects using QDs

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J. Appl. Phys.
vol. 96, no. 2, pp. 1115-1119, 2004

Stark effect in semiconductor quantum dots

S. I. Pokutnyi, L. Jacak, J. Misiewicz, W. Salejda, G. G. Zegrya

A theory of the Stark effect in semiconductor quantum dots has been developed for the case of dominating polarization interaction of an electron and a hole with the nanocrystal surface. A shift of electron and hole quantum well levels in a nanocrystal in the interband absorption range in a uniform external electric field is determined by the quantum-confinement quadratic Stark effect. An electro-optical method is proposed, making it possible to estimate the characteristic quantum dot radius at which three-dimensional excitons can exist.

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Appl. Phys. Lett.
vol. 82, no. 16, pp. 2571-2573, 2003

Nonradiative recombination in quantum dots via Coulomb interaction with carriers in the barrier region

I. Yu. Solov’ev, G. G. Zegrya

A mechanism of nonradiative recombination of nonequilibrium carriers in semiconductor quantum dots (QDs) is suggested and discussed. Recombination of an electron-hole pair localized in a QD occurs via Coulomb (Auger) interaction with carriers in the barrier region. It is shown that the characteristic time of such an Auger process depends on QD parameters, temperature, and carrier density in the barrier region and, under certain conditions, is shorter than the characteristic time of radiative recombination.

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Proc. SPIE
vol. 5023, pp. 235-238, 2003

On the zero phonon line homogeneous broadening in semiconductor QDs

S. V. Goupalov, R. A. Suris, P. Lavallard, D. S. Citrin

Dephasing of optical excitations in semiconductor quantum dots (QDs) has recently received much attention. A common model used for understanding such processes is a two-level electronic system interacting with phonons. In our work we construct a consistent non-perturbative theory of the ZPL homogeneous broadening and resolve the contradictions by pointing out the limits of validity of the theoretical papers mentioned.

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Semiconductors
vol. 37, no. 3, pp. 317-321, 2003

Structure of energy quantum levels in a quantum dot shaped as an oblate body of revolution

G. G. Zegrya, O. V. Konstantinov, A. V. Matveentsev

It was shown that the electron energy spectrum in a disk-shaped potential well is characterized by two types of levels. One is characterized by a quantum number corresponding to carrier motion mainly along the disk axis. Energy intervals between such levels are large. As a rule, only a single electron level of this type can fit into the InAs quantum dot with GaAs surroundings. The second-type levels form a substructure with quantum numbers corresponding to carrier rotation about the polar axis and motion along the major disk axis. The distances between such levels are rather short. The theory makes it possible to determine the number of such levels as a function of the disk thickness and diameter and the conditions of the quantum dot transition into the quantum well with a large number of substructure levels.

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Semiconductors
vol. 36, no. 12, pp.1375-1384, 2002

Damping of Bloch oscillations in one-, two-, and three-dimensional quantum-dot superlattices

I. A. Dmitriev, R. A. Suris

In the preceding paper by the same authors, the density-matrix formalism was used to derive a quantum kinetic equation describing the damping of Bloch oscillations (BOs) in perfect one-, two-, and three-dimensional quantum-dot superlattices (QDSLs) and the conditions were determined under which the only process of the charge-carrier scattering by phonons in 2D and 3D QDSLs that contributes to the BO damping is the acoustic-phonon scattering within the transverse minibands of the Stark ladder of the carrier states. In this paper, the possibilities of suppressing this remaining scattering channel are analyzed. It is shown that the BO damping time in 2D and 3D QDSLs at room temperature may exceed the oscillation period by a factor of several hundreds and the conditions necessary for such strong suppression of the scattering are revealed. This makes a considerable difference between the QDSLs and the quantum-well superlattices, where, in reality, the BOs damping over a single oscillation period at room temperature.

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Semiconductors
vol. 36, no. 12, pp.1364-1374, 2002

Damping of Bloch oscillations in quantum dot superlattices: A general approach

I. A. Dmitriev, R. A. Suris

A quantum kinetic equation describing damping of the Bloch oscillations in ideal quantum-dot (QD) superlattices of various dimensionalities (1D, 2D, 3D) has been derived using the density matrix formalism. The

possibility of suppressing completely single-phonon scattering by optical phonons and considerably suppressing the acoustic-phonon scattering in the QD superlattice by effectively controlling the spectrum by varying the DC electric field magnitude and orientation is demonstrated. Conditions ensuring that the only photon-scattering mechanism responsible for damping of the Bloch oscillations is scattering by acoustic phonons within transverse minibands of the Stark carrier-state ladder are obtained.

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Tech. Phys. Lett.
vol. 28, no. 8, pp. 693-695, 2002

The energy spectrum of charge carriers in a strongly oblate ellipsoidal quantum dot

G. G. Zegrya, O. V. Konstantinov, A. V. Matveentsev

A new method of introducing curvilinear coordinates for an oblate ellipsoid of revolution is developed, which is valid for charge carriers obeying a parabolic isotropic dispersion law. Using this method, simple analytical formulas are derived for the energy spectrum of carriers in an oblate ellipsoidal quantum dot. According to these expressions, there are energy levels of two types. The first type is characterized by a quantum number corresponding to the motion of carriers predominantly along the minor axis of the ellipsoid. The distances between levels of the first type are large: only one such level is found in an InAs quantum well confined between GaAs layers. The second type is characterized by a quantum number corresponding to the motion of carriers along the major axis of the ellipsoid. The distances between levels of the second type are small and many such levels can be sometimes accommodated in a quantum dot, their number rapidly increasing with the degree of oblateness of the ellipsoid.

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Int. J. of High Speed Electronics and Systems
vol. 12, pp.583-592, 2002

Quantum dot superlattices in a constant electric field: localization and Bloch oscillations

R. A. Suris, I. A. Dmitriev

An analysis has been presented of electron localization in ideal 2D and 3D quantum dot superlattices (QDSL) in a homogeneous dc electric field and of Bloch oscillations in such structures. A very strong dependence of the ideal QDSL spectrum and wave functions on the field orientation is demonstrated. Bloch oscillations (BO) in QDSL are performed at two (or three for 3D QDSL) main Stark frequencies, which can be independently tuned by variation of field value and orientation. Due to the strong dependence of spectrum on field orientation, in QDSL intraminiband scattering processes can be almost totally suppressed. That allows to enlarge the BO lifetime by two orders of magnitude as compared with conventional quantum well superlattices.

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IEEE J. Sel. Top. Quantum Electron.
vol. 8, no. 5, pp. 1009-1014, 2002

Exciton dephasing and absorption line shape in semiconductor quantum dots

S. V. Goupalov, R. A. Suris, P. Lavallard, D. S. Citrin

The homogeneous broadening of exciton absorption spectral lines in semiconductor quantum dots (QDs) in the strong confinement regime is studied theoretically. It is shown that the term linear in nuclear displacements in the difference of the phonon Hamiltonians of the ground and optically excited states does not lead to the zero-phonon line (ZPL) broadening. The ZPL width is contributed by the term quadratic in

nuclear displacements associated with short-living optical phonons. This contribution is estimated for CdSe nanocrystals (NCs) and found to be much less than the linewidth observed in recent experiments. We conclude that the experimentally observed linewidth is due to the longitudinal lifetime associated with the exciton relaxation to the dark state. The shape of spectral wings originating from the exciton interaction with long-living acoustic phonons is studied at various temperatures for a CdSe NC embedded in a glass matrix.

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Semiconductors
vol. 36, no. 5, pp. 511-518, 2002

Electrons, holes, and excitons in a superlattice composed of cylindrical quantum dots with extremely weak coupling between quasiparticles in neighboring layers of quantum dots

N. V. Tkach, A. M. Makhanets, G. G. Zegrya

The spectrum of electrons, holes, and excitons in a superlattice composed of cylindrical quantum dots with extremely weak coupling between quasiparticles in neighboring layers of quantum dots was studied theoretically. Calculations were performed for the example of cylindrical β-HgS quantum dots embedded in β-CdS in the form of a superlattice. It is shown that electrons and holes in such a system form quasi-twodimensional energy minibands, whereas excitons can be described in terms of the Shinoda–Sugano model. The dependence of the quasiparticle spectra on geometric parameters of a superlattice with cylindrical quantum dots was studied. It is shown that the positions of minibands for all quasiparticles are very sensitive to the height of quantum dots, which should manifest itself in the experimental excitonic absorption spectrum.

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Nanotechnology,
vo. 12, no. 4, pp. 518-522, 2001

Homogeneous broadening of the zero-optical-phonon spectral line in semiconductor quantum dots

S. V. Goupalov, R. A. Suris, P. Lavallard, D. S. Citrin

Two different mechanisms of homogeneous broadening of the zero-optical-phonon spectral line in CdSe nanocrystal quantum dots are analysed. The first mechanism is due to modulation of the optical-phonon mode frequencies. The second one is caused by multiple-acoustic-phonon-assisted transitions. We show that homogeneous broadening due to acoustic phonons dominates at low temperatures and for small nanocrystal radii. For large nanocrystal radii and at room temperature, the two mechanisms become comparable.

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Semiconductors
vol. 35, no. 2, pp.212-219, 2001

Electron localization and Bloch oscillations in quantum-dot superlattices under a constant electric field

I. A. Dmitriev, R. A. Suris

It is demonstrated that the electron spectrum in ideal two-dimensional and three-dimensional quantum-dot superlattices (SLs) under a constant electric field can be either discrete or continuous depending on the field orientation with respect to the SL crystallographic axes. In the latter case, the width of the resulting transverse miniband depends exponentially on the crystallographic index corresponding to the direction of the field. The electron localization area undergoes dramatic variations with the field orientation in the vicinity of the directions corresponding to the continuous energy spectrum. The Bloch oscillations in this kind of SL are considered. It is established that the scattering of oscillating electrons can be strongly suppressed by an appropriate choice of the field strength and direction.

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Semicond. Sci. Technol.
vol. 15, no. 4, pp. 395-398, 2000

Energy spectrum of electron in quasiplane superlattice of cylindrical quantum dots

N. V. Tkach, A. M. Makhanets, G. G. Zegrya

The energy spectrum of an electron in a quasiplane superlattice of cylindrical β-HgS quantum dots in a β-CdS matrix has been calculated using the modified augmented plane wave method. The electronic miniband responsible for the electron motion in the superlattice plane is formed solely if the cylinder height to radius ratio exceeds a certain minimal value. The dependence of band parameters (bottom energy E_0 and the effective mass of an electron m) on geometrical dimensions of dots and the distance between them is established.

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Semiconductors
vol. 33, no. 5, pp. 564-568, 1999

Electron and hole spectra in a superlattice of cylindrical quantum wires

V. M. Golovach, G. G. Zegrya, A. M. Makhanets, I. V. Pronishin, N. V. Tkach

The electron and hole spectra in a superlattice of cylindrical quantum wires are calculated by the augmented-plane-wave method. The energy component due to the motion of quasiparticles in a direction perpendicular to the long axis of a wire consists of an alternation of bands with positive and negative effective mass. The potential of the quantum-wire superlattice lifts the degeneracy with respect to the magnetic quantum number away from the Γ point of the Brillouin zone. The energies of the main bands are investigated as functions of the radius of the quantum wires and the distance between wires for planar motion of quasiparticles.

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Auger recombination
in bulk semiconductors
and quantum wells

J. Phys.: Conf. Ser.
vol. 929, no. 1, 012089, 2017

Effect of carrier spectra nonsphericity and subband mixing on CHHS Auger process rate in deep quantum wells

N. V. Pavlov, G. G. Zegrya

The Kane's equations are written and solved with taking into account nonsphericity of the ***kp*** Hamiltonian. Charge carrier energy spectra and wave functions are obtained and analized. Subbands of dimensional quantization in the $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ system are calculated with taking subband mixing into account. CHHS Auger process coefficient in the $AlSb/InAs_{0.84}Sb_{0.16}/AlSb$ system is calculated with and without taking energy spectra nonsphericity and subband mixing into account. It is obtained that energy spectra nonsphericity and subband mixing lead to Auger matrix element and CHHS Auger process rate decrease.

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JETP Lett.
vol. 105, no. 9, pp. 586-590, 2017

Impact ionization rate in direct gap semiconductors

A. N. Afanasiev, A. A. Greshnov, G. G. Zegrya

In the framework of the 14-band ***k·p*** model, the intensity of the impact ionization processes in direct gap semiconductors is studied and explicit expressions for the impact ionization rate are obtained. It is shown that the rate of the process near the threshold energy is determined by the sum of the isotropic and strongly anisotropic contributions. The former contribution is proportional to the cube of the distance from the threshold, whereas the latter is a quadratic one arising only because of the coupling with remote bands. The comparison of these contributions under averaging over the nondegenerate isotropic distribution of nonequilibrium

electrons characterized by some effective temperature T^* demonstrates that the cubic contribution rather than the commonly used quadratic one is dominant in the direct gap semiconductors with $E_g < 1-1.5$ eV up to $T^* = 300$ K. This should be taken into account in the calculations of the operating characteristics of the devices based on the avalanche multiplication of charge carriers.

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J. Phys.: Conf. Ser.
vol. 661, no. 1, 012051, 2015

Generation of the pure spin current via Auger recombination in Rashba quantum wells

A. N. Afanasiev, A. A. Greshnov, G. G. Zegrya

We propose new non-optical mechanism of the pure spin current generation via Auger recombination in the quantum wells with Rashba spin-orbit coupling. It is shown that such process is allowed due to interference between the Coulomb matrix elements corresponding to two different transitions during Auger recombination, leading to non-diagonal transversal components of the spin current tensor, $J_R = J^{xy} = -J^{yx}$. In the limit of low temperatures the total spin current is proportional to the Rashba constant γ_R , spin relaxation time τ_s and the third power of both the concentration n, inverse quantum well width a^{-1} and E_g^{-2}. Estimations show that typical magnitude of the generated spin current by this way is much greater than the ones obtained using intraband optical excitation mechanisms and comparable with spin currents driven by interband optical excitation, provided that the quantum well bandgap is narrow enough ($E_g < 0.5$ eV).

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JETP
vol. 121, no. 4, pp. 640-646, 2015

Generation of pure spin currents via Auger recombination in quantum wells with Rashba splitting

A. N. Afanasiev, A. A. Greshnov, G. G. Zegrya

We propose a nonoptical mechanism for generating spin current via Auger recombination in semiconductor quantum wells (QWs) with spin–orbit splitting associated with structural QW asymmetry. It is shown that Auger recombination in narrow-bandgap semiconductors makes it possible to produce spin currents that exceed those that are obtained in the case of intraband as well as interband optical excitation. Analysis shows that the interference term in the expression for the Auger-recombination rate is responsible for the generation of spin currents.

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Semiconductors
vol. 49, no. 4, pp. 432-436, 2015

Temperature dependence of the carrier lifetime in $Cd_xHg_{1-x}Te$ narrow-gap solid solutions with consideration for Auger processes

N. L. Bazhenov, K. D. Mynbaev, G. G. Zegrya

The temperature dependence of the carrier lifetime in $Cd_xHg_{1-x}Te$ narrow-gap solid solutions in the temperature range 5 K < T < 300 K is analyzed within the scope of a microscopic model. Main attention is given to an analysis of the Auger recombination mechanism governing the carrier lifetime at high temperatures. The Auger-recombination rates are calculated with consideration for specific features of the band structure of the narrow-gap semiconductor in microscopic theory. It is shown that strict account of the non parabolicity of the electronic structure in terms of Kane's model leads to a substantially different temperature dependence of the Auger-recombination rates, compared with the approach in which nonparabolicity is dis regarded.

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Semiconductors
vol. 46, no. 1, pp. 29-34, 2012

Radiative recombination of hot carriers in narrow-gap semiconductors

N. V. Pavlov, G. G. Zegrya

The mechanism of the radiative recombination of hot carriers in narrow-gap semiconductors is analyzed using the example of indium antimonide. It is shown that the CHCC Auger recombination process may lead to pronounced carrier heating at high excitation levels. The distribution functions and concentrations of hot carriers are determined. The radiative recombination rate of hot carriers and the radiation gain coefficient are calculated in terms of the Kane model. It is demonstrated that the radiative recombination of hot carriers will make a substantial contribution to the total radiative recombination rate at high carrier con centrations.

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Semiconductors
vol. 42, no. 5, pp. 550-556, 2008

Theoretical study of auger recombination processes in deep quantum wells

L. V. Danilov, G. G. Zegrya

The basic processes and mechanisms of Auger recombination of nonequilibrium carriers in a semiconductor heterostructure with deep $InAs_{0.84}Sb_{0.16}$/AlSb quantum wells (QWs) are analyzed. It is shown that a zero-threshold Auger recombination process involving two heavy holes predominates in sufficiently narrow QWs, and a resonant process involving two electrons is dominant in wide QWs. The range of QW widths at which the Auger recombination is suppressed in a given structure to the greatest extent (suppression region) is determined. In this case, the threshold process involving two electrons remains the

basic nonradiative recombination process, with its probability being several orders of magnitude lower than those for the zero-threshold and resonant mechanisms. In turn, the zero-threshold mechanism involving two electrons is totally impossible in the heterostructure under study because of the large conduction-band offset (which markedly exceeds the energy gap). Also, the range of emission wavelengths that corresponds to the suppression region is estimated. It is shown that the interval calculated belongs to the mid-IR range.

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JETP
vol. 104, no. 6, pp. 951-965, 2007

Mechanisms of Auger recombination in semiconducting quantum dots

G. G. Zegrya, D. M. Samosvat

Microscopic calculation of the probability of Auger recombination of charge carriers localized in a semiconducting quantum dot (QD) is carried out. It is shown that two mechanism of Auger recombination (nonthreshold and quasi-threshold) operate in the QD. The nonthreshold Auger recombination mechanism is associated with scattering of a quasimomentum from a heterobarrier, while the quasi-threshold mechanism is connected with spatial confinement of the wave functions of charge carriers to the QD region; scattering of carriers occurs at the short-range Coulomb potential. Both mechanisms lead to a substantial enhancement of Auger recombination at the QD as compared to a homogeneous semiconductor. A detailed analysis of the dependence of Auger recombination coefficient on the temperature and QD parameters is carried out. It is shown that the nonthreshold Auger recombination process dominates at low temperatures, while the quasi-threshold mechanism prevails at high temperatures. The dependence of the Auger recombination coefficient on the QD radius experiences noticeable changes as compared to quantum wells and quantum filaments.

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Tech. Phys. Lett.
vol. 32, no. 8, pp. 670-673, 2006

Relationship between quasi-threshold and thresholdless Auger recombination processes in InAs/GaAs quantum dots

A. S. Shkolnik, V. P. Evtikhiev, G. G. Zegrya

The principal mechanisms of the nonradiative (Auger) recombination of nonequilibrium charge carriers in semiconductor heterostructures with quantum dots (QDs) are considered. It is shown that the Auger recombination process in QDs can proceed, in addition to a threshold mechanism, by means of two other substantially different mechanisms—thresholdless and quasi-threshold—and either of these can predominate, depending on the QD size. For a QD radius of ~30 Å, the probability of Auger recombination is comparable with that of radiative recombination.

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Semiconductors
vol. 39, no. 4, pp. 481-484, 2005

Temperature dependence of the effective coefficient of Auger recombination in 1.3 µm InAs/GaAs QD lasers

I. I. Novikov, N. Yu. Gordeev, M. V. Maksimov, Yu. M. Shernyakov, E. S. Semenova, A. P. Vasil'ev, A. E. Zhukov, V. M. Ustinov, G. G. Zegrya

Semiconductor laser heterostructures containing five and ten sheets of InAs/GaAs QDs on GaAs substrates, with an emission wavelength of ~1.3 µm, have been studied. Dependences of the nonradiative lifetime and effective Auger coefficient in QDs are obtained from an analysis of temperature and current dependences of the efficiency of spontaneous radiative recombination. The zero-threshold Auger recombination channel in QDs is shown to dominate at low (below 200 K) temperature, whereas at higher temperatures the quasithreshold channel becomes dominant. The effective 3D Auger coefficient is estimated in the

approximation of a spherical QD, and a good agreement with the experimental data is obtained.

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Phys. Rev. B
vol. 64, 073205, 2001

Electron-electron relaxation effect on Auger recombination in direct-band semiconductors

A. Polkovnikov, G. Zegrya

Influence of electron-electron relaxation processes on Auger recombination rate in direct band semiconductors is investigated. Comparison between carrier-carrier and carrier-phonon relaxation processes is provided. It is shown that relaxation processes are essential if the free path length of carriers does not exceed a certain critical value, which exponentially increases with temperature. For illustration of obtained results a typical InGaAsP compound is used.

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Phys. Rev. B
vol. 63, 075317, 2001

Auger recombination in semiconductor quantum wells in a magnetic field

G. G. Samsonidze, G. G. Zegrya

Auger process involving two electrons from the conduction band and a heavy hole from the valence band in semiconductor heterostructures with quantum wells is investigated for the case of a magnetic field applied normal to heteroboundaries. It is shown that there exist three different mechanisms of Auger recombination, associated with (I) electron scattering at interface with transition into the continuous spectrum, (II) short-range Coulomb interaction in the quantum well with transition into the continuous spectrum, and (III) resonance transition into

the discrete spectrum. All these processes are thresholdless. The Auger recombination coefficients analytically calculated for the processes I, II, and III show different dependencies on temperature, magnetic field, and quantum well parameters. In the limit of an infinitely wide quantum well, processes I and II merge to form a bulk threshold Auger process, while process III remains thresholdless resonance one. In the limit of infinitely weak magnetic field, process I remains thresholdless, process II becomes a quasithreshold process (i.e., its threshold energy slightly depends on temperature), and process III transforms into a nonresonance process with a threshold. The results obtained are new and have no analogies in the literature.

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Proc. of the 8th Int. Symposium
Nanostructures: Physics and Technology,
St.Petersburg, Russia, 2000
pp. 399-401, 2000

Theoretical investigation of Auger recombination in spherical quantum dots

E. B. Dogonkine, V. N. Golovatch, A. S. Polkovnikov,
A. V. Pozdnyakov, G. G. Zegrya

The principal mechanisms of Auger recombination (AR) of nonequilibrium carriers in spherical quantum dots (QDs) are investigated theoretically. It is shown that there exist two Auger recombination mechanisms of (i) quasithreshold and (ii) thresholdless types. These mechanisms originate from the existence of barriers but have different nature. The quasithreshold mechanism is caused by confinement of carriers within the region of a quantum dot which makes the quasimomentum conservation law approximate and enhances AR process. With increase of the dot radius this process turns to the threshold one. The thresholdless mechanism relates to the violation of the momentum conservation law at the heteroboundary and disappears with the radius tending to infinity.

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JETP
vol. 90, no. 2, pp. 378-388, 2000

Microscopic theory of Auger recombination in quantum wires

E. B. Dogonkin, G. G. Zegrya, A. S. Polkovnikov

An analysis is made of mechanisms for Auger recombination of nonequilibrium carriers in cylindrical quantum wires. It is shown that two different Auger recombination mechanisms take place in these wires: a quasi-threshold and a nonthreshold mechanism. Both mechanisms are associated with the presence of heterobarriers but are of a different nature. The quasi-threshold mechanism is attributed to the spatial confinement of the carrier wave functions to the region of the quantum wire and in this case the quasi-momentum conservation law is violated and the Auger recombination process is intensified. As the radius of the wire increases, the quasi-threshold Auger recombination process goes over to a threshold process. The nonthreshold mechanism is caused by the scattering of an electron (hole) at the heterojunction; the rate of this nonthreshold Auger recombination tends to zero in the limit of an infinite-radius wire.

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Semiconductors
vol. 34, no. 4, pp. 448-452, 2000

A numerical calculation of Auger recombination coefficients for InGaAsP/InP quantum well heterostructures

N. A. Gun’ko, A. S. Polkovnikov, G. G. Zegrya

Auger recombination coefficients are calculated numerically for InGaAsP/InP quantum well heterostructures. In narrow quantum wells, the quasi-threshold and thresholdless mechanisms mainly contribute to the Auger recombination coefficient. For the processes involving two electrons and a heavy hole (CHCC) or an electron and two heavy holes

with a transition of one of the holes to the spin–orbit split-off band (CHHS), the Auger recombination coefficients depend on temperature only slightly in a wide temperature range. The dependence of the Auger coefficient on the quantum well width is analyzed and found to be nonmonotonic.

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Two-dimensional electron gas

Phys. Rev. B
vol. 96, 235148, 2017

Sensitivity of the anomalous Hall effect to disorder correlations

I. Ado, I. A. Dmitriev, P. M. Ostrovsky, M. Titov

Both longitudinal and anomalous Hall conductivities are computed in the model of two-dimensional Dirac fermions with a mass in the presence of weak Gaussian spin-independent disorder with an arbitrary correlation function. The anomalous Hall conductivity is shown to be highly sensitive to the correlation properties of the random potential, such as the correlation length, while it remains independent of the integral disorder strength. This property extends beyond the Dirac model making the anomalous Hall effect an interesting tool to probe disorder correlations.

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Phys. Rev. B
vol. 96, 155306, 2017

Evidence for non-Markovian electron dynamics in the microwave absorption of a two-dimensional electron system

S. I. Dorozhkin, A. A. Kapustin, I. A. Dmitriev, V. Umansky, K. von Klitzing, J. H. Smet

We have studied the absorption of monochromatic microwave radiation in high-quality two-dimensional electron systems for the frequency span from 10 to 380 GHz using a bolometric method. For frequencies above 100 GHz the absorption exhibits an anomalous magnetic field dependence. Minima form at harmonics of the cyclotron resonance frequency. The results contrast previously reported data for other frequency ranges. Quasiclassical memory effects originating from the non-Markovian dynamics of electrons in a disorder potential containing short-range scatterers on top of a smooth potential background favorably account for the observed behavior.

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Phys. Rev. B
vol. 96, 115449, 2017

Magnetoresistance oscillations induced by high-intensity terahertz radiation

T. Herrmann, Z. D. Kvon, I. A. Dmitriev, D. A. Kozlov, B. Jentzsch, M. Schneider, L. Schell, V. V. Bel'kov, A. Bayer, D. Schuh, D. Bougeard, T. Kuczmik, M. Oltscher, D. Weiss, S. D. Ganichev,

We report on observation of pronounced terahertz radiation-induced magnetoresistivity oscillations in AlGaAs/GaAs two-dimensional electron systems, the terahertz analog of the microwave induced resistivity oscillations (MIRO). Applying high-power radiation of a pulsed molecular laser we demonstrate that MIRO, so far observed at low power only, are not destroyed even at very high intensities. Experiments with radiation intensity ranging over five orders of magnitude from 0.1 to 10^4 W/cm^2 reveal high-power saturation of the MIRO amplitude, which is well described by an empirical fit function $I/(1+I/I_s)^{\beta}$ with $\beta \sim 1$. The saturation intensity I_s is of the order of tens of watts per square centimeter and increases by a factor of 6 by increasing the radiation frequency from 0.6 to 1.1 THz. The results are discussed in terms of microscopic mechanisms of MIRO and compared to nonlinear effects observed earlier at significantly lower excitation frequencies.

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Phys. Rev. B
vol. 96, 121301(R), 2017

Hall field-induced resistance oscillations in a tunable-density GaAs quantum well

M. A. Zudov, I. A. Dmitriev, B. Friess, Q. Shi, V. Umansky, K. von Klitzing, and J. Smet

We report on Hall field-induced resistance oscillations (HIROs) in a 60-nm-wide GaAs/AlGaAs quantum well with an in situ grown back gate, which allows tuning the carrier density *n*. At low *n*, when all electrons are

confined to the lowest subband (SB1), the HIRO frequency, proportional to the product of the cyclotron diameter and the Hall field, scales with $n^{-1/2}$ as expected. Remarkably, the population of the second subband (SB2) significantly enhances the HIROs, whereas their frequency now scales as n^{-1}. We demonstrate that in this two-subband regime HIROs still originate solely from backscattering of SB1 electrons. The unusual density dependence occurs because the population of SB2 steadily increases, whereas that of SB1 remains essentially unchanged. The enhancement of the HIROs manifests an unexpected steplike increase in the quantum lifetime of SB1 electrons, which reaches a record value of 52 ps in the two-subband regime.

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Phys. Rev. B
vol. 95, 041403(R), 2017

Fine structure of high-power microwave-induced resistance oscillations

Q. Shi, M. A. Zudov, I. A. Dmitriev, K. W. Baldwin, L. N. Pfeiffer, K. W. West

We report on observation of a fine structure of microwave-induced resistance oscillations in an ultraclean two-dimensional electron gas. This fine structure is manifested by multiple secondary sharp extrema, residing beside the primary ones, which emerge at high radiation power. Theoretical considerations reveal that this fine structure originates from multiphoton-assisted scattering off short-range impurities. Unique properties of the fine structure allow us to access all experimental parameters, including microwave power, and to separate different contributions to photoresistance. Furthermore, we show that the fine structure offers a convenient means to quantitatively assess the correlation properties of the disorder potential in high-quality systems, allowing separation of short- and long-range disorder contributions to the electron mobility.

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Semiconductors
vol. 51,no. 6, pp 766–776, 2017

Classical magnetoresistance of a two-component system induced by thermoelectric effects

P. S. Alekseev, I. V. Gornyi, A. P. Dmitriev,
V. Yu. Kachorovskii, M. A. Semina

Magnetotransport in a two-dimensional two-component system consisting of electrons and holes with the same concentrations is studied. Balance equations to describe charge carrier and heat transfer are derived from the classical kinetic equation. The charge-carrier density and temperature distributions and electric-current densities are calculated by solving the balance equations for a long strip sample. In a sufficiently high magnetic field, regions of increased and decreased charge-carrier density, temperature, and fluxes are formed near the sample edges. This leads to nontrivial positive magnetoresistance.

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Phys. Rev. Lett.
vol. 117, 046601, 2016

Anomalous Hall effect in 2D Rashba ferromagnet

I. Ado, I. A. Dmitriev, P. M. Ostrovsky, M. Titov

Skew scattering on rare impurity configurations is shown to dominate the anomalous Hall effect in a 2D Rashba ferromagnet. The mechanism originates in scattering on rare impurity pairs separated by distances of the order of the Fermi wavelength. The corresponding theoretical description goes beyond the conventional noncrossing approximation. The mechanism provides the only contribution to the anomalous Hall conductivity in the most relevant metallic regime and strongly modifies previously obtained results for lower energies in the leading order with respect to impurity strength.

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Phys. Rev. B
vol. 94, 081301(R), 2016

MIRO-like oscillations of magneto-resistivity in GaAs heterostructures induced by THz radiation

T. Herrmann, I. A. Dmitriev, D. A. Kozlov, M. Schneider, B. Jentzsch, Z. D. Kvon, P. Olbrich, V. V. Bel'kov, A. Bayer, D. Schuh, D. Bougeard, T. Kuczmik, M. Oltscher, D. Weiss, S. D. Ganichev

We report on the study of terahertz radiation-induced MIRO-like oscillations of magnetoresistivity in GaAs heterostructures. Our experiments provide an answer on two most intriguing questions—effect of radiation helicity and the role of the edges—yielding crucial information for an understanding of the MIRO (microwave-induced resistance oscillations) origin. Moreover, we demonstrate that the range of materials exhibiting radiation-induced magneto-oscillations can be largely extended by using high-frequency radiation.

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Phys. Rev. B
vol. 93, 041410(R), 2016

Observation of microwave induced resistance oscillations in MgZnO/ZnO heterostructures

D. F. Kärcher, A. V. Shchepetilnikov, Yu. A. Nefyodov, J. Falson, I. A. Dmitriev, Y. Kozuka, D. Maryenko, A. Tsukazaki, S. I. Dorozhkin, I. V. Kukushkin, M. Kawasaki, J. H. Smet

Microwave induced resistance and photovoltage oscillations were investigated in $Mg_xZn_{1-x}O/ZnO$ heterostructures. The physics of these oscillations is controlled significantly by scattering mechanisms, and therefore these experiments were motivated by the recently achieved high quality levels in this material and the apparent dominance of large angle, short-range scattering, which is distinct from the prevailing small

angle scattering in state-of-the-art GaAs structures. Within the studied frequency range of 35–120 GHz, up to four oscillations were resolved at 1.4 K temperature, but only in high density samples. This allowed us to extract the value of the effective electron mass $m^{*}=(0.35\pm0.01)m_0$, which is enhanced over the bare band mass, and estimate a local quantum scattering time of about 5 ps.

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Phys. Rev. Lett.
vol. 115, 197601, 2015

Spin-selective electron quantum transport in nonmagnetic MgZnO/ZnO heterostructures

D. Maryenko, J. Falson, M. S. Bahramy, I. A. Dmitriev, Y. Kozuka, A. Tsukazaki, M. Kawasaki

We report magnetotransport measurements on a high-mobility two-dimensional electron system at the nonmagnetic MgZnO/ZnO heterointerface showing distinct behavior for electrons with spin-up and spin-down orientations. The low-field Shubnikov–de Haas oscillations manifest alternating resistance peak heights which can be attributed to distinct scattering rates for different spin orientations. The tilt-field measurements at a half-integer filling factor reveal that the majority spins show usual diffusive behavior, i.e., peaks with the magnitude proportional to the index of the Landau level at the Fermi energy. By contrast, the minority spins develop “plateaus” with the magnitude of dissipative resistivity that is fairly independent of the Landau level index and is of the order of the zero-field resistivity.

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Europhys. Lett.
vol. 111, 37004, 2015

Anomalous Hall effect with massive Dirac fermions

I. Ado, I. A. Dmitriev, P. M. Ostrovsky, M. Titov

The anomalous Hall effect arises in systems with both spin-orbit coupling and magnetization. Generally, there are three mechanisms contributing to anomalous Hall conductivity: intrinsic, side jump, and skew scattering. The standard diagrammatic approach to the anomalous Hall effect is limited to computation of ladder diagrams. We demonstrate that this approach is insufficient. An important additional contribution comes from diagrams with a single pair of intersecting disorder lines. This contribution constitutes an inherent part of skew scattering on pairs of closely located defects and essentially modifies previously obtained results for anomalous Hall conductivity. We argue that this statement is general and applies to all models of anomalous Hall effect. We illustrate it by an explicit calculation for two-dimensional massive Dirac fermions with weak disorder. In this case, inclusion of the diagrams with crossed impurity lines reverses the sign of the skew scattering term and strongly suppresses the total Hall conductivity at high electron concentrations.

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Phys. Rev. B
vol. 90, 205415, 2014

Quantum oscillations of photocurrents in HgTe quantum wells with Dirac and parabolic dispersions

C. Zoth, P. Olbrich, P. Vierling, K.-M. Dantscher, V. V. Bel'kov,
M. A. Semina, M. M. Glazov, L. E. Golub, D. A. Kozlov, Z. D. Kvon,
N. N. Mikhailov, S. A. Dvoretsky, S. D. Ganichev, ,

We report on the observation of magneto-oscillations of terahertz radiation induced photocurrent in HgTe/HgCdTe quantum wells of different widths, which are characterized by a Dirac-like, inverted, and

normal parabolic band structure. The photocurrent data are accompanied by measurements of photoresistance (photoconductivity), radiation transmission, as well as magnetotransport. We develop a microscopic model of a cyclotron-resonance assisted photogalvanic effect, which describes main experimental findings. We demonstrate that the quantum oscillations of the photocurrent are caused by the crossing of Fermi level by Landau levels resulting in the oscillations of spin polarization and electron mobilities in spin subbands. Theory explains a photocurrent direction reversal with the variation of magnetic field observed in experiment. We describe the photoconductivity oscillations related with the thermal suppression of the Shubnikov–de Haas effect.

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Phys. Rev. B
vol. 89, 075414, 2014

Relaxation of optically excited carriers in graphene: Anomalous diffusion and Lévy flights

U. Briskot, I. A. Dmitriev, A. D. Mirlin

We present a theoretical analysis of the relaxation cascade of a photoexcited electron in graphene in the presence of screened electron-electron interaction in the random phase approximation. We calculate the relaxation rate of high energy electrons and the jump-size distribution of the random walk constituting the cascade which exhibits fat tails. We find that the statistics of the entire cascade are described by Lévy flights with constant drift instead of standard drift diffusion in energy space. The Lévy flight manifests nontrivial scaling relations of the fluctuations in the cascade time, which is related to the problem of the first passage time of Lévy processes. Furthermore we determine the transient differential transmission of graphene after an excitation by a laser pulse taking into account the fractional kinetics of the relaxation dynamics.

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Phys. Rev. Lett.
vol. 111, 206801, 2013

Emergence of domains and nonlinear transport in the zero-resistance state

I. A. Dmitriev, M. Khodas, A. D. Mirlin, D. G. Polyakov

We study transport in the domain state, the so-called zero-resistance state, that emerges in a two-dimensional electron system in which the combined action of microwave radiation and magnetic field produces a negative absolute conductivity. We show that the voltage-biased system has a rich phase diagram in the system size and voltage plane, with second- and first-order transitions between the domain and homogeneous states for small and large voltages, respectively. We find the residual negative dissipative resistance in the stable domain state.

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Phys. Rev. B
vol. 87, 195432, 2013

Quantum magnetooscillations in the ac conductivity of disordered graphene

U. Briskot, I. A. Dmitriev, A. D. Mirlin

The dynamic conductivity $\sigma(\omega)$ of graphene in the presence of diagonal white noise disorder and quantizing magnetic field B is calculated. We obtain analytic expressions for $\sigma(\omega)$ in various parametric regimes ranging from the quasiclassical Drude limit corresponding to strongly overlapping Landau levels (LLs) to the extreme quantum limit where the conductivity is determined by the optical selection rules of the clean graphene. The nonequidistant LL spectrum of graphene renders its transport characteristics quantitatively different from conventional 2D electron systems with parabolic spectrum. Since the magneto-oscillations in the semiclassical density of states are anharmonic and are described by a quasicontinuum of cyclotron frequencies, both the ac Shubnikov-de Haas oscillations and the quantum corrections to $\sigma(\omega)$ that survive to higher temperatures manifest a slow beating on top of fast

oscillations with the local energy-dependent cyclotron frequency. Both types of quantum oscillations possess nodes whose index scales as ω^2. In the quantum regime of separated LLs, we study both the cyclotron resonance transitions, which have a rich spectrum due to the nonequidistant spectrum of LLs, and disorder-induced transitions, which violate the clean selection rules of graphene. We identify the strongest disorder-induced transitions in recent magnetotransmission experiments. We also compare the temperature and chemical-potential dependence of $\sigma(\omega)$ in various frequency ranges from the dc limit allowing intra-LL transition only to the universal high-frequency limit where the Landau quantization provides a small B-dependent correction to the universal value of the interband conductivity $\sigma=e^2/4\hbar$ of the clean graphene.

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Rev. Mod. Phys.
vol. 84, pp.1709-1763, 2012

Nonequilibrium phenomena in high Landau levels

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov, and M. A. Zudov

Developments in the physics of 2D electron systems during the last decade revealed a new class of nonequilibrium phenomena in the presence of a moderately strong magnetic field. The hallmark of these phenomena is magnetoresistance oscillations generated by the external forces that drive the electron system out of equilibrium. The rich set of dramatic phenomena of this kind, discovered in high-mobility semiconductor nanostructures, includes, in particular, microwave radiation-induced resistance oscillations and zero-resistance states, as well as Hall field-induced resistance oscillations and associated zero-differential resistance states. The experimental manifestations of these phenomena and the unified theoretical framework for describing them in terms of a quantum kinetic equation are reviewed. This survey also contains a thorough discussion of the magnetotransport properties of 2D electrons in the linear-response regime, as well as an outlook on future directions, including related nonequilibrium phenomena in other 2D electron systems.

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Journal of Physics: Conf. Ser.
vol. 334, 012015, 2011

Nonequilibrium magnetooscillations in spatially non-uniform quantum Hall systems

I. A. Dmitriev

A theory of nonequilibrium magnetotransport in high Landau levels of inhomogeneous quantum Hall systems is presented. A nonlinear current is calculated in response to given local gradients of the chemical and electrostatic potential in the presence of moderately strong microwave radiation. In the regime of high temperature, theory generalizes previously obtained results describing microwave- and Hall-induced oscillations of magnetoresistivity for the case of spatially non-uniform systems. Additionally, the regime of low temperatures is studied, where strong modification of Shubnikov-de Haas oscillations by the ac and dc fields is demonstrated.

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Phys. Rev. B
vol. 84, 125448, 2011

Negative conductivity and anomalous screening in two-dimensional electron systems subjected to microwave radiation

S. I. Dorozhkin, I. A. Dmitriev, A. D. Mirlin

A two-dimensional electron system in a quantizing magnetic field can be driven by microwave radiation into a nonequilibrium state with strong magneto-oscillations of the dissipative conductivity. We demonstrate that in such a system a negative conductivity can coexist with a positive diffusion coefficient. In a finite system, the solution of coupled electrostatic and linear transport problems shows that the diffusion can

stabilize a state with negative conductivity. Specifically, this happens when the system size is smaller than the absolute value of the nonequilibrium screening length that diverges at the point where the conductivity changes sign. We predict that a negative resistance can be measured in such a state. Furthermore, for a nonzero difference between the work functions of two contacts, we explore the distribution of the electrostatic potential and of the electron density in the sample. We show that in the diffusion-stabilized regime of negative conductivity the system splits into two regions with opposite directions of electric field. This effect is a precursor of the domain structure that has been predicted to emerge spontaneously in the microwave-induced zero-resistance states.

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Phys. Rev. B
vol. 82, 201311(R), 2010

Phonon-induced resistance oscillations of two-dimensional electron systems drifting with supersonic velocities

I. A. Dmitriev, R. Gellmann, and M. G. Vavilov

We present a theory of the phonon-assisted nonlinear dc transport of two-dimensional electrons in high Landau levels. The nonlinear dissipative resistivity displays quantum magneto-oscillations governed by two parameters which are proportional to the Hall drift velocity v_H of electrons in electric field and the speed of sound s. In the subsonic regime, $v_H < s$, the theory quantitatively reproduces the oscillation pattern observed in recent experiments. We also find the $\pi/2$ phase change in oscillations across the sound barrier $v_H = s$. In the supersonic regime, $v_H > s$, the amplitude of oscillations saturates with lowering temperature while the subsonic region displays exponential suppression of the phonon-assisted oscillations with temperature.

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Phys. Rev. B
vol. 81, 201302(R), 2010

Quantum oscillations in the microwave magneto-absorption of a two-dimensional electron gas

O. M. Fedorych, M. Potemski, S. A. Studenikin, J. A. Gupta, Z. R. Wasilewski, I. A. Dmitriev

We report on the experimental observation of the quantum oscillations in microwave magnetoabsorption of a high-mobility two-dimensional electron gas induced by Landau quantization. Using original resonance-cavity technique, we observe two kinds of oscillations in the magnetoabsorption originating from inter-Landau-level and intra-Landau-level transitions. The experimental observations are in full accordance with theoretical predictions. Presented theory also explains why similar quantum oscillations are not observed in transmission and reflection experiments on high-mobility structures despite of very strong effect of microwaves on the dc resistance in the same samples.

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Physica E
vol. 42, pp.1159-1162, 2010

Photogalvanic effects originating from the violation of the Einstein relation in a 2D electron gas in high Landau levels

I. A. Dmitriev, S. I. Dorozhkin, and A. D. Mirlin

Recent experiment [S.I. Dorozhkin et al., Phys. Rev. Lett. 102 (2009) 036602] on quantum Hall structures with strongly asymmetric contact configuration discovered microwave-induced photocurrent and photovoltage magnetooscillations in the absence of dc driving. We show that in an irradiated sample the Landau quantization leads to violation of the Einstein relation between the dc conductivity and diffusion coefficient. Then, in the presence of a built-in electric field in a sample, the microwave illumination causes photo-galvanic signals which oscillate as

a function of magnetic field with the period determined by the ratio of the microwave frequency to the cyclotron frequency, as observed in the experiment.

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Phys. Rev. B
vol. 80, 165327, 2009

Mechanisms of the microwave photoconductivity in quantum hall systems with mixed disorder

I. A. Dmitriev, M. Khodas, A. D. Mirlin, D. G. Polyakov, M. G. Vavilov

We present a systematic study of the microwave-induced oscillations in the magnetoresistance of a two-dimensional electron gas for mixed disorder including both short-range and long-range components. The obtained photoconductivity tensor contains contributions of four distinct transport mechanisms. We show that the photoresponse depends crucially on the relative weight of the short-range component of disorder. Depending on the properties of disorder, the theory allows one to identify the temperature range within which the photoresponse is dominated by one of the mechanisms analyzed in the paper.

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Phys. Rev. B
vol. 80, 125418, 2009

Theory of the microwave-induced photocurrent and photovoltage magnetooscillations in a spatially non-uniform 2D electron gas

I. A. Dmitriev, S. I. Dorozhkin, and A. D. Mirlin

Recent experiment [S. I. Dorozhkin et al., Phys. Rev. Lett. 102, 036602 (2009)] on quantum Hall structures with strongly asymmetric contact configuration discovered microwave-induced photocurrent and photovoltage magneto-oscillations in the absence of dc driving. We show that in an irradiated sample the Landau quantization leads to violation of

the Einstein relation between the dc conductivity and diffusion coefficient. Then, in the presence of a built-in electric field in a sample, the microwave illumination causes photogalvanic signals which oscillate as a function of magnetic field with the period determined by the ratio of the microwave frequency to the cyclotron frequency, as observed in the experiment.

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Int. J. of Mod. Phys. B.
vol. 23, p.2678-2683, 2009

Integer and fractional magnetooscillations in irradiated quantum Hall systems

I. A. Dmitriev, A. D. Mirlin, and D. G. Polyakov

Recent results on nonequilibrium magnetotransport of electrons in irradiated quantum Hall systems are reviewed. The phenomena discussed include integer and fractional microwave-induced resistance oscillations as well as quantum magnetooscillations in DC and AC conductivity and in local compressibility of a 2D electron gas.

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Phys. Stat. Sol. B
vol. 245, pp.239-259, 2008

Magnetotransport of electrons in quantum Hall systems

I.A. Dmitriev, F. Evers, I.V. Gornyi, A.D. Mirlin, D.G. Polyakov, P. Wölfle

Recent theoretical results on magnetotransport of electrons in a 2D system in the range of moderately strong transverse magnetic fields are reviewed. The phenomena discussed include: quasiclassical memory effects in systems with various types of disorder, transport in lateral superlattices, interaction-induced quantum magnetoresistance, quantum magnetooscillations in dc and ac transport, and oscillatory microwave photoconductivity.

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Physica E
vol. 40, pp.1332-1334, 2008

Fractional microwave-induced resistance oscillations

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov

We develop a systematic theory of microwave-induced oscillations in magnetoresistivity of a 2D electron gas in the vicinity of fractional harmonics of the cyclotron resonance, observed in recent experiments. We show that in the limit of well-separated Landau levels the effect is dominated by the multiphoton inelastic mechanism. At moderate magnetic field, two single-photon mechanisms become important. One of them is due to resonant series of multiple single-photon transitions, while the other originates from microwave-induced sidebands in the density of states of disorder-broadened Landau levels.

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Phys. Rev. Lett.
vol. 99, 206805, 2007

Theory of the fractional microwave-induced resistance oscillations

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov

We develop a systematic theory of microwave-induced oscillations in magnetoresistivity of a 2D electron gas in the vicinity of fractional harmonics of the cyclotron resonance, observed in recent experiments. We show that in the limit of well-separated Landau levels the effect is dominated by a change of the distribution function induced by multiphoton processes. At moderate magnetic field, a single-photon mechanism originating from the microwave-induced sidebands in the density of states of disorder-broadened Landau levels becomes important.

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Phys. Rev. B
vol. 75, 245320, 2007

Microwave photoconductivity of a 2D electron gas: Mechanisms and their interplay at high radiation power

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov

We develop a systematic theory of microwave-induced oscillations in the magnetoresistivity of a two-dimensional electron gas, focusing on the regime of strongly overlapping Landau levels. At linear order in microwave power, two mechanisms of the oscillations ("quadrupole" and "photovoltaic") are identified, distinctly different from those studied before ("displacement" and "inelastic"). The quadrupole and photovoltaic mechanisms are shown to be the only ones that give rise to oscillations in the nondiagonal part of the photoconductivity tensor. In the diagonal part, the inelastic contribution dominates at moderate microwave power, while at elevated power the other mechanisms become relevant. We demonstrate the crucial role of feedback effects, which lead to a strong interplay of the four mechanisms in the nonlinear photoresponse and yield, in particular, a nonmonotonic power dependence of the photoconductivity, narrowing of the magnetoresonances, and a nontrivial structure of the Hall photoresponse. At ultrahigh power, all effects related to the Landau quantization decay due to a combination of the feedback and multiphoton effects, restoring the classical Drude conductivity.

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JETP Lett.
vol. 85, no. 1, pp.86-91, 2007

Fractional features in radiation-induced oscillations of the magnetoresistance of two-dimensional electron systems

I. V. Pechenezhskii, S. I. Dorozhkin, I. A. Dmitriev

The magnetoresistance of two-dimensional electron systems irradiated by microwave radiation is calculated. It exhibits oscillatory features at fractional values of the ratio ω/ω_c of the circular frequency of microwave

radiation to the cyclotron frequency. The calculation explains existing experimental data by nonequilibrium population of electron states that appears due to one-photon processes and predicts ω/ω_c values near which the basic features in magnetoresistance are expected. In the framework of the mechanism under consideration, the fractional features can be observed only in the crossover from strongly overlapping to separate Landau levels and only at radiation frequencies below the threshold frequencies depending on a fractional value.

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Phys. Rev. B
vol. 71, 115316, 2005

Theory of the microwave-induced oscillations in the magnetoconductivity of a 2D electron gas

I. A. Dmitriev, M. G. Vavilov, I. L. Aleiner, A. D. Mirlin, D. G. Polyakov

We develop a theory of magneto-oscillations in the photoconductivity of a two-dimensional electron gas observed in recent experiments. The effect is governed by a change of the electron distribution function induced by the microwave radiation. We analyze a nonlinearity with respect to both the dc field and the microwave power, as well as the temperature dependence determined by the inelastic relaxation rate.

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Appl. Phys. Lett.
vol. 86, no. 3, 032108, 2005

Suppression of intrinsic bistability in resonant-tunneling diode by in-plane magnetic field

A. Yu. Serov, G. G. Zegrya

Using the Bardeen formalism, we calculated the electron tunneling through a double barrier structure with an in-plane magnetic field. It is shown that the in-plane magnetic field has two effects on the current–

voltage characteristics. First, it reduces the width of the bistable region. At high magnetic fields, the bistability can be completely suppressed. This can provide a method for tuning the bistable region in a double barrier structure. Second, it modifies the peak current. The dependence of the peak current on the magnetic field is different in the cases of high and low electron concentrations in the quantum well.

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JETP Lett.
vol. 80, no. 5, pp. 412-415, 2004

Absolute negative conductivity and zero-resistance states in two dimensional electron systems: A plausible scenario

V. Ryzhii, A. Chaplik, R. Suris

We present a model which provides a plausible explanation of the effect of zero-resistance and zero-conductance states in two-dimensional electron systems subjected to a magnetic field and irradiated with microwaves observed in a number of experiments and of the effect main features. The model is based on the concept of absolute negative conductivity associated with photon-assisted scattering of electrons on impurities. It is shown that the main features of the effect can be attributed to the interplay of different electron scattering mechanisms.

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Physica E
vol. 22, no. 1-3, pp. 13-18, 2004

Mechanisms of absolute negative conductivity in a two-dimensional electron system stimulated by microwave radiation and zero-resistance and zero-conductance states

V .Ryzhii, R. Suris, B. Shchamkhalova

We review the mechanisms resulting in absolute negative conductivity in two-dimensional electron systems subjected to a magnetic field which

can be relevant to the so-called zero-resistance and zero-conductance states stimulated by microwaves observed in recent experiments.

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Phys. Rev. B
vol. 70, 161306(R), 2004

Compressibility of a 2D electron gas under microwave radiation

M. G. Vavilov, I. A. Dmitriev, I. L. Aleiner, A. D. Mirlin, D. G. Polyakov

Microwave irradiation of a two-dimensional electron gas (2DEG) produces a non-equilibrium distribution of electrons, and leads to oscillations in the dissipative part of the conductivity. We show that the same non-equilibrium electron distribution induces strong oscillations in the 2DEG compressibility, measured by local probes. Local probe measurements of the compressibility are expected to provide information about the domain structure of the zero resistance state of a 2DEG under microwave radiation.

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Advances in Solid State Physics
vol. 44, pp.147-156, 2004

Oscillatory photoconductivity of a two-dimensional electron gas in a magnetic field

I. A. Dmitriev, M. G. Vavilov, I. L. Aleiner, A. D. Mirlin, D. G. Polyakov

We develop a theory of magneto-oscillations in the photoresistivity of a two-dimensional electron gas observed in recent experiments. It is shown that the effect is governed by a change of the electron distribution function induced by the microwave radiation. We analyze a nonlinearity with respect to both the dc field and the microwave power, as well as the temperature dependence determined by the inelastic relaxation rate.

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Phys. Rev. B
vol. 70, 165305, 2004

Oscillatory ac- and photoconductivity of a 2D electron gas: Quasiclassical transport beyond the Boltzmann equation

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov

We have analyzed the quasiclassical mechanism of magneto-oscillations in the ac conductivity and photoconductivity, related to non-Markovian dynamics of disorder-induced electron scattering. While the magneto-oscillations in the photoconductivity are found to be weak, the effect manifests itself much more strongly in the ac conductivity, where it may easily dominate over the oscillations due to the Landau quantization. We argue that the damping of the oscillatory photoconductivity provides a reliable method of measuring the homogeneous broadening of Landau levels (single-particle scattering rate) in high-mobility structures.

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Physica E
vol. 25, pp.205-211, 2004

Theory of the oscillatory photoconductivity of a two-dimensional electron system

I. A. Dmitriev, M. G. Vavilov, I. L. Aleiner, A. D. Mirlin, D. G. Polyakov

We develop a theory of magnetooscillations in the photoresistivity of a two-dimensional electron gas observed in recent experiments. According to our theory, the effect is governed by a change of the electron distribution function induced by the microwave radiation. We analyze a nonlinearity with respect to both the DC field and the microwave power, as well as the temperature dependence determined by the inelastic relaxation rate.

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J. Phys. Condensed Matter.
vol. 15, no. 40, pp. 6855-6869, 2003

Nonlinear effects in microwave photoconductivity of two-dimensional electron systems

V .Ryzhii, R. Suris

We present a model for microwave photoconductivity of two-dimensional electron systems in a magnetic field which describes the effects of strong microwave and steady-state electric fields. Using this model, we derive an analytical formula for the photoconductivity associated with photon- and multi-photon-assisted impurity scattering as a function of the frequency and power of microwave radiation. According to the developed model, the microwave conductivity is an oscillatory function of the frequency of microwave radiation and the cyclotron frequency which turns zero at the cyclotron resonance and its harmonics. It exhibits maxima and minima (with absolute negative conductivity) at the microwave frequencies somewhat different from the resonant frequencies. The calculated power dependence of the amplitude of the microwave photoconductivity oscillations exhibits pronounced sublinear behavior similar to a logarithmic function. The height of the microwave photoconductivity maxima and the depth of its minima are nonmonotonic functions of the electric field. It is pointed to the possibility of a strong widening of the maxima and minima due to a strong sensitivity of their parameters on the electric field and the presence of strong long-range electricfield fluctuations. The obtained dependences are consistent with the results of the experimental observations.

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Phys. Rev. Lett.
vol. 91, 226802, 2003

Cyclotron-resonance harmonics in the ac response of a 2D electron gas with smooth disorder

I. A. Dmitriev, A. D. Mirlin, D. G. Polyakov

The frequency-dependent conductivity $\sigma_{xx}(\omega)$ of 2D electrons subjected to a transverse magnetic field and smooth disorder is calculated. The interplay of Landau quantization and disorder scattering gives rise to an oscillatory structure that survives in the high-temperature limit. The relation to recent experiments on photoconductivity by Zudov et al. and Mani et al. is discussed.

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Excitons and excitonic complexes

Phys. Rev. B
vol. 98, 075204, 2018

Third harmonic generation on exciton-polaritons in bulk semiconductors subject to a magnetic field

W. Warkentin, J. Mund, D. R. Yakovlev, V. V. Pavlov,
R. V. Pisarev, A. *V. Rodina, M. A. Semina, M. M. Glazov,*
E. L. Ivchenko, M. Bayer

We report on a comprehensive experimental and theoretical study of optical third harmonic generation (THG) on the exciton-polariton resonances in the zinc-blende semiconductors GaAs, CdTe, and ZnSe subject to an external magnetic field, representing a topic that had remained unexplored so far. In these crystals, crystallographic THG is allowed in the electric-dipole approximation, so that substantial magnetic-field-induced changes of the THG are unexpected: the symmetry reduction due to magnetic field, corresponding change of the selection rules, and the Zeeman effect are expected to play a minor role. Surprisingly, we observe a strong enhancement of the THG intensity by a factor of 50 for the 1s exciton-polariton in GaAs in magnetic fields up to 10 T. In contrast, the corresponding enhancement is moderate in CdTe and almost absent in ZnSe. In order to explain this strong variation, we develop a microscopic theory accounting for the optical harmonics generation on exciton-polaritons and analyze the THG mechanisms induced by the magnetic field. The calculations show that the increase of THG intensity is dominated by the magnetic field enhancement of the exciton oscillator strength, which is particularly strong for GaAs in the studied range of field strengths. The much weaker increase of THG intensity in CdTe and ZnSe is explained by the considerably larger exciton binding energies, leading to a weaker modification of their oscillator strengths by the magnetic field.

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Semiconductors
vol. 52, Issue 5, pp 554–557, 2018

Biexciton binding energy in spherical quantum dots with Γ8 valence band

A. A. Golovatenko, M. A. Semina, A. V. Rodina, T. V. Shubina

The biexciton binding energy in spherical CdSe/ZnSe quantum dots is calculated variationally in the framework of *kp* -perturbation theory. Smooth and abrupt confining potentials with the same localization area of carriers are compared for two limiting cases of lighthole to heavy hole mass ratio $\beta = m_{lh}/m_{hh}$: β=1 and β=0. Accounting for correlations between carriers results in their polarized configuration and significantly increases the biexciton binding energy in comparison with the first order perturbation theory. For β =0 in smooth confining potentials there are three nearby biexciton states separated by small energy gap between $1S_{3/2}$ and $1P_{3/2}$ hole states

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Phys. Rev. Materials
vol. 2, 011001(R), 2018

Optical spectroscopy of excited exciton states in MoS_2 monolayers in van der Waals heterostructures

C. Robert, M. A. Semina, F. Cadiz, M. Manca, E. Courtade, T. Taniguchi, K. Watanabe, H. Cai, S. Tongay, B. Lassagne, P. Renucci, T. Amand, X. Marie, M. M. Glazov, B. Urbaszek

The optical properties of MoS_2 monolayers are dominated by excitons, but for spectrally broad optical transitions in monolayers exfoliated directly onto SiO_2 substrates detailed information on excited exciton states is inaccessible. Encapsulation in hexagonal boron nitride (hBN) allows approaching the homogenous exciton linewidth, but interferences in the van der Waals heterostructures make direct comparison between transitions in optical spectra with different oscillator strength more challenging. Here we reveal in reflectivity and in photoluminescence excitation spectroscopy the presence of excited states of the A exciton in

MoS_2 monolayers encapsulated in hBN layers of calibrated thickness, allowing us to extrapolate an exciton binding energy of ≈220 meV. We theoretically reproduce the energy separations and oscillator strengths measured in reflectivity by combining the exciton resonances calculated for a screened two-dimensional Coulomb potential with transfer matrix calculations of the reflectivity for the van der Waals structure. Our analysis shows a very different evolution of the exciton oscillator strength with principal quantum number for the screened Coulomb potential as compared to the ideal two-dimensional hydrogen model.

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Phys. Rev. B
vol. 98, 035302, 2018

Observation of exciton-phonon coupling in $MoSe_2$ monolayers

S. Shree, M. Semina, C. Robert, B. Han, T. Amand, A. Balocchi, M. Manca, E. Courtade, X. Marie, T. Taniguchi, K. Watanabe, M. M. Glazov, B. Urbaszek

We study experimentally and theoretically the exciton-phonon interaction in $MoSe_2$ monolayers encapsulated in hexagonal BN, which has an important impact on both optical absorption and emission processes. The exciton transition linewidth down to 1 meV at low temperatures makes it possible to observe high-energy tails in absorption and emission extending over several meV, not masked by inhomogeneous broadening. We develop an analytical theory of the exciton-phonon interaction accounting for the deformation potential induced by the longitudinal acoustic phonons, which plays an important role in exciton formation. The theory allows fitting absorption and emission spectra and permits estimating the deformation potential in $MoSe_2$ monolayers. We underline the reasons why exciton-phonon coupling is much stronger in two-dimensional transition metal dichalcogenides as compared to conventional quantum well structures. The importance of exciton-phonon interactions is further highlighted by the observation of a multitude of Raman features in the photoluminescence excitation experiments.

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Phys. Rev. B
vol. 96, 125142, 2017

Scaling laws of Rydberg excitons

J. Heckötter, M. Freitag, D. Fröhlich, M. Aßmann, M. Bayer, M. A. Semina, M. M. Glazov

Rydberg atoms have attracted considerable interest due to their huge interaction among each other and with external fields. They demonstrate characteristic scaling laws in dependence on the principal quantum number n for features such as the magnetic field for level crossing or the electric field of dissociation. Recently, the observation of excitons in highly excited states has allowed studying Rydberg physics in cuprous oxide crystals. Fundamentally different insights may be expected for Rydberg excitons, as the crystal environment and associated symmetry reduction compared to vacuum give not only optical access to many more states within an exciton multiplet but also extend the Hamiltonian for describing the exciton beyond the hydrogen model. Here we study experimentally and theoretically the scaling of several parameters of Rydberg excitons with n, for some of which we indeed find laws different from those of atoms. For others we find identical scaling laws with n, even though their origin may be distinctly different from the atomic case. At zero field the energy splitting of a particular multiplet n scales as n^{-3} due to crystal-specific terms in the Hamiltonian, e.g., from the valence band structure. From absorption spectra in magnetic field we find for the first crossing of levels with adjacent principal quantum numbers a $B_r \propto n^{-4}$ dependence of the resonance field strength, B_r, due to the dominant paramagnetic term unlike for atoms for which the diamagnetic contribution is decisive, resulting in a $B_r \propto n^{-6}$ dependence. By contrast, the resonance electric field strength shows a scaling as $E_r \propto n^{-5}$ as for Rydberg atoms. Also similar to atoms with the exception of hydrogen we observe anticrossings between states belonging to multiplets with different principal quantum numbers at these resonances. The energy splittings at the avoided crossings scale roughly as n^{-4}, again due to crystal specific features in the exciton Hamiltonian. The data also allow us to assess the susceptibility of Rydberg excitons to the external fields: The crossover field strength in magnetic field from a hydrogenlike exciton to a magnetoexciton dominated by electron and hole Landau level

quantization scales as n^{-3}. In electric field, on the other hand, we observe the exciton polarizability to scale as n^7. At higher fields, the exciton ionization can be studied with ionization voltages that demonstrate an n^{-4} scaling law. Particularly interesting is the field dependence of the width of the absorption lines which remains constant before dissociation for high enough n, while for small $n \lesssim 12$ an exponential increase is found. These results are in excellent agreement with theoretical predictions.

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Phys. Rev. B
vol. 96, 085302, 2017

Charged excitons in monolayer WSe_2: Experiment and theory

E. Courtade, M. Semina, M. Manca, M. M. Glazov, C. Robert, F. Cadiz, G. Wang, T. Taniguchi, K. Watanabe, M. Pierre, W. Escoffier, E. L. Ivchenko, P. Renucci, X. Marie, T. Amand, B. Urbaszek

Charged excitons, or $X^{\pm}$ trions, in monolayer transition-metal dichalcogenides have binding energies of several tens of meV. Together with the neutral exciton X^0 they dominate the emission spectrum at low and elevated temperatures. We use charge-tunable devices based on WSe_2 monolayers encapsulated in hexagonal boron nitride to investigate the difference in binding energy between X^+ and X^- and the X^- fine structure. We find in the charge-neutral regime, the X^0 emission accompanied at lower energy by a strong peak close to the longitudinal optical (LO) phonon energy. This peak is absent in reflectivity measurements, where only the X^0 and an excited state of the X^0 are visible. In the n-doped regime, we find a closer correspondence between emission and reflectivity as the trion transition with a well-resolved fine-structure splitting of 6 meV for X^- is observed. We present a symmetry analysis of the different X^+ and X^- trion states and results of the binding energy calculations. We compare the trion binding energy for the n- and p-doped regimes with our model calculations for low carrier concentrations. We demonstrate that the splitting between the X^+ and X^- trions as well as the fine structure of the X^- state can be related to the short-range Coulomb-exchange interaction between the charge carriers.

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Physics of the Solid State
vol. 59, no. 6, pp 1215–1224, 2017

Biexciton in II–VI quantum dots with different localization potentials

A. A. Golovatenko, M. A. Semina, A. V. Rodina, T. V. Shubina

We present a comparative study of the influence of the form of a localization potential on the binding energy of the biexciton in spherically symmetric quantum dots based on II–VI compounds. The proposed criterion for the comparison of potentials of different forms—the box potential, the harmonic oscillator, and the Gaussian potential—is based on the identical localization of charge carriers of the same sign in these potentials. Calculations of the biexciton binding energy have been performed using the variational method within the framework of the *kp*-perturbation theory taking into account additional polarization terms in the wave functions of the electron and hole subsystems, as well as the complex structure of the valence band. The obtained results have demonstrated that the presence of a smoothly varying finite-height potential in Cd(Zn)Se/ZnSe quantum dots can lead to a more efficient localization in the case of the biexciton in comparison with the exciton, which is of interest for the implementation of fast-acting quantum light emitters.

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Phys. Rev. B
vol. 95, 035210, 2017

High-resolution study of the yellow excitons in Cu_2O subject to an electric field

J. Heckötter, M. Freitag, D. Fröhlich, M. Aßmann, M. Bayer, M. A. Semina, M. M. Glazov

We have used high-resolution transmission spectroscopy to study the exciton level spectrum in Cu_2O subject to a longitudinal external electric field, i.e., in the geometry where the transmitted light is propagating along the field direction. Different experimental configurations given by

the field orientation relative to the crystal and the light polarization have been explored. We focus on the range of small principal quantum numbers $n \leq 7$. The number of exciton states belonging to a particular principal quantum number increases with n, leading to an enhanced complexity of the spectra. Still, in particular, for n=3..5, a spectral separation of the different lines is feasible and identification as well as assignment of the dominant state character are possible. We find a strong dependence of the spectra on the chosen light propagation direction and polarization configuration, reflecting the inadequacy of the hydrogen model for describing the excitons. With increasing the field excitonic states with different parity become mixed, leading to optical activation of states that are dark in zero field. As compared with atoms, due to the reduced Rydberg energy states with different n can be brought into resonance in the accessible electric field strength range. When this occurs, we observe mostly crossing of levels within the experimental accuracy showing that the electron and hole motion remains regular. The observed features are well described by detailed calculations accounting for the spin-orbit coupling, the cubic anisotropy effects, and the symmetry-imposed optical selection rules.

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Phys. Rev. Lett.
vol. 115, 027402, 2015

Observation of high angular momentum excitons in cuprous oxide

*J. Thewes, J. Heckötter, T. Kazimierczuk, M. Aßmann,
D. Fröhlich, M. Bayer, M. A. Semina, M. M. Glazov*

The recent observation of dipole-allowed *P* excitons up to principal quantum numbers of n=25 in cuprous oxide has given insight into exciton states with unprecedented spectral resolution. While so far, the exciton description as a hydrogenlike complex has been fully adequate for cubic crystals, we demonstrate here distinct deviations: The breaking of rotational symmetry leads to mixing of high angular momentum *F* and *H* excitons with the *P* excitons so that they can be observed in absorption. The *F* excitons show a threefold splitting that depends systematically on n, in agreement with theoretical considerations. From detailed comparison of experiment and theory we determine the cubic anisotropy parameter of the Cu2O valence band.

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JETP Letters
vol. 94, no. 7, pp. 574-578, 2011

Coulomb states in nanostructures, accidental degeneracy, and the Laplace-Runge-Lenz operator

M. A. Semina, R. A. Suris

The energy-level structure of spatially indirect Coulomb complexes is investigated. Two limiting cases that correspond to the two-dimensional hydrogen atom and planar isotropic harmonic oscillator are characterized by accidental degeneracy are considered. Numerical calculations are used to trace the evolution of the energy-level structure between these two limiting cases.

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Semiconductors
vol. 47, no. 7, pp 917–925, 2011

Effect of localization in quantum wells and quantum wires on heavy-light hole mixing and acceptor binding energy

M. A. Semina, R. A. Suris

The variational method taking into account the complex valence band structure is used to study the effect of localization in quantum wells and quantum wires on the acceptor binding energy. Trial functions that make possible tracing of the transition from the bulk material to narrow quantum wells and quantum wires of small radius are constructed. The possibility of the appearance of an unsteadily varying dependence of the acceptor binding energy on the characteristic dimension of the system is shown.

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Semiconductors
vol. 43, no. 9, pp 1182–1192, 2009

The simplest electron-hole complexes localized at longitudinal fluctuations in quantum wires

M. A. Semina, R. A. Sergeev, R. A. Suris

The variational method is used to study how the states of electron-hole complexes in the quantum wires of a semiconductor are influenced by extra localization along the axis of the structure. Simple trial functions involving a small number of physically substantiated adjustable parameters are suggested, which provides reasonable accuracy in calculating the binding energies of ground states of the complexes in a wide range of parameters of the system. The general form of the trial functions is independent of the specific shape of the irregularity potential. The applicability of the method is demonstrated by the examples of excitons and X^+ and X^- trions localized at an irregularity described by a parabolic potential. The error of the method developed here to describe localization of the complexes at arbitrarily shaped potential irregularities is estimated. The accuracy of the variational calculations of the binding energy of localized excitons is estimated by comparing the results with those obtained by direct diagonalization of the Hamiltonian.

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Physica E
vol. 40, no. 5, pp.1357-1359, 2008

Binding energies of 2D laterally-confined trions

M. A. Semina, R. A. Sergeev, R. A. Suris

The localization of two-dimensional (2D) trions on the attractive potential of the arbitrary shape and strength is studied theoretically. We suggest a general method for the construction of a simple and descriptive trial function suitable for the calculation of the ground state binding energy for electron–hole complexes. The limiting cases corresponding to different relations between characteristic parameters are analyzed. Binding

energy of the 2D trions, localized on parabolic potential, is calculated in a wide range of values of its parameters.

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Semiconductors
vol. 42, no. 12, pp 1427–1433, 2008

The binding energy of excitons and X^+ and X^- trions in one-dimensional systems

M. A. Semina, R. A. Sergeev, R. A. Suris

The exciton and trion states in semiconductor quantum wires are treated by the variational method. Simple trial functions provide an adequate precision of the calculation over a wide region of wire radii, with an arbitrary relation between the effective masses of charge carriers. The precision of the results obtained by the variational method is checked by numerical diagonalization of the Hamiltonian of excitons and positively and negatively charged trions. The asymptotic behavior of the binding energies of excitons and trions in narrow quantum wires is established in the analytical form. The structure of the excited X^+ trion states is analyzed in the context of the adiabatic approximation.

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Phys. Status Solidi C
vol. 4, pp. 363-365, 2006

Electron-hole complexes localized on the quantum well interface roughnesses

M. A. Semina, R. A. Sergeev, R. A. Suris

The localization of two-dimensional electron-hole complexes on the attractive potential of an arbitrary shape is studied theoretically. General method of a simple and vivid trial function construction for calculation of the ground state binding energy for such complexes is suggested. The limiting cases corresponding to different relations between characteristic

parameters are analyzed. The developed method is illustrated by the particular calculations for the case of exciton in two-dimensional quantum well with an additional lateral confinement potential.

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Semiconductors
vol. 40, no. 11, pp 1338–1345, 2006

Localization of electron-hole complexes at fluctuations of interfaces of quantum dots

M. A. Semina, R. A. Sergeev, R. A. Suris

The localization of two-dimensional electron-hole complexes at the attractive potential of arbitrary shape is treated theoretically. A general method of construction of simple descriptive trial functions is suggested to calculate the binding energy of the ground state of such complexes. The limiting cases corresponding to different relations between the characteristic parameters of the system are analyzed. The developed approach is illustrated by particular calculations for the exciton in a two-dimensional quantum well with an additional lateral potential.

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Eur. Phys. J. B
vol. 47, no. 4, pp. 541-547, 2005

Universal estimation of X^- trion binding energy in semiconductor quantum wells

R. A. Sergeev, R. A. Suris, G. V. Astakhov, W. Ossau, D. R. Yakovlev

We have analyzed the binding energy (EBT) of negatively charged excitons (X^-) in GaAs, CdTe and ZnSe quantum wells, which differ considerably in exciton and trion binding energy. Surprisingly, the EBT in these materials plotted against quantum well width in Bohr units is found to group around one universal curve described by a simple phenomenological equation. An illustrative model is suggested to calculate the binding energy EBT in a general case, and the results of

calculations are in agreement with experimental data. The EBT dependencies on the mass ratio and the barriers height are also obtained from the general model and compared with other calculations available.

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NATO Science series II
vol.119 (Optical Properties of 2D Systems
with Interacting Electrons)
pp. 111-124, 2003

Correlation between trion and hole in Fermi distribution in process of trion photo-excitation in doped QWs

R. A. Suris

The problem of correlation between a trion and a hole in the electron Fermi distribution created in the process of trion photo-excitation in doped quantum wells is under consideration. The hole in the Fermi distribution appears in the trion creation process consisting of picking of the Fermi Sea electron up by the exciton created in virtual state due to photon absorption. It is demonstrated that the interaction results in formation of a correlated state of the trion and the hole in the Fermi Sea. The state has excitation energy which is less then trion energy minus Fermi energy that can be obtained as a lower edge of trion excitation band using the simple energy conservation low in the picture of independent trion and electrons. The wave function of the correlated state is real and decreases with increase of distance between the trion and the Fermi Sea hole, r, as $1/r^{3/2}$. The wave function can be normalized to unity and it corresponds to correlated state of the trion and Fermi Sea hole. In contrast to this state, the states with excitation energies in the absorption band between the trion energy and the trion energy minus Fermi energy have complex wave functions that decrease as $1/r^{1/2}$. These states correspond to the trion and the Fermi Sea hole that is running away from the trion. The correlated state described above is supposed to be responsible for the narrow trion absorption line that was observed experimentally.

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NATO Science series II
vol.119 (Optical Properties of 2D Systems
with Interacting Electrons)
pp. 279-288, 2003

The heavy-hole X^+ trion in double quantum wells

R. A. Sergeev, R. A. Suris

The system of two heavy holes in 2D Quantum Well bound by an electron in the adjacent 2D Quantum Well is considered. Simple variational wave function with a few variational parameters is suggested to calculate the ground state energy of such X^+ trion in the whole range of the distances between the wells. The trion appears to be bound up to unexpectedly large distance values. The critical value of the latter is found to be more than 34 (in atomic units) which is 68 times of the distance between the holes in 2D X^+ trion. The resonant state of the trion at the distances between QWs greater than the critical is also considered. A few simple estimations of the trion binding energy for GaAs and ZnSe double quantum well structures are proposed.

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Semiconductors
vol. 37, no. 10, pp. 1205-1210, 2003

The X^+ trion in a system with spatial separation of the charge carriers

R. A. Sergeev, R. A. Suris

A system composed of two heavy holes located in a two-dimensional (2D) quantum well (QW) and bound via mediation of an electron in a neighboring 2D QW is considered. Using a simple qualitative trial wave function, the ground-state energy of this kind of X^+ trion is determined in the infinite-hole-mass approximation as a function of the QW spacing. Coordinate dependence of the effective potential binding the holes to each other is calculated for different values of QW spacing. In the adiabatic approximation, a set of dependences describing the X^+ trion

binding energy as a function of the electron mass to the hole mass ratio is obtained. Several estimates for the trion binding energy in GaAs-and ZnSe-based double-QW heterostructures are given.

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Nanotechnology
vol. 12, pp. 597–601, 2001

Singlet and triplet states of X^+ and X^- trions in two-dimensional quantum wells

R. A. Sergeev, R. A. Suris

A new simple variational wavefunction with a few variational parameters for two-dimensional X^+ and X^- trions is suggested. The function gives accurate results for the singlet and triplet state energies of X^+ and X^- trions in the whole range of electron-to-hole mass ratio. The mass ratio range where the triplet state exists has been found, and the behaviour of the triplet state energy has been examined near the critical mass ratio. The other excited states of the trion are analysed in the vicinity of their critical mass ratios.

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Phys.Solid State
vol. 43, no. 4, pp. 746-751, 2001

Ground-state energy of X^- and X^+ trions in a two-dimensional quantum well at an arbitrary mass ratio

R. A. Sergeev, R. A. Suris

A simple model variational function is proposed for an adequate unified description of X^+ and X^- two-dimensional trions over the entire range of electron-to-hole mass ratios with the use of a minimum number of variable parameters.

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Phys. Status Solidi B
vol. 227, no. 2, pp. 387-396, 2001

The triplet state of X^+ trion in 2D quantum wells

R. A. Sergeev, R. A. Suris

A simple variational calculation of the trion triplet state energy is presented. In zero magnetic field, the triplet state of the hole trion (X^+) in two dimensions appears to be bound in a considerable mass ratio range close to the H_2^+-like trion. The critical value of electron-to-hole mass ratio estimated by various methods is found to be between 0.35 and 0.39. The energy behavior near the critical mass ratio is analytically examined.

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Phys. Status Solidi B
vol. 227, no. 2, pp. 343-352, 2001

Excitons and trions modified by interaction with a two-dimensional electron gas

R. A. Suris, V. P. Kochereshko, G. V. Astakhov, D. R. Yakovlev, W. Ossau, J. Nurnberger, W. Faschinger, G. Landwehr, T. Wojtowicz, G. Karczewski, J. Kossut

A concept of mixed exciton-trion states is formulated theoretically and proved experimentally for II–VI semiconductor quantum wells with a two-dimensional electron gas. The concept considers the resonances of neutral excitons and charged excitons (trions) as mixed (with each other) via their interaction with free electrons. Reflectivity spectra of modulation-doped ZnSe/(Zn,Mg)(S,Se) and CdTe/(Cd,Mg)Te quantum wells are analyzed. A good qualitative agreement of the experimental results with model calculations is achieved.

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Proc. of the 8th Int. Symposium Nanostructures:
Physics and Technology, St Petersburg, Russia
pp. 260-263, 2000

Reflectivity studies of trion (X^-) and exciton (X) states in ZnSe/(Zn,Mg)(S,Se) QWs

G. V. Astakhov, V. P. Kochereshko, D. R. Yakovlev, R. A. Suris, W. Ossau, J. Nurnberger, W. Faschinger, G. Landwehr

The oscillator strength of negatively charged exciton (trion) in ZnSe/(Zn,Mg)(S,Se) quantum-well structures with n-type modulation doping is studied by reflection spectroscopy as a function of electron concentration and temperature. The trion oscillator strength is found to increase linearly with increasing electron concentration up to $6x10^{10}$ cm^{-2}. The effect of oscillator strength "shearing" between the exciton and trion states is observed. The value of the oscillator strength shearing is found to be not more than 20%.

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Proc. of the 8th Int. Symposium Nanostructures:
Physics and Technology, St Petersburg, Russia
pp. 248-251, 2000

Spectroscopy of negatively charged excitons interacting with 2DEG in CdTe/(Cd,Mg)Te QWs

G. V. Astakhov, V. P. Kochereshko, D. R. Yakovlev, R. A. Suris, W. Ossau, G. Landwehr, T. Wojtowicz, G. Karczewski, J. Kossut

We report on experimental observation of a combined exciton-electron processes in which an incident photon creates a trion (negatively charged exciton-electron complex) and promotes an inter-Landau level transition of an additional electron.

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Quantum Hall effect

Semiconductors
vol. 49, no. 4, pp. 483-491, 2015

Quantum Hall effect in semiconductor systems with quantum dots and antidots

Ya. M. Beltukov, A. A. Greshnov

The integer quantum Hall effect in systems of semiconductor quantum-dots and antidots is stud ied theoretically as a factor of temperature. It is established that the conditions for carrier localization in quantum-dot systems favor the observation of the quantum Hall effect at higher temperatures than in quantum-well systems. The obtained numerical results show that the fundamental plateau corresponding to the transition between the ground and first excited Landau levels can be retained up to a temperature of T ~ 50 K, which is an order of magnitude higher than in the case of quantum wells. Implementation of the quantum Hall effect at such temperatures requires quantum-dot systems with controllable characteristics, including the optimal size and concentration and moderate geometrical and composition fluctuations. In addition, ordered arrangement is desirable, hence quantum antidots are preferable.

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J. Phys.: Conf. Ser.
vol. 568, 052011, 2014

The quantum Hall effect in quantum dot systems

Y. M. Beltukov, A. A. Greshnov

It is proposed to use quantum dots in order to increase the temperatures suitable for observation of the integer quantum Hall effect. A simple estimation using Fock-Darwin spectrum of a quantum dot shows that good part of carriers localized in quantum dots generate the intervals of plateaus robust against elevated temperatures. Numerical calculations employing local trigonometric basis and highly efficient kernel polynomial

method adopted for computing the Hall conductivity reveal that quantum dots may enhance peak temperature for the effect by an order of magnitude, possibly above 77 K. Requirements to potentials, quality and arrangement of the quantum dots essential for practical realization of such enhancement are indicated. Comparison of our theoretical results with the quantum Hall measurements in InAs quantum dot systems from two experimental groups is also given.

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J. Phys.: Conf. Ser.
vol. 568, 052010, 2014

Room-temperature quantum Hall effect in graphene:
The role of the two-dimensional nature of phonons

A. A. Greshnov

We consider two-dimensional nature of the electron-phonon coupling in graphene as a source for the room-temperature quantum Hall effect discovered in 2007. It is shown that magnetic field introduces strong cut-off for coupling with the two-dimensional acoustic phonons, viz. the processes with energy transfer exceeding $\hbar s l_B^{-1}$ are exponentially suppressed, while for three-dimensional phonons the cut-off is set by a temperature T (here s is the sound velocity and $l_B \propto B^{-1/2}$ is the magnetic length). Consequently, at sufficiently high temperatures and magnetic fields only a small part ($\sim\hbar s l_B^{-1}/T$) of the electron states is involved in coupling with a given electron state in comparison with the case of three-dimensional phonons. Hence, the percolation threshold is postponed, and the quantum Hall effect survives up to T = 300 K.

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Semiconductors
vol. 48, no. 2, pp. 228-234, 2014

On the effect of electron-phonon interaction on the temperature dependences of magnetotransport in quantum hall systems

A. A. Greshnov, Y. M. Beltukov

The effect of electron–phonon interaction on the temperature dependences of conductivity is studied in the mode of the integer quantum Hall effect. It is shown that electron–phonon interaction leads to the possibility of transport in the region of localized states, thus forming the shape of magnetotransport curves at a given temperature. The relation between scaling indices in the power laws describing the dependences of the widths of transition regions between successive plateaus of the quantum Hall effect on the temperature and localization length is determined within an analytical model as a function of the energy measured from a certain Landau-level center. Direct numerical calculations of the magnetotransport curves are performed at various temperatures. The results are in good agreement with theory and experimental data on the integer quantum Hall effect.

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JETP Lett.
vol. 100, no. 8, pp. 518-522, 2014

On the role of two-dimensional phonons in the possibility of the observation of the quantum hall effect in graphene at room temperature

A. A. Greshnov

An explanation of the possibility of the observation of the quantum Hall effect in graphene at room temperature with allowance for the two-dimensional nature of the electron and phonon excitations has been pro posed. It has been shown that the two-dimensional character of the

electron–phonon interaction under conditions of a strong magnetic field establishes the threshold for the energy of the emitted or absorbed phonon, thus reducing the fraction of the electronic states involved in the percolation process. The number of mixed states is proportional to the root of the magnetic field rather than to the temperature. Therefore, the percolation threshold in a rather strong magnetic field no longer depends on the temperature and the limitation on the maximum observation temperature with allowance for exclusively two-dimensional phonons arises owing to the temperature smearing of the Fermi distribution function. The contribution of three-dimensional phonons, as well as the quantitative agreement with the experiment, has also been discussed.

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Proc. Int. Conf. Nanomeeting 2013
(International Conference on Physics, Chemistry
and Applications of Nanostructures, Minsk, Belarus)
pp. 24-27, 2013

Quantum Hall effect in semiconductor nanostructures at finite temperatures: modelling of electron-phonon interaction

A. A. Greshnov, Y. M. Beltukov

We present a theory and numerical modelling of the integer quantum Hall effect at finite temperatures considering electron-phonon interaction as a source of decoherence. Current approach is a unique tool for quantitative description of magnetotransport at low temperatures and high magnetic fields. Good agreement with the experimental data has been achieved by exploiting sophisticated numerical method of kernel polynomials.

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Semiconductors
vol. 46, no. 6, pp. 759-761, 2012

Quantum corrections to conductivity under conditions of the integer quantum Hall effect

A. A. Greshnov

Quantum corrections to the conductivity of a two-dimensional electron gas under conditions of the integer quantum Hall effect have been studied. It is shown that violation of the one-parameter scaling under conditions of quantizing magnetic fields, $\omega_c\tau \gg 1$, occurs at a level of the perturbation theory. The results of diagrammatic calculation of the quantum correction are in agreement with the numerical dependences of the peaks in the longitudinal conductivity on the effective size of the sample, in contrast to earlier calculations based on the unitary nonlinear σ-model. Due to this, consideration of Landau quantization rep resents a criterion for correct description of the quantum Hall effect.

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Physica E
vol. 40, no. 5, pp. 1185-1188, 2008

Theory of σ_{xx} peaks in the IQHE regime with correlated disorder potential

A. A. Greshnov, G.G. Zegrya

The problem of σ_{xx} peaks has been studied theoretically in the regime of integer quantum Hall effect (IQHE) for disorder potentials with arbitrary correlation length to magnetic length ratio λ/a_H. We obtained analytical solutions for two limiting cases of long-wavelength disorder potential, $\lambda \gg r_c = a_H\sqrt{(n+1)}$, and short-wavelength disorder potential, $\lambda \ll a_H$. The case

of intermediate λ/a_H ratio has been studied numerically. Our results are in good agreement with available experimental data but not with the hypothesis of universality due to Khmelnitskii and Pruisken.

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JETP
vol. 107, no. 3, pp. 491-500, 2008

Peak values of the longitudinal conductivity under integer quantum Hall effect conditions for sharp and smooth chaotic potentials

A. A. Greshnov, G. G. Zegrya, É. N. Kolesnikova

The problem of the peak values of the longitudinal conductivity under integer quantum Hall effect conditions is studied. The limiting cases of sharp and smooth chaotic potentials are considered. In the case of a sharp chaotic potential, the first longitudinal conductivity peak ($\sigma_{xx}^{(0)}$) obtained by the extrapolation of numerical data to an infinite sample size $L \to \infty$ is $(0.55\pm0.03)e^2/h$. In the case of a smooth chaotic potential, the peak values of the longitudinal conductivity are independent of the Landau level number and decrease as the chaotic-potential correlation length λ increases. The results obtained for sharp and smooth chaotic potentials agree with the reported experimental and numerically calculated data.

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Semiconductors
vol. 41, no. 11, pp. 1329-1334, 2007

Integer quantum Hall effect and correlated disorder

A. A. Greshnov, G. G. Zegrya

The effect of the form of the random potential of impurities and defects on the longitudinal σ_{xx} and Hall σ_{xy} components of conductivity in the mode of the integer quantum Hall effect is theoretically investigated. It is

shown that the width of the Hall conductivity plateau as well as the peak values of the longitudinal conductivity heavily depend on the ratio λ/a_H between the random potential correlation length and the magnetic length. For the first time, it is established that in the case of the short-wavelength potential $\lambda \ll a_H$, the peak values of $\sigma_{xx}^{(N)}$ are directly proportional to the Landau level number $N \geq 1$, $\sigma_{xx} = 0.5Ne^2/h$, whereas the peak values of $\sigma_{xx}^{(N)}$ are independent of the Landau level number in the case of the long-wavelength potential $\lambda \gg a_H$, and their magnitude is much lower than $0.5e^2/h$. The obtained results are in good agreement with the available experimental data.

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Semiconductors
vol. 40, no. 1, pp. 89-93, 2006

Precision of quantization of the Hall conductivity in a finite-size sample: Power law

A. A. Greshnov, É. N. Kolesnikova, G. G. Zegrya

A microscopic calculation of the conductivity in the integer quantum Hall effect (IQHE) mode is carried out. The precision of quantization is analyzed for finite-size samples. The precision of quantization shows a power-law dependence on the sample size. A new scaling parameter describing this dependence is introduced. It is also demonstrated that the precision of quantization linearly depends on the ratio between the amplitude of the disorder potential and the cyclotron energy. The data obtained are compared with the results of magnetotransport measurements in mesoscopic samples.

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Semiconductors
vol. 33, no. 9, pp. 1043-1046, 1999

Quantization of magnetic induction in a 2D system under conditions of the quantum Hall effect

G. G. Zegrya

In this paper we show that in a 2D system situated in an external transverse magnetic field *H* the magnetic induction *B* can under certain conditions, as a result of the de Haas-van Alfvén effect, take only certain discrete values, i.e., it is “quantized.” In this case the dependence *B(H)* consists of jumps and a plateau. At the plateau *B(H)*=const. As a consequence of quantization of the magnetic induction *B(H)*, quantization of the Hall resistivity $\rho_{xy}(H)$ is possible.

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Electronic, magnetic and optical properties of materials

J. Magn. Magn. Mater.
vol. 342, pp. 120-127, 2014

Universal effect of Mn-site doping on charge ordering in $La_{1/3}Ca_{2/3}MnO_3$

T. S. Orlova, J. Y. Laval, Ph. Monod, J. G. Noudem, A. A. Greshnov

Comparison of doping effect on the charge ordering in $La_{1/3}Ca_{2/3}Mn_{1-y}M_yO_3$ (M: Fe, Ga, Cr, Ni, Cu, Ru, Mg and $0 \leq y \leq 0.07$) has been investigated by combining magnetic and transport measurements and local compositional analysis in situ in transmission electron microscope. The effect of Mn-site doping on the charge ordering temperature T_{CO} is shown for the first time to be universal for a given dopant valence and $y \leq 0.05$. T_{CO} is governed by the effective relative concentration $n_{Mn3+}=Mn^{3+}/(Mn^{3+}+Mn^{4+})$ of Mn^{3+} ions, $T_{CO} \sim Cn_{Mn3+}$, where the coefficient C depends on the valence but not on d-shell filling of a dopant ion. This dependence indicates that any of the considered dopants do not participate in charge transfer during charge ordering formation, however, indirectly affects the charge redistribution between manganese ions. Consideration of Mn-site doping effect on charge ordering temperature using a simple order–disorder model supports the concept of universality for a given dopant valence and dominating role of the factor of entropy over energy change. Analysis of the remanent magnetization together with the obtained behavior of $T_{CO}(n_{Mn3+})$ testify that it is the dopant valence (Ru^{5+}), but not formation of Rubased magnetic clusters, that is responsible for antiferromagnetic (AFM) insulator–ferromagnetic (FM) 'bad-metal' phase transition observed in the Ru-doped system at y=0.07.

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Mater. Phys. Mech.
vol. 18, no. 2, pp. 171-178, 2013

Modeling recombination processes in solid solutions with large-scale composition fluctuations

A. V. Shilyaev, A. A. Greshnov, N. L. Bazhenov, K. D. Mynbaev

A model describing recombination processes in a solid solution containing large- scale compositional fluctuations is developed. Modeling considered carrier injection, their dynamics in a random potential, energy relaxation via phonon scattering, carrier capture by defects, and radiative and non-radiative recombination. The results of modeling show that intensive luminescence from the samples of solid solutions with large-scale compositional fluctuations, which is observed experimentally, is a substantial increase of carrier concentration in fluctuation-induced potential minima of the energy gap.

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Tech. Phys.
vol. 57, no. 9, pp. 1219-1224, 2012

High-frequency modulation of light in diffraction by the Bragg grating with a refractive index traveling wave

A. A. Greshnov, V. V. Lebedev, A. V. Shamrai

The diffraction by a Bragg grating with high-frequency modulation of the refractive index of the medium is analyzed theoretically. The effect of the grating parameters and parameters of an *rf* signal on the efficiency of modulation of optical signals at frequencies above 10 GHz is investigated.

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Tech. Phys.
vol. 57, no. 2, pp. 167-173, 2012

Heisenberg-Dirac-van Vleck vector model for a 1D antiferromagnetic chain of localized spins *S* = 1

F. E. Orlenko, G. G. Zegrya, E. V. Orlenko

Magnetic properties of anisotropic crystals with localized spins $S = 1$ are investigated; for these crystals, the Hamiltonian is derived in the Heisenberg–Dirac–van Vleck form, which includes biquadratic contributions apart from bilinear terms. The ground-state energy of the antiferromagnetic chain of spins $S = 1$ is calculated in the model of nearest neighbors, and the interaction constant is renormalized using the renorm group method in the case of coarsening of the system. The temperature criterion for the formation of long-range order in the system is obtained. The excitations of this chain in the linear approximation have a dispersion relation differing from that for antiferromagnets with spin $S = 1/2$ and are separated by an energy gap from the ground state. Allowance for nonlinear contribution leads to the formation of a solitary wave in the form of a dark–bright soliton.

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Adv. Phys. Chem.
vol. 2011, 868610, 2011

Exchange perturbation theory for multiatomic electron system and its application to spin arrangement in manganite chains

E. V. Orlenko, T. S. Orlova, F. E. Orlenko, G. G. Zegrya

A new methodology of binding energy calculation with respect to different spin arrangements for a multiatomic electron system is developed from the first principle in the frame of the exchange perturbation theory (EPT). We developed EPT formalism in the general form of the Rayleigh-Schrodinger expansion with a symmetric Hamiltonian, taking into

account an exchange and nonadditive contributions of a superexchange interaction. The expressions of all corrections to the energy and wave function were reduced to the nonsymmetric Hamiltonian form. The EPT method is extended for the case of degeneracy in the total spin of a system. As an example of the application of the developed EPT formalism for the degeneracy case, spin arrangements were considered for the key Mn–O–Mn (Mn: Mn^{3+} or Mn^{4+}) fragments in manganites. In Mn–O–Mn for $La_{1/3}Ca_{2/3}MnO_3$ are in good agreement the obtained estimations of Heisenberg parameter and binding energy with the available experimental data.

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JETP
vol. 110, no. 5, pp. 805-810, 2010

Effects of the reduction of the dimension of a system upon spin ordering in a degenerate electron gas

F. E. Orlenko, S. I. Chelkak, E. V. Orlenko, G. G. Zegrya

Collective effects of spin ordering in a quasi-one-dimensional degenerate electron gas are discussed. The total energy of the quasi-one-dimensional system, as well as the exchange contribution per particle, has been calculated by the Hartree–Fock method. It has been shown that spontaneous polarization can be observed in the system when a universal parameter related to the density of the particles satisfies the ine quality $r_s \geq 0.476$. A comparative analysis of one-, two-, and three-dimensional systems has been performed. A general expression has been obtained for the total energy per particle as a function of the degree of polarization and dimension of the system. According to this expression, the possibility of spontaneous polarization in the system is closely correlated with the dimension of the system.

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Tech. Phys.
vol. 53, no. 8, pp. 978-984, 2008

Enhancement of paramagnetic effects during spin alignment in 2D semiconductors

F. E. Orlenko, G. G. Zegrya, E. V. Orlenko

Effects of magnetic ordering associated with the Coulomb exchange interaction of free electrons in a 2D Fermi system are considered. It is shown that the paramagnetic response is substantially enhanced by Fermi-liquid effects. The phase transition to a state with spontaneous polarization of spins can be observed when Heisenberg parameter J is not smaller than $\mu_F/3.06$ (approximately one-third of the Fermi energy) and not larger than half the Fermi energy ($J \leq \mu_F/2$).

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Physica E
vol. 34, pp. 308-310, 2006

Photomagnetic effect in bilayer two-dimensional electron–hole systems

Yu. B. Vasilyev, C. Stellmach, G. Nachtwei, R. A. Suris, S. D. Suchalkin, B. Ya, Meltser, S. V. Ivanov, P. S. Kop’ev

In tilted magnetic fields a bilayer electron-hole system is found to generate a photocurrent under terahertz radiation as the system is tuned to electron cyclotron resonance conditions. The photoinduced current amplitude oscillates with the magnetic field in correlation with Shubnikov-de Haas oscillations for electrons. The phenomenon is accounted for by a photomagnetic effect in electron-hole systems in the quantum Hall regime and has potentialities for terahertz detection and spectroscopy.

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Phys. Rev. B
vol. 62, no. 24, pp. 16566-16571, 2000

Reflection of light and heavy holes from a linear potential barrier

A. Polkovnikov, R. A. Suris

In this paper we study reflection of holes in direct-band semiconductors from the linear potential barrier. It is shown that light-heavy hole transformation matrix is universal. It depends only on a dimensionless product of the light hole longitudinal momentum and the characteristic length determined by the slope of the potential and doesn't depend on the ratio of light and heavy hole masses, provided this ratio is small. It is shown that the transformation coefficient goes to zero both in the limit of small and large longitudinal momenta, however the phase of a reflected hole is different in these limits. An approximate analytical expression for the light-heavy hole transformation coefficient is found.

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Luminescence in semiconductors and nanostructures

Mater. Sci. Forum
vol. 924, pp. 310-313, 2018

Thz emission from sic natural superlattice diodes induced by strong electrical field

V. I. Sankin, A. V. Andrianov, A. G. Petrov, A. O. Zachar'in, S. S. Nagalyuk, P. P. Shkrebiy, A. A. Lebedev

Recently the intense terahertz electroluminescence from monopolar n^{++}–n^{-}–n^{+} structures of 6H- and 8H-SiC of natural superlattices at helium temperatures due to Bloch oscillations was discovered. In the present work we present the THz emission spectra of bipolar n^{++}–π–n^{+} structures (π is a high-resistance layer of p-type conductivity) of natural superlattices 4H-, 8H- and 15R-SiC at 7 K. The bipolar n^{++}–π–n^{+} structures of 4H- and 8H-SiC were analogous to those of structures for which the negative differential conductivity effect was observed earlier for three polytypes (4H, 6H and 8H) at T=300 K. We demonstrate resemblance and differences of the spontaneous THz emission spectra for the monopolar and bipolar 4H-, 6H- 8H- and 15R-SiC natural superlattices caused by Bloch oscillations of electrons in the SiC natural superlattice.

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JETP Letters
vol. 107, no. 9, pp.540-543, 2018

Intraexciton and intracenter terahertz radiation from doped silicon under interband photoexcitation

A. V. Andrianov, A. O. Zachar'in, A. G. Petrov

Terahertz photoluminescence of boron- and phosphorus-doped silicon at low temperatures under interband photoexcitation is investigated. The lines of radiative transitions between free-exciton levels and between the levels of shallow impurity centers are observed. The intensities of these lines exhibit different dependences on temperature and excitation intensity. At temperatures near the temperature of liquid helium ($T \sim 5\ K$), the terahertz radiation spectrum features a broad band (about 18–20 meV wide) with a peak at an energy of about 20–22 meV. This band is apparently associated with radiative transitions of nonequilibrium charge carriers from the states of the continuum to the state of an electron–hole liquid.

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J. Infrared Millim. Terahertz Waves
vol. 38, no. 12, pp.1530-1541, 2017

Terahertz luminescence and electrical characteristics of sic structures with natural superlattice in strong electric fields

V. I. Sankin, A. V. Andrianov, A. G. Petrov, A. O. Zakhar'in, S. S. Nagalyuk, P. P. Shkrebiy

Recently, the intense terahertz electroluminescence from monopolar n^{++}–n^{-}–n^{+} structures of 8H-SiC natural superlattice at helium temperatures due to Bloch oscillations was found out. In the present work, we compare the THz emission and electrical characteristics of monopolar n^{++}–n^{-}–n^{+} and bipolar n^{++}–π– n^{+} 8H-SiC structures at 7 K. The bipolar n^{++}–π–n^{+} 8H-SiC structures were analogous to those on which the negative differential conductivity effect was observed earlier for three polytypes (4H, 6H, and 8H) at T = 300 K. The obtained results allow one to draw a conclusion about common nature of the negative differential conductivity and THz emission effects in the natural superlattice of SiC caused by Bloch oscillations. These results give the proof of fundamental importance supporting the objectivity of postulates of the F. Bloch – C. Zener – G. N. Wannier theory.

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Tech. Phys.
vol. 62, no. 3, pp. 441-448, 2017

Effect of composition fluctuations on radiative recombination in narrow-gap semiconductor solid solutions

A. V. Shilyaev, K. D. Mynbaev, N. L. Bazhenov, A. A. Greshnov

The photoluminescence of the epitaxial structures based on the narrow-gap CdHgTe solid solutions has been experimentally investigated and the presence of large-scale composition fluctuations localizing carriers in the structures has been established. A model has been proposed for describing the effect of the fluctuations on the radiative recombination rate, the shape of the luminescence spectra, and their peak position. The model describes carrier transport and recombination at the strongly inhomogeneous composition of the solid solution and demonstrates the manifestation of carrier localization in the luminescence spectra.

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Mater. Sci. Forum
vol. 897, pp.242-245, 2017

New efficient canal of thz emission from sic natural superlattices in conditions of wannier-stark localization

*V. I. Sankin, A. V. Andrianov, P. P. Shkrebiy, A. G. Petrov,
A. O. Zachar'in, S. S. Nagalyuk*

The comprehensive study of the terahertz electroluminescence caused by the Bloch oscillations of the electrons in the natural superlattices of 8H-, 6H-SiC with strong electrical field applied along the natural superlattices axis is represented. The electroluminescence spectra become much broader when the bias field exceeds substantially the threshold field of the Bloch oscillations. This spectral broadening can be explained by an appearance of a new spectral line that is much wider and its maximum is localized at higher energy than lines induced by Bloch oscillations. This line has no link with the Bloch oscillations mechanism and it is a result of the presumed changes in the SiC

conduction band with complex electron spectrum structure by applied electrical field.

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Semiconductors
vol. 50, no. 6, pp. 778-784, 2016

Features of high-temperature electroluminescence in an LED n-GaSb/n-InGaAsSb/p-AlGaAsSb heterostructure with high potential barriers

L. V. Danilov, A. A. Petukhov, M. P. Mikhailova, G. G. Zegrya, E. V. Ivanov, Yu. P. Yakovlev

The electroluminescent properties of a light-emitting diode n-GaSb/n-InGaAsSb/p-AlGaAsSb heterostructure with high potential barriers are studied in the temperature range of 290–470 K. An atypical temperature increase in the power of the long-wavelength luminescence band with an energy of 0.3 eV is experimentally observed. As the temperature increases to 470 K, the optical radiation power increases by a factor of 1.5–2. To explain the extraordinary temperature dependence of the radiation power, the recombination and carrier transport processes are theoretically analyzed in the heterostructure under study.

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Appl. Phys. Lett.
vol. 108, no. 21, 211108, 2016

Terahertz emission from sic natural superlattices in strong electrical field

V. I. Sankin, A. V. Andrianov, A. G. Petrov, A. O. Zakhar'in

Results are reported from a study of the terahertz electroluminescence from 8H-, 6H-, and 4H-SiC natural superlattices under the action of an electrical field applied along the natural superlattice axis. It is shown that

the single, relatively narrow emission lines (*L1*-lines) dominate in the electroluminescence spectrum at moderate bias voltages and follow the increase of the width of the first mini-band of the superlattice in accordance with the criterion for Bloch oscillations. At bias voltages well above the Bloch oscillation threshold, the structure of the terahertz emission spectra undergoes considerable changes, which occur due to the appearance of a new intense, broader emission line (*L2*-line) with a maximum at about 12–13 meV. Tentatively, this latter emission is attributed to optical transitions between Wannier-Stark ladders formed from degenerate states in a side minimum of the SiC conduction band under strong electric field conditions.

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Semiconductors
vol. 49, no. 9, pp. 1206-1211, 2015

Temperature dependence of the carrier lifetime in narrow-gap $Cd_xHg_{1-x}Te$ solid solutions: Radiative recombination

N. L. Bazhenov, K. D. Mynbaev, G. G. Zegrya

The probability of the radiative recombination of carriers in narrow-gap semiconductors is analyzed for the example of $Cd_xHg_{1-x}Te$ solid solutions. Expressions are derived for the imaginary part of the dielectric permittivity in terms of the three-band Kane’s model with consideration for the nonparabolic dependence of the carrier energy on the wave vector. It is shown that taking into account this nonparabolicity of the energy spectrum of carriers modifies the dependence of the imaginary part of the dielectric permittivity on frequency. Expressions for the probability of radiative recombination, derived in terms of the simple parabolic model and Kane’s model with and without the nonparabolicity effect taken into account, are compared. It is shown that the contributions to recombination from electron transitions to heavy- and light-hole bands are close and the contribution from light holes cannot be neglected when calculating the radiative recombination probability.

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Semiconductors
vol. 49, no. 2, pp.242-246, 2015

Terahertz-emission generation caused by new effects in the 6H-SiC natural superlattice

V. I. Sankin, A. V. Andrianov, A. O. Zakhar'in, A. G. Petrov

It is demonstrated that the 6H-SiC natural superlattice has two simultaneously electroluminescence channels in the terahertz range: narrow lines at frequencies of 1.6-2.3 THz and broader lines at frequencies of about 3.25 THz. The first channel is formed by transitions between the localized states of the Wannier-Stark ladder in the Bloch oscillation mode in the first conduction miniband at point *M* of the hexagonal Brillouin zone. The second channel is probably caused by transitions between Wannier-Stark ladders formed by electric-field mixing of degenerate states of the conduction band at point *K* of the hexagonal Brillouin zone. The conduction-band minimum at point *K* is higher than that at point *M* by 100-200 meV.

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Proc. SPIE
vol. 9450, 94501Q, 2015

High-temperature luminescence in light-emitting heterostructures with a high potential barriers based on GaSb

A. Petukhov, L. Danilov, E. Ivanov, K. Kalinina, M. Mikhailova, G. Zegrya, N. Stoyanov, Yu. Yakovlev

The electroluminescent properties of an n-GaSb/n-InGaAsSb/p-AlGaAsSb heterostructure with a high potential barrier in the conduction band (large conduction-band offset) at the n-GaSb/n-InGaAsSb type-II heterointerface (ΔE_c = 0.79 eV) are studied. Two bands with peaks at 0.28 and 0.64 eV at 300 K, associated with radiative recombination in n-InGaAsSb and n-GaSb, respectively, are observed in the

electroluminescence spectrum. In the entire temperature range under study, T = 290 – 480 K, additional electron-hole pairs are formed in the n-InGaAsSb active region by impact ionization with hot electrons heated on the large the conduction-band offset. These pairs contribute to radiative recombination, which leads to a nonlinear increase in the electroluminescence intensity and output optical power with increasing pump current. A superlinear increase in the emission power of the long-wavelength band is observed upon heating in the temperature range T = 290 – 345 K, and a linear increase is observed at T > 345 K. Theoretical calculations have shown that this behavior of the temperature dependence of the optical power caused by competition between the radiative recombination, thermionic emission and Auger recombination.

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Mater. Sci. Forum
vol. 821-823, pp.277-280, 2015

The bloch oscillations and thz electroluminescence in natural superlattices of 6h-, 8h-sic polytypes

V. I. Sankin, A. V. Andrianov, A.G. Petrov, A.O. Zakhar'in,
S. S. Nagalyuk, P. P. Shkrebiy, N. I. Sablina

We report on the observation of the THz electroluminescence in 6H-SiC and 8H-SiC n^{++}–n^{-}–n^{+} structures of hexagonal crystals with natural superlattice, caused by applied electrical field along the lattice and natural superlattice axis. It is shown that there are the terahertz electro-luminescence correspond to the narrow lines at 5.3–12.7 meV. The emission channel can be well explained by the optical intraladder transitions in the Bloch oscillations regime.

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JETP Lett.
vol. 102, no. 12, pp. 796-802, 2015

Anharmonic Bloch oscillation of electrons in biased superlattices

K. A. Ivanov, A. G. Petrov, M. A. Kaliteevskii, A. J. Gallant.

The oscillatory motion of electrons in a periodic potential under a constant applied electric field, known as Bloch oscillations (BO), is one of the most striking and intriguing quantum effects and was predicted more than eighty years ago. Oscillating electrons emit electromagnetic radiation and here we consider this BO effect for emission in the THz region. To date, it has been assumed that the Bloch oscillation of an electron is anharmonic oscillation, therefore with radiation emitted at the single Bloch frequency. We analyze scenarios when Bloch oscillations can be accompanied by the emission of radiation not only at the Bloch frequency but also with double and triple Bloch frequencies. The first scenario means that electrons could jump over neighboring Stark states. The second scenario of anharmonic emission is coupled to an opening of the minigap in the miniband.

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J. Appl. Phys.
vol. 115, no. 22, 223102, 2014

Two-band superlinear electroluminescence in GaSb based nanoheterostructures with AlSb/InAs$_{1-x}$Sb$_{x}$/AlSb deep quantum well

M. P. Mikhailova, E. V. Ivanov, L. V. Danilov, A. A. Petukhov, K. V. Kalinina, S. I. Slobozhanyuk, G. G. Zegrya, N. D. Stoyanov, Yu. P. Yakovlev, A. Hospodková, J. Pangrác, J. Oswald, M. Zíková, E. Hulicius

We report on superlinear electroluminescent structures based on AlSb/InAs$_{1-x}$Sb$_{x}$/AlSb deep quantum wells grown by MOVPE on n-GaSb:Te substrates. Dependence of the electroluminescence (EL) spectra and optical power on the drive current in nanoheterostructures

with $AlSb/InAs_{1-x}Sb_x/AlSb$ quantum well at 77–300 K temperature range was studied. Intensive two-band superlinear EL in the 0.5–0.8 eV photon energy range was observed. Optical power enhancement with the increasing drive current at room temperature is caused by the contribution of the additional electron-hole pairs due to the impact ionization by the electrons heated at the high energy difference between AlSb and the first electron level E_{e1} in the InAsSb QW. Study of the EL temperature dependence at 90–300 K range enabled us to define the role of the first and second heavy hole levels in the radiative recombination process. It was shown that with the temperature decrease, the relation between the energies of the valence band offset and the second heavy hole energy level changes due to the temperature transformation of the energy band diagram. That is the reason why the EL spectrum revealed radiative transitions from the first electron level E_{e1} to the first hole level E_{h1} in the whole temperature range (90–300 K), while the emission band related with the transitions to the second hole level occurred only at T > 200 K. Comparative examination of the nanostructures with high band offsets and different interface types (AlAs-like and InSb-like) reveals more intense EL and optical power enhancement at room temperature in the case of AlAs-like interface that could be explained by the better quality of the heterointerface and more efficient hole localization.

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J. Appl. Phys.
vol. 114, no. 6, 063704, 2013

Impact ionization of nitrogen in 4h- and 6h-sic.

V. I. Sankin, A. G. Petrov, M. Kaliteevski

A natural superlattice (NSL) in silicon carbide polytypes induces a miniband structure within the conduction band along the NSL axis C. It was found that the presence of NSL leads to an anisotropy of a nitrogen impurity impact ionization in SiC. For an electric field direction F∥C, the nitrogen impurity breakdown at temperature 4.2 K has not been observed up to the field 1.6 MV/cm for the polytype 6H-SiC. However, for the polytype 4H-SiC dependence breakdown field on impurity concentration

demonstrates its usual behavior, which has also been observed for other semiconductor materials. Therewith, the impurity breakdown at the electric field perpendicular to the axis in 4H- and 6H-SiC demonstrates consistency with traditional conceptions. These results are explained theoretically.

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Phys. Status Solidi C.
vol. 10, no. 3, pp. 332-334, 2013

Mechanisms behind efficiency droop and degradation in InGaN/GaN LEDs

N. Shmidt, A. Greshnov, A. Chernyakov, M. Levinshtein, A. Zakgeim, E. Shabunina

The results of low frequency noise studies in power blue InGaN/GaN LEDs with external quantum efficiency 30-45% classified by leakage current (LC) values before and after degradation are reported. The LC values at $V < 2V$ integrally characterize electrical properties of extended defect system (EDS) that is typical for InGaN/GaN LEDs. The smaller concentration of extended defects and length of dilatation, dislocation boundaries, the lower LC value is. It has been demonstrated that non-radiative recombination processes (NRRP) localized in extended defect system (EDS) contribute in efficiency droop of LEDs at $j \geq 10$ A/cm^2 . The main characteristics of degradation processes such as: (1) increase in tunneling current values related with EDS, at $U \leq 2$ V, (2) strong deterioration of p-n junction rectification properties, (3) formation of conductive paths along EDS; (4) increase in nonuniformity of current distribution, and (5) the formation of local overheating channels at $j > 10$ A/cm^2 along EDS had been revealed. The NRRP are localized along EDS and can be considered as a general mechanism of efficiency droop and the ambiguous degradation process in power InGaN/GaN LEDs.

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AIP Conf. Proc.
vol. 1566, pp. 53-54, 2013

Wannier-stark localization and terahertz electroluminescence of natural sic superlattice

V. I. Sankin, A. V. Andrianov, A. G. Petrov, A. O. Zakhar`in

We report on efficient terahertz electroluminescence in the region of 1.5-2 THz from high electric field biased 6H-SiC n+−n-−n+ structures with a natural superlattice at 7 K. The properties of the terahertz emission allow it to be attributed to spontaneous radiation resulting from electron Bloch oscillations in SiC natural superlattice. The use of the unique object, namely, natural superlattice of SiC allowed us to demonstrate a whole series of remarkable effects of Wannier-Stark localization and to get the intensive terahertz emission under steady-state electrical excitation of Bloch oscillations.

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Appl. Phys. Lett.
vol. 100, no. 11, 111109, 2012

Terahertz electroluminescence from 6c-sic structures with natural superlattice.

V. I. Sankin, A. V. Andrianov, A. O. Zakhar`in, A. G. Petrov

We report on efficient terahertz emission in the region of 1.5-2 THz from high electric field biased 6H-SiC structures with a natural superlattice (NSL) at liquid helium temperatures. The shape of the THz emission spectrum, the linear dependence of its maximum on the bias, the characteristic field strength required to achieve the emission, and the linear polarization of the emission along the natural superlattice axis allow it to be attributed to steady-state Bloch oscillations of electrons in the 6H-SiC natural superlattice.

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J. Surf. Invest.: X-Ray, Synchrotron Neutron Tech.
vol. 6, no. 5, pp, 722-725, 2012

Photoluminescence of single quantum wires and quantum dots

V.P. Kochereshko, V.N. Kats, A.V. Platonov, R.A. Suris,
G.E. Cirlin, A.D. Buravlev, Yu. B. Samsonenko,
L. Besombes, C. Le Gal, H. Mariette

The results of a study into the photoluminescence spectra of a set of quantum dots based on GaAs enclosed in AlGaAs nanowires are presented. The steady state and time resolved spectra of photoluminescence under optical excitation both from an array of quantum wires/dots and a single quantum wire/dot have been measured. In the photoluminescence spectra of single quantum dots, emission lines of excitons, biexcitons and tritons have been found. The binding energy of the biexciton in the studied structures was deduced to be 8 meV.

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J. Appl. Phys.
vol. 112, no. 2, 023108, 2012

Superlinear electroluminescence due to impact ionization in GaSb-based heterostructures with deep Al(As)Sb/InAsSb/Al(As)Sb quantum wells

M. P. Mikhailova, E. V. Ivanov, L. V. Danilov, K. V. Kalinina,
N. D. Stoyanov, G. G. Zegrya, Yu. P. Yakovlev, E. Hulicius,
A. Hospodkova, J. Pangrac, M. Zikova

We report on the observation of superlinear electroluminescence (EL) in nanoheterostructures based on GaSb with a deep narrow Al(As)Sb/InAsSb/Al(As)Sb quantum well (QW) in the active region, grown by metal organic vapor phase epitaxy. Electroluminescence spectra for different driving currents were measured at temperatures of 77 and 300 K. It is shown that such structure exhibits superlinear

dependence of optical power on the drive current and its increase of 2–3 times in the current range 50–200 mA. This occurs due to impact ionization in the Al(As)Sb/InAsSb quantum well in which a large band offset at the interface ΔE_C = 1.27 eV exceeds ionization threshold energy for electrons in the narrow-gap well. Calculation of the size quantization energy levels is presented, and possible cases of impact ionization, depending on the band offset ΔE_C at the interface and on the quantum well width, are considered. This effect can be used to increase quantum efficiency and optical power of light emitting devices (lasers), as well as for photovoltaic elements.

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Nanoscale Res. Lett.
vol. 7, no. 1, 560, 2012

The intensive terahertz electroluminescence induced by bloch oscillations in sic natural superlattices

V. Sankin, A. Andrianov, A. Petrov, A. Zakhar\`in, A. Lepneva, P. Shkrebiy

We report on efficient terahertz (THz) emission from high-electric-field-biased SiC structures with a natural superlattice at liquid helium temperatures. The emission spectrum demonstrates a single line, the maximum of which shifts linearly with increases in bias field. We attribute this emission to steady-state Bloch oscillations of electrons in the SiC natural superlattice. The properties of the THz emission agree fairly with the parameters of the Bloch oscillator regime, which have been proven by high-field electron transport studies of SiC structures with natural superlattices.

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Mater. Sci. Forum
vol. 717-720, pp.553-556, 2012

Terahertz electroluminescence of 6h-sic natural sic superlattice in bloch oscillations regime

V. I. Sankin, A. V. Andrianov, A. G. Petrov, P. P. Shkrebiy, A. O. Zakhar`in

We report on efficient terahertz emission in the region of 1.5-2 THz from high electric field biased 6H-SiC structures with a natural superlattice at liquid helium temperatures. The shape of the emission spectrum, the linear dependence of its maximum on the bias and the characteristic field strength required to achieve the emission allow the emission to be attributed to steady-state Bloch oscillations of electrons in the SiC natural superlattice.

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JETP Lett.
vol. 94, no. 5, pp. 362-365, 2011

Terahertz radiation induced by the wannier-stark localization of electrons in a natural silicon carbide superlattice

V. I. Sankin, A. V. Andrianov, A. O. Zakhar`in, A. G. Petrov

Intense terahertz electroluminescence from SiC structures with a miniband electron spectrum caused by the natural superlattice has been observed. The shape of the terahertz radiation line, the linear dependence of the position of its maximum on the bias voltage, the typical value of the field required to induce the radiation, and the prevailing polarization of the radiation along the superlattice axis indicate that the observed radiation results from to the excitation of stationary Bloch oscillations of electrons in the natural silicon carbide superlattice.

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36th International Conference on
Infrared, Millimeter and Terahertz Waves
(IRMMW-THz), 2011

Terahertz emission induced by electron bloch oscillations in sic natural superlattice

A. V. Andrianov, A. O. Zakhar`in, A. G. Petrov, V. I. Sankin

We report on efficient terahertz electroluminescence from SiC structures with the natural superlattice. The emission spectrum demonstrates a single line, the maximum of which shifts linearly with increase in bias field. We attribute this emission to steady-state Bloch oscillations of electrons in SiC natural superlattice.

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Semiconductors
vol. 45, no. 3, pp. 415-421, 2011

Effect of the silicon doping level and features of nanostructural arrangement on decrease in external quantum efficiency in InGaN/GaN light-emitting diodes with increasing current

B. Ya. Ber, E. V. Bogdanova, A. A. Greshnov, A. L. Zakgeim, D. Yu. Kazanzev, A. P. Kartashova, A. S. Pavluchenko, A. E. Chernyakov, E. I. Shabunina, N. M. Shmidt, E. B. Yakimov

A comprehensive study of blue light-emitting diodes based on quantum-well InGaN/GaN structures with external quantum efficiencies η of up to 40% has been carried out. It is shown that, in the general case, the manner in which the efficiency depends on the current density j is determined by the competition of contributions to the radiative recombination of localized and delocalized carriers. The contribution of the latter grows with worsening structural organization of the nanomaterial, increasing temperature and drive current, and decreasing

width of the depleted layer in the active region (under zero bias). The steepest efficiency droop relative to the maximum value (by up to a factor of 2 at $j \approx 50$ A cm^{-2}) is observed in the case of heavy doping of the n$^+$-region (to 10^{19} cm^{-3}) and upon appearance of compensated layers in the active or p+region. At $j > 50$ A cm^{-2}, the contribution of delocalized carriers is predominant and the current dependences of efficiency are of uniform type, approximated with $\eta(j) \propto j^{-b}$, where $0.2 < b < 0.3$.

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Semicond. Sci. Technol.
vol. 23, no. 12, 125026, 2008

Novel materials GaInAsPSb/GaSb and GaInAsPSb/InAs for room-temperature optoelectronic devices for a 3–5 μm wavelength range (GaInAsPSb/GaSb and GaInAsPSb/InAs for 3–5 μm)

G. S. Gagis, V. I. Vasil'ev, A. G. Deryagin, V. V. Dudelev, A. S. Maslov, R. V. Levin, B. V. Pushnyi, V. M. Smirnov, G. S. Sokolovskii, G. G. Zegrya, V. I. Kuchinskii

A novel class of narrow-bandgap semiconductor materials is proposed as well as heterostructures based on these materials and suitable for the fabrication of mid-infrared optoelectronic devices, such as room-temperature laser diodes and thermo-photovoltaic converters. Our experimental data on infrared emission of such materials demonstrate high effectiveness of photoluminescence in a wavelength range 3–3.4 μm at room temperature. Simulations of the operating characteristics of room-temperature laser diodes, based on suggested heterostructures, show that their threshold current does not exceed 1 kA cm^{-2} due to suppression of the CHHS Auger-recombination process.

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Phys. Status Solidi C.
vol. 4, no. 8, pp. 2981-2985, 2007

Comparative study of quantum efficiency of blue LED with different nanostructural arrangement

A. A. Greshnov, A. E. Chernyakov, B. Y. Ber, D. V. Davydov, A. P. Kovarskyi, N. M. Shmidt, F. M. Snegov, O. A. Soltanovich, P. S. Vergeles, E. B. Yakimov, A. L. Zakgeim

Current–voltage characteristics and quantum efficiency dependence on injected current for blue light emitting diodes with different nanostructural arrangement were studied. The Electron Beam Induced Current (EBIC) technique was used to monitor the hole recombination inside the quantum wells and to reveal the lateral inhomogeneities in the recombination velocity. The bright EBIC contrast associated with extended defects was revealed. This contrast was explained by a formation of channels with enhanced conductivity near the extended defects penetrating the active device region.

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Semiconductors
vol. 41, no. 2, pp. 184-189, 2007

Dielectric function of quasi-2D semiconductor nanostructures

N. L. Bazhenov, K. D. Mynbaev, G. G. Zegrya

The spatial and temporal dispersion of the dielectric function of the electron gas in quasi-2D quantum nanostructures has been studied. Analytical expressions for the dielectric function for a quantum well in the form of a δ function and a rectangular well of finite depth are derived for the first time. A criterion for transition to strictly 2D and strictly 3D cases was obtained.

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Appl. Phys. Lett.
vol. 88, no.13, 132102, 2006

Room-temperature electroluminescence of AlSb/InAsSb single quantum wells grown by metal organic vapor phase epitaxy

K. D. Moiseev, E. V. Ivanov, G. G. Zegrya, M. P. Mikhailova, Yu. P. Yakovlev, E. Hulicius, A. Hospodková, J. Pangrác, K. Melichar, T. Šimeček

Intense mid-infrared (λ ~ 2 μm) room temperature electroluminescence from metal organic vapor phase epitaxy (MOVPE) grown type-I single AlSb/InAsSb/AlSb quantum wells (QWs) is reported. The spectral position of the electroluminescent peaks is in good agreement with *k·p* envelope function calculation in the frame of four-band Kane's model taking into account the intermixing of *s* and *p* states in the deep quantum well. A four times increase of the emission intensity with temperature increasing from 77 to 300 K can be explained by highly efficient radiative recombination of the electrons injected into the narrow AlSb/InAsSb/AlSb QW due to its specific design, leading to Auger process suppression.

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Proc. SPIE
vol. 5725, 45, 2005

Time-resolved photoluminescence measurements of InAs self-assembled quantum dots

S. Pellegrini, G. S. Buller, L. Ya. Karachinsky, A. S. Shkolnik, N. Yu. Gordeev, G. G. Zegrya, V. P. Evtikhiev, I. R. Sellers, M. S. Skolnick, H. Y. Liu, M. Hopkinson

Time-resolved photoluminescence decay measurements have been performed on samples with varying sized selfassembled InAs/GaAs quantum dot ensembles, formed by substrate mis-orientation alone, but

otherwise under identical growth conditions. Ground-state radiative recombination lifetimes from 0.8 to 5.3 ns in the incident energy density range of 0.79 $pJcm^{-2}$ - 40 $nJcm^{-2}$ at a temperature of 77 K were obtained. It was found that a reduction of the quantum dot size led to a corresponding reduction of the radiative lifetime. The evident bi-exponential decay was obtained for the ground state emission of the quantum dot array, with the slower second component attributed to a carrier re-capturing and indirect radiative recombination processes. Also experimental evidence of the effect of the AlGaAs barrier in InAs QDs emitting in the wavelength range 1200-1300 nm is presented. Time-resolved photoluminescence measurements have been performed on samples with different compositions of Al in the barrier. A full discussion of the lifetimes of these near infra-red emitting dots will be presented.

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Semiconductors
vol. 38, no. 7, pp. 837-841, 2004

Mechanism of dicke superradiance in semiconductor heterostructures

L. Ya. Karachinsky, I. I. Novikov, N. Yu. Gordeev, G. G. Zegrya

Dicke superradiance is regarded as an intermediate phase in the transition from spontaneous to stimulated emission in semiconductor laser heterostructures. A phenomenological model that describes the formation of superradiant domains (“macrodipoles”) in the active region of heterostructures is suggested. It is shown that the characteristic emission time of these domains falls within the subpicosecond range.

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Proc. SPIE
vol. 5036, no. 1, pp. 218-223, 2003

Superradiance as a transition phase from spontaneous to stimulated emission in low-dimensional semiconductor heterostructures

L. Ya. Karachinsky, N. Yu. Gordeev, I. I. Novikov, G. G. Zegrya

Dicke superradiance mechanism is suggested as a transition phase from spontaneous to stimulated emission in semiconductor laser heterostructures. Model, which describes "macrodipoles" formation in the active layer of heterostructures is proposed. Estimated characteristic radiation time of these "microdipoles" was obtained in suppicosecond range, which is in a good agreement with our previous experimental results.

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Semicond. Sci. Technol.
vol. 16, no. 9, pp. 812-815, 2001

Numerical analysis of the energy-band diagram of type-II p-GaInAsSb/p-InAs heterojunction and size-quantization levels at the interface

N. L. Bazhenov, G. G. Zegrya, M. P. Mikhailova, K. D. Mynbaev, V. A. Smirnov, Yu. P. Yakovlev

The equilibrium energy-band diagram of a broken-gap p−GaInAsSb/p−InAs heterojunction was calculated by solving the Poisson equation with account of the charge of free carriers and ionized impurities and the built-in charge at the heterointerface. The quantum level energies were found within the quasi-classical approximation for electrons in the self-consistent potential well. The calculated energies are close to those observed in electroluminescence spectra of such heterojunctions.

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Semiconductors
vol. 33, no. 9, pp. 1007-1009, 1999

InGaAs/InP heterostructures with strained quantum wells and quantum dots (λ=1.5–1.9 μm)

Z. N. Sokolova, D. A. Vinokurov, I. S. Tarasov, N. A. Gun'ko, G. G. Zegrya

Strongly strained $In_xGa_{1-x}As/In_{0.53}Ga_{0.47}As/InP$ heterostructures with indium content x=0.69−1.0 in the active region were investigated experimentally and theoretically. Two types of structures were obtained by vapor-phase epitaxy from metalorganic compounds: 1) with isolated compression-strained quantum wells and 2) with self-organized nanosize InAs clusters (quantum dots). The temperature dependence of the quantum radiation efficiency of samples with quantum wells in the temperature range 77–265 K is characterized by T_0=43 K. One reason for the low value of T_0 is electron delocalization in the active region. The maximum radiation wavelength obtained in structures with quantum dots is 1.9 μm at 77 K.

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J. Appl. Phys.
vol. 32, no. 7, pp. 765-769, 1998

Low temperature laser cooling with a rare-earth doped glass

G. Lamouche, P. Lavallard, R. Suris, R. Grousson

A theoretical study of laser cooling at low temperature by anti-Stokes luminescence in a rare-earth doped glass is performed. A model is developed to evaluate the absorption and emission spectra of rare-earth ions in a glass matrix. This model allows the evaluation of the inhomogeneously broadened spectra at any temperature. It takes into account the saturation effects that occur at high excitation. The model is used to evaluate the cooling capability at low temperature of a ytterbium-

doped fluorozirconate glass, the latter having been proposed in the literature as a good candidate for the cooling element of a cryocooler. Results are compared with previous estimations, confirming that one could expect a useful cooling efficiency from this material, but with smaller performances than previously estimated. Limitations to the cooling process are discussed. The reabsorption of luminescence is identified as one of the main limitations to the performance of a potential cryocooler.

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Heterojunction lasers

Tech. Phys. Lett.
vol. 39, no. 6, pp. 520-524, 2013

A quantum cascade laser in a transverse magnetic field. A model of the open triple-barrier active region

N. V. Tkach, I. V. Boyko, Ju. A. Seti, G. G. Zegrya

A theory of spectral parameters and active dynamic conductivity of the quantum cascade laser is proposed in the model of a triplebarrier active region of an individual cascade in a transverse magnetic field. In correspondence with the experiment, it is shown that, with an increase in the magnetic field to 8 T, the radiation peak is shifted to the region of higher energies and its integral intensity sharply decreases.

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Phys. Status Solidi B
vol. 249, no. 5, pp. 885-895, 2012

Theoretical analysis of free carrier absorption in the cavity of a quantum cascade laser

A. A. Bogdanov, R. A. Suris

In this work we analyze free carrier absorption (FCA) and polarization ratio (transversality degree) for eigenmodes of a quantum cascade laser (QCL) waveguide. We consider the dielectric function and conductivity of the waveguide core and cladding layers within the Drude–Lorentz approximation. We show that the entire spectrum of a QCL cavity consists of three kinds of eigenmodes: volume, surface, and Langmuir modes. We perform an analytical analysis and numerical calculations of FCA and polarization ratio for each type of the eigenmodes within a wide frequency range from the microwave up to the ultraviolet spectrum. We make a comparative analysis of FCA in the cladding layers and waveguide core. We specify frequency intervals where absorption in the core or in the cladding layers is dominant. Identification of the most

favorable modes for lasing is carried out for each part of the spectrum. So, we identify that the main Langmuir mode is the most favorable mode for the lasing at the long-wave edge of the terahertz (THz) region: (i) it has no frequency cutoff and can be excited at arbitrarily low frequency, (ii) it is nearly transversal that is very favorable for the QCL operation, and (iii) it is almost totally confined within the waveguide core. The model analyzed is directly related to one-dimensional photonic crystals and metamaterials consisting of alternating anisotropic layers.

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Phys. Rev. B
vol. 82, 125316, 2011

Mode structure of a quantum cascade laser

A. A. Bogdanov, R. A. Suris

We analyze the mode structure of a quantum cascade laser (QCL) cavity considering the surface plasmon-polariton modes and familiar modes of hollow resonator jointly, within a single model. We present a comprehensive mode structure analysis of the laser cavity, varying its geometric parameters and free electron concentration inside cavity layers within a wide range. Our analysis covers, in particular, the cases of metal-insulator-metal and insulator-metal-insulator waveguides. We discuss the phenomenon of negative dispersion for eigenmodes in detail and explain the nature of this phenomenon. We specify a waveguide parameters domain in which negative dispersion exists. The mode structure of QCL cavity is considered in the case of the anisotropic electrical properties of the waveguide materials. We show that anisotropy of the waveguide core results in propagation of Langmuir modes that are degenerated in the case of the isotropic core. Comparative analysis of optical losses due to free carrier absorption is presented for different modes within the frequency range from terahertz to ultraviolet frequencies.

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Semiconductors
vol. 40, no. 4, pp. 481-485, 2006

Effect of intraband carrier relaxation on the threshold characteristics of quantum well lasers

I. A. Kostko, N. A. Gun'ko, N. L. Bazhenov, K. D. Mynbaev, G. G. Zegrya

The effect of intraband carrier relaxation on the threshold characteristics of InGaAsP quantum well (QW) lasers is studied. The dependence of the intraband hole–hole relaxation time τ_{int} on temperature and carrier density is analyzed. It is shown that taking into account the finiteness of τ_{int} and its dependence on temperature and carrier density strongly affects the gain and the threshold current density of QW lasers.

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Semiconductors
vol. 39, no. 10, pp. 1210-1214, 2005

Temperature dependence of the threshold current of QW lasers

N. L. Bazhenov, K. D. Mynbaev, V. I. Ivanov-Omski, V. A. Smirnov, V. P. Evtikhiev, N. A. Pikhtin, M. G. Rastegaeva, A. L. Stankevich, I. S. Tarasov, A. S. Shkol'nik, G. G. Zegrya

The temperature dependence of the threshold current in GaInAs-based laser structures has been studied in a wide temperature range ($4.2 \leq T \leq 290$ K). It is shown that this dependence is monotonic in the entire temperature interval studied. Theoretical expressions for the threshold carrier density are derived and it is demonstrated that this density depends on temperature linearly. It is shown that the main contribution to the threshold current comes from monomolecular (Shockley–Read) recombination at low temperatures. At $T > 77$ K, the threshold current is determined by radiative recombination. At higher temperatures, close to room temperature, Auger recombination also makes a contribution. The threshold current grows with temperature linearly in the case of radiative recombination and in accordance with T^3 in the case of Auger recombination.

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Semiconductors
vol. 39, no. 5, pp. 603-607, 2005

The influence of gain saturation on the output power of quantum-well semiconductor lasers

G. G. Zegrya, I. Yu. Solov'ev

The light-power characteristic of a quantum-well semiconductor laser is theoretically studied taking into account the gain saturation effect. It is shown that, at high drive current densities, this light-current characteristic becomes nonlinear. The results obtained are in a good agreement with the experimental data.

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CAS 2004 Proc. (2004 International
Semiconductor conference, Sinaia, Romania)
vol. 1, pp. 209-212, 2004

Theoretical and experimental study of the effect of carrier relaxation on threshold and power-current characteristics of quantum well lasers

G. G. Zegrya, N. L. Bazhenov, D. V. Dorofeyev, V. P. Evtikhiev,
E. Yu. Kotelnikov, K. D. Mynbaev, I. Yu. Solovyev, A.S. Shkolnik

In this paper, the effect of intraband relaxation processes of non-equilibrium carriers on the threshold and power-current characteristics of quantum-well lasers is studied both theoretically and experimentally. Special attention is paid to the study of physical mechanisms, which affect the maximum laser power. It is shown that at high excitation levels, the maximum laser power gets affected, apart from lattice and carrier heating, by the phenomenon of gain saturation. Power-current characteristics of a quantum well laser are calculated with gain saturation effect being taken into account. It is shown that at high excitation levels the characteristic becomes non-linear. Calculated behavior of power-current characteristics agrees well with experimental observations.

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Proc. SPIE
vol. 5023, no. 1, pp. 395-397, 2003

Influence of intraband relaxation processes on threshold and power-current characteristics of quantum well lasers

G. G. Zegrya, I. A. Kostko, N. A. Gunko, E. B. Dogonkin

The effect of carrier-carrier relaxation on threshold and power-current characteristics of InAs and GaAs quantum well (QW) lasers is studied. Dependence of carrier relaxation time on temperature and carrier density is considered. It is shown that in this case the gain coefficient becomes a more pronounced function of temperature and carrier density, and threshold current density increases drastically.

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Proc. SPIE
vol. 5023, no. 1, pp. 379-382, 2003

SC DHS InGaAsP/InP lasers (λ = 1.5-1.6 μm) with above-threshold internal quantum efficiency η_i^{st} about 100%

I. S. Tarasov, G. G. Zegrya, G. V. Skrynnikov,
N. A. Pikhtin, S. O. Slipchenko

InGaAsP/InP SC DHS lasers with different waveguide design were fabricated and studied. Extremely high values of internal quantum efficiency of stimulated emission η_i^{st} about 97% was demonstrated experimentally in structures with step-like waveguide design which is related to lowest leakage currents above threshold and reduced threshold carriers concentration. Theoretically was shown, that it is possible to create lasers emitting at λ = 1.5 μm, with an internal quantum efficiency of stimulated emission close to 100%. η_i^{st} for structure with different waveguide design was calculated and prove to be in good agreement with experimental data.

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Proc. SPIE
vol. 5023, no. 1, pp. 365-367, 2003

Non-linear power-current characteristics of quantum well lasers at high injection

V. P. Evtikhiev, E. Yu. Kotelnikov, D. V. Dorofeyev, G. C. Zegrya

Mechanisms causing non-linearity of power-current characteristics (PCC) of quantum-well lasers at high injection levels were studied both experimentally and theoretically. A critical injection current that switch on a nonlinear PCC mode was found to depend to a great extend on the resonator length (on the threshold concentration). The PCC non-linearity is well described within the framework of the gain saturation mechanism where a dependence of the gain coefficient on the radiation intensity at high injected carriers concentration is taken into account.

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J. Appl. Phys.
vol. 93, no. 5, pp. 2349-2352, 2003

Injection cascade lasers with graded gap barriers

Yu. B. Vasilyev, S. D. Suchalkin, A. S. Polkovnikov, G. G. Zegrya

We propose cascade structures based on type-II heterostructures with graded barriers separating electron and hole layers. The electron–hole separation is controlled by an external bias due to modification of the barrier shape. This principle can be used for fabrication of a class of devices. In particular, bipolar interband cascade lasers are considered in which an external bias changes the rate of electron–hole radiative recombination by several orders of magnitude. Theoretical calculations predict the feasibility of these lasers.

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Semiconductors
vol. 37, no. 2, pp. 233-238, 2003

Internal quantum efficiency of stimulated emission of (λ =1.55 µm) InGaAsP/InP laser diodes

G. V. Skrynnikov, G. G. Zegrya, N. A. Pikhtin, S. O. Slipchenko, V. V. Shamakhov, I. S. Tarasov

The stimulated emission (η_i^{st}) of InGaAsP/InP separate-confinement double heterostructure lasers operating at λ = 1.5–1.6 μm has been studied experimentally and theoretically. Laser heterostructures with a varied design of the waveguide layer were grown by MOCVD. The maximum internal quantum efficiency η_i^{st} ≈ 97% was obtained in a structure with a double-step waveguide characterized by minimum leakage into the p-emitter above the generation threshold. The high value of η_i^{st} is provided by low threshold and nonequilibrium carrier concentrations at the interface between the waveguide and p-emitter. The calculation yields η_i^{st} values correlating well with the experimental data.

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Mater. Sci. Forum
vol. 384-385, no.3, pp. 209-212, 2002

Injection lasers based on intraband carrier transitions

E. Towe, D. Pal, L. E. Vorobjev, A. V. Glukhovskoy, S.N. Danilov, V. L. Zerova, V. Y. Panevin, D. A. Firsuv, V.A. Shalygin, G. G. Zegrya, A. Weber, M. Grundmann

Novel designs of mid-infrared lasers based on intersubband electron transitions in funnel shaped quantum wells are suggested. The calculated laser parameters as well as results of photoluminescence and mid-infrared emission studies are presented.

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Proc. SPIE
vol. 4651, no. 1, pp. 264-268, 2002

Influence of intraband relaxation processes on threshold and power-current characteristics of semiconductor lasers

G. G. Zegrya, N. A. Gunko, E. B. Dogonkin

The effect of carrier-carrier relaxation and carrier-phonon relaxation on threshold characteristics of quantum well (QW) lasers is studied. Carrier relaxation time considerably depends on temperature, carrier density, and quantum well width. It is shown that in this case the gain coefficient becomes a more pronounced function of temperature and carrier density.

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Electron. Lett.
vol. 37, no. 22, pp. 1339-1341, 2001

Design of semiconductor laser with current-induced cooling

E. B. Dogonkin, G. G. Zegrya

A novel design of semiconductor lasers and photodiodes with cooling by injection current is proposed. Carriers are injected into the active region via tunnelling with absorption of optical phonons. An expression for the optimal emitter lengths in a current-cooled system is obtained.

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JETP Lett.
vol. 74, no. 6, pp. 312-317, 2001

New mechanism of current-induced cooling of quantum systems

E. B. Dogonkin, G. G. Zegrya

A new mechanism of current-induced cooling of heterostructures is proposed and studied. As an example, a structure with two quantum wells was taken to determine the conditions under which electric current can flow in the situation where electrons and holes transfer from one well to another via indirect phonon-assisted tunneling. It is shown that this system can be used to create an inverse electron and hole population and simultaneously cool the laser active region by injection current. The universal relation is obtained according to which the cooling temperature of a quantum system is expressed only in terms of energy difference between the carrier size-quantization levels.

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Bull. Russ. Acad. Sci.: Phys.
vol. 65, no. 2, pp. 253-256, 2001

Middle-IR Auger laser, based on charge carrier intersubband transitions in quantum wells

L.E. Vorobiev, G.G. Zegrya, D.A. Firsov

We describe a new type of a middle-IR semiconductor laser with electric or optical pumping based on intersubband optical transitions of electrons in quantum wells of II-type heterostructures. The population inversion is achieved due to a special quantum well shape and resonant Auger recombination maintaining additional pumping of the excited level.

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Semiconductors
vol. 35, no. 8, pp. 962-969, 2001

Threshold characteristics of λ=1.55 μm InGaAsP/InP heterolasers

G. G. Zegrya, N. A. Pikhtin, G. V. Skrynnikov,
S. O. Slipchenko, I. S. Tarasov

Temperature dependences of the threshold characteristics of InGaAsP/InP quantum well (QW) lasers have been studied. The main contribution to the threshold current is made by the thresholdless Auger recombination. The observed power-law temperature dependence of the threshold current is explained by the predominance of the thresholdless Auger recombination in QWs over the threshold Auger process.

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CAS 2001 Proc. (2001 International
Semiconductor conference, Sinaia, Romania)
vol. 1, pp. 169-172, 2001

The effect of carrier relaxation on quantum well laser threshold characteristics

G. G. Zegrya, N. A. Gunko, I. A. Kostko, E. B. Dogonkin

The effect of carrier-carrier relaxation and carrier - phonon relaxation on threshold characteristics of quantum well (QW) lasers is studied. Carrier relaxation time considerably depends on temperature, carrier density, and quantum well width. It is shown that in this case the gain coefficient becomes a more pronounced function of temperature and carrier density.

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Proc. of the 8th Int. Symposium
Nanostructures: Physics and Technology,
St.Petersburg, Russia, 2000
pp. 84-87, 2000

Mid infrared range laser based on intersubband transitions and resonant Auger processes in quantum wells

L. E. Vorobjev, G. G. Zegrya, D. A. Firsov

A new type of mid infrared semiconductor laser based on intersubband optical electron transitions in type II quantum wells with electrical or optical pumping is suggested. Inversion of population is created due to special shape of quantum well and resonant Auger recombination providing additional pumping of excited level.

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Appl. Phys. Lett.
vol. 74, no. 7, pp. 905-907, 1999

Power rise in broad-waveguide diode laser with inclined facet

I. A. Kostko, V. P. Evtikhiev, E. Yu. Kotelnikov, G. G. Zegrya

A method of transverse mode selection in high-power broad-waveguide separate confinement heterostructure quantum-well lasers by placing the front mirror at the angle other than the normal to the radiation propagation direction is proposed. Optimal values of facet inclination angles and widths and the refractive indices of the dielectric coating at which the fundamental guided mode dominates are found. The possibility of increasing the output power 1.2 times of a broad-waveguide separate confinement heterostructure quantum-well diode laser with inclined facet is shown.

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Semiconductors
vol. 33, no. 6, pp. 693-699, 1999

Increasing the power of broad-waveguide lasers by additional selection of transverse modes

I. A. Kostko, V. P. Evtikhiev, E. Yu. Kotelnikov, G. G. Zegrya

A new method is proposed for transverse mode selection in high-power, broad-waveguide, separate-confinement, heterostructure quantum-well lasers by orienting the front mirror at an angle other than normal to the direction of radiation propagation. The dependence of the mode reflection coefficients on the laser mirror parameters is investigated. Optimal values are found for the mirror inclination angles and the thicknesses and refractive indices of the dielectric coating at which the fundamental guide mode dominates. The possibility of a 1.2-fold increase in the output power of a broad-waveguide, separate-confinement, heterostructure quantum-well diode laser is demonstrated.

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J. Appl. Phys.
vol. 84, no. 1, pp. 547-554, 1999

Optical loss in InAs-based long-wavelength lasers

N. A. Gun'ko, V. B. Khalfin, Z. N. Sokolova, G. G. Zegrya

A microscopic quantum-mechanical analysis of the intervalence band absorption of radiation (IVA) with hole transition into the spin-orbit split-off band has been made. It was found that IVA can heavily influence the threshold characteristics and quantum efficiency of heterolasers based on InAs. A detailed study of the threshold characteristics as functions of temperature and heterostructure parameters has been analyzed taking into account IVA.

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Semiconductors
vol. 33, no. 5, pp. 564-568, 1999

Suppression of Auger recombination in diode lasers utilizing InAsSb/InAsSbP and InAs/GaInAsSb type-II heterojunctions

G. G. Zegrya, M. P. Mikhaılova, T. N. Danilova, A. N. Imenkov, K. D. Moiseev, V. V. Sherstnev, Yu. P.Yakovlev

The results of a comparative study of the temperature dependence of the threshold current, the differential quantum efficiency, and the polarization of light are reported for type-I and type-II InAsSb/InAsSbP heterostructures and for a tunneling injection laser utilizing a type-II GaInAsSb/InGaAsSb separate-confinement heterojunction. The theoretically predicted suppression of nonradiative Auger recombination in type-II InAsSb/InAsSbP lasers with a large ratio of band discontinuities at the interface $\Delta E_v/\Delta E_c$ = 3.4 is verified experimentally. Weakening of the temperature dependence of the threshold current is established for both type-II laser configurations. The maximum working temperatures T[sub lim] = 203 and 195 *K* and the characteristic temperatures T_0 = 40 and 47 *K* are attained for (respectively) a conventional type-II InAsSb/InAsSbP laser and a type-II p-GaInAsSb/n-InGaAsSb tunneling injection laser.

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Quantum dot lasers

Appl. Phys. Lett.
vol. 102, no. 19, 191102, 2013

Effect of excited states on the ground-state modulation bandwidth in quantum dot lasers

Y. Wu, R. A. Suris, L. V. Asryan

We consider direct and indirect (excited-state-mediated) capture of carriers from the waveguide region into the lasing ground state in quantum dots (QDs) and calculate the modulation response of a QD laser. We show that, when only indirect capture is involved, the excited-to-ground-state relaxation delay strongly limits the ground-state modulation bandwidth of the laser—at the longest tolerable relaxation time, the bandwidth becomes zero. When direct capture is also involved, the effect of excited-to-ground-state relaxation is less significant and the modulation bandwidth is considerably higher.

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Appl. Phys. Lett.
vol. 100, no. 13, 131106, 2012

Effect of internal optical loss on the modulation bandwidth of a quantum dot laser

Y. Wu, R. A. Suris, L. V. Asryan

We show that the internal optical loss, which increases with free-carrier density in the waveguide region, considerably reduces the modulation bandwidth ω_{-3dB} of a quantum dot laser. At a certain optimum value j_0^{opt} of the *dc* component of the injection current density, the maximum bandwidth ω^{max}_{-3dB} is attained and the modulation response function becomes as flat as possible. With internal loss cross-section σ_{int} increasing and approaching its maximum tolerable value, ω^{max}_{-3dB} decreases and becomes zero. As with j_0^{opt} , there also exists the optimum cavity length, at which ω_{-3dB} is highest; the larger is σ_{int}, the longer is the optimum cavity.

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Appl. Phys. Lett.
vol. 98, no. 13, 131108, 2011.

Carrier capture delay and modulation bandwidth in an edge-emitting quantum dot laser

L. V. Asryan, Y. Wu, R. A. Suris

We show that the carrier capture from the optical confinement layer into quantum dots (QDs) can strongly limit the modulation bandwidth ω_{-3dB} of a QD laser. As a function of the cross-section n of carrier capture into a QD, ω_{-3dB} asymptotically approaches its highest value when $\sigma_n \to \infty$ (the case of instantaneous capture). With reducing σ_n, ω_{-3dB} decreases and becomes zero at a certain nonvanishing σ_n^{min}. The use of multiple-layers with QDs significantly improves the laser modulation response — ω_{-3dB} is considerably higher in a multilayer structure as compared to a single-layer structure at the same *dc* current.

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Proc. SPIE
vol. 7947, 794708, 2011

Capture delay and modulation bandwidth in a quantum dot laser

L. V. Asryan, Y. Wu, R. A. Suris

We show that the carrier capture from the optical confinement layer into quantum dots (QDs) can strongly limit the modulation bandwidth ω_{-3dB} of a QD laser. Closed-form analytical expressions are obtained for ω_{-3dB} in the limiting cases of fast and slow capture. ω_{-3dB} is highest in the case of instantaneous capture into QDs, when the cross-section of carrier capture into a QD $\sigma_n = \infty$. With reducing σn, ω_{-3dB} decreases and becomes zero at a certain non-vanishing value σ_n^{min}. This σ_n^{min} presents the minimum tolerable capture cross-section for the lasing to occur at a given dc component j_0 of the injection current density. The higher is j_0, the smaller is σ_n^{min} and hence the direct modulation of the output power is possible at a slower capture. The use of multiple layers with QDs is shown to considerably improve the modulation response of the laser –

the same ω_{-3dB} is obtained in a multi-layer structure at a much lower j_0 than in a single-layer structure. At a plausible value of σn = 10–11 cm2, ω –3 dB as high as 19 GHz is attainable in a 5-QD-layer structure.

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IEEE Winter Topicals
vol. 43, pp.43-44, 2011

Quantum-dot based quantum cascade lasers: Arguments in favor

R. A. Suris, I. A. Dmitriev

Advantages of quantum dot cascade lasers over quantum well devices are demonstrated. Discrete spectrum of quantum dots enables suppression of non-radiative relaxation and optical losses and provides flexibility in optical and electrical design of lasers.

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Appl. Phys. Lett.
vol. 96, no. 22, 221112, 2010

Upper limit for the modulation bandwidth of a quantum dot laser

L. V. Asryan, R. A. Suris

We derive a closed-form expression for the upper limit for the modulation bandwidth of a semiconductor quantum dot (QD) laser. The highest possible bandwidth increases directly with overlap integral of the electron and hole wave functions in a QD, number of QD-layers, and surface density of QDs in a layer, and is inversely proportional to the inhomogeneous line broadening caused by the QD-size dispersion. At 10% QD-size fluctuations and 100% overlap, the upper limit for the modulation bandwidth in a single QD-layer laser can be as high as 60 GHz.

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Proc. SPIE
vol. 7610, 76100R, 2010

Theory of relaxation oscillations and modulation response of a quantum dot laser

L. V. Asryan, R. A. Suris

Dynamic effects in a quantum dot (QD) laser are studied theoretically. The frequency and decay rate of relaxation oscillations, and the modulation response are calculated as functions of injection current density, cavity length, and parameters of the QD structure. The highest possible bandwidth is calculated and shown to increase with increasing overlap integral between the electron and hole wave functions in a QD, number of QD-layers and surface density of QDs in a layer, and with reducing QD-size dispersion.

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Physica E
vol. 40, pp. 2007-2009, 2008

Quantum dot cascade laser: Arguments in favor

I. A. Dmitriev, R. A. Suris

Quantum cascade lasers are recognized as propitious candidates for future terahertz optoelectronics. Here we demonstrate several definite advantages of quantum dot cascade structures over quantum well devices, which suffer fundamental performance limitations owing to continuous carrier spectrum. The discrete spectrum of quantum dots opens an opportunity to control the non-radiative relaxation and optical loss and also provides for more flexibility in the choice of an optical and electrical design of the laser.

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Phys. Status Solidi A
vol. 202, pp.987-991, 2005

Quantum cascade lasers based on quantum dot superlattice

I.A. Dmitriev, R.A. Suris

A theory of threshold characteristics of novel quantum cascade lasers with an active medium made of a regular array of quantum dots is presented. Very low threshold current density for the room-temperature operation is predicted.

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Semiconductors
vol. 38, no. 10, pp. 1207-1211, 2004

Effect of nonradiative recombination centers on photoluminescence efficiency in quantum dot structures

M. V. Maksimov, D. S. Sizov, A. G. Makarov, I. N. Kayander, L. V. Asryan, A. E. Zhukov, V. M. Ustinov, N. A. Cherkashin, N. A. Bert, N. N. Ledentsov, D. Bimberg

The influence of dislocations on photoluminescence (PL) intensity in structures with InAs–GaAs quantum dots (QD) has been studied. The structural characteristics of samples were studied by transmission electron microscopy in bright-field and weak-beam dark-field diffraction conditions. At temperatures below room temperature and for moderate excitation density, the PL intensity in a structure containing large clusters with dislocations was about the same as in a structure with a significantly lower density of clusters. In contrast, the measurement of PL intensity at elevated temperatures and high excitation densities allows an accurate estimation of the structural perfection of QD structures. The overgrowth of QDs with a thin (1–2 nm) GaAs layer with subsequent annealing reduces the density of clusters with dislocations and significantly improves the temperature stability of the PL intensity.

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IEEE J. Quantum Electron.
vol. 40, no. 7, pp. 833-843, 2004

Effect of internal optical loss on threshold characteristics of semiconductor lasers with a quantum-confined active region

L. V. Asryan, S. Luryi

We develop a general approach to including the internal optical loss in the description of semiconductor lasers with a quantum-confined active region. We assume that the internal absorption loss coefficient is linear in the free-carrier density in the optical confinement layer and is characterized by two parameters, the constant component and the net cross section for all absorption loss processes. We show that, in any structure where the free-carrier density does not pin in the presence of light generation, the free-carrier-density dependence of internal loss gives rise to the existence of a second lasing threshold above the conventional threshold. Above the second threshold, the light–current characteristic is two-valued up to a maximum current at which the lasing is quenched. We show that the presence of internal loss narrows considerably the region of tolerable structure parameters in which the lasing is attainable; for example, the minimum cavity length is significantly increased. Our approach is quite general but the numerical examples presented are specific for quantum dot (QD) lasers. Our calculations suggest that the internal loss is likely to be a major limiting factor to lasing in short-cavity QD structures.

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Semiconductors
vol. 38, no. 1, pp. 1-22, 2004

Theory of threshold characteristics of semiconductor quantum dot lasers

L. V. Asryan, R. A. Suris

A comprehensive theory of threshold characteristics of quantum dot (QD) lasers, which provides a basis for optimization of their design, is

reviewed. The dependences of the gain, transparency current, threshold current, characteristic temperature, and multimode generation threshold on the parameters of the QD ensemble (surface density and size dispersion of QDs), cavity (stripe length and thickness of the waveguide region), heterocontacts (band offsets), and temperature are considered in detail. The limiting characteristics of the laser (optimum structure parameters, minimum threshold current density, and characteristic temperature of the optimized structure) are discussed at length. The results of the analysis may serve as direct recommendations for the development of QD lasers that significantly outperform the semiconductor lasers currently in use.

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Proc. SPIE
vol. 5349, pp. 69-80, 2004

Internal optical loss and threshold characteristics of semiconductor lasers with a reduced-dimensionality active region

L. V. Asryan, S. Luryi

We develop a general approach to including the internal optical loss in the description of semiconductor lasers with a quantum-confined active region. We assume that the internal absorption loss coefficient is linear in the free-carrier density in the optical confinement layer and is characterized by two parameters, the constant component and the net cross-section for all absorption loss processes. We show that the free-carrier-density dependence of internal loss gives rise, in general, to the existence of a second lasing threshold above the conventional threshold. Above the second threshold, the light-current characteristic is two-valued up to a maximum current at which the lasing is quenched. We show that the presence of internal loss narrows considerably the region of tolerable structure parameters in which the lasing is attainable; for example, the minimum cavity length is significantly increased. Our approach is quite general but the numerical examples presented are specific for quantum dot (QD) lasers. Our calculations suggest that the internal loss is likely to be a major limiting factor to lasing in short-cavity QD structures.

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Appl. Phys. Lett.
vol. 83, no. 26, pp. 5368-5370, 2003

Two lasing thresholds in semiconductor lasers with a quantum-confined active region

L.V. Asryan, S. Luryi

We show that the free-carrier-density dependence of internal optical loss gives rise, in general, to the existence of a second lasing threshold above the conventional threshold. Above the second threshold, the light-current characteristic is two-valued up to a maximum current at which the lasing is quenched.

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IEEE J. Quantum Electron.
vol. 39, no. 3, pp. 404-418, 2003

Internal efficiency of semiconductor lasers with a quantum-confined active region

L. V. Asryan, S. Luryi, R. A. Suris

We discuss in detail a new mechanism of nonlinearity of the light–current characteristic (LCC) in heterostructure lasers with reduced-dimensionality active regions, such as quantum wells (QWs), quantum wires (QWRs), and quantum dots (QDs). It arises from: 1) noninstantaneous carrier capture into the quantum-confined active region and 2) nonlinear (in the carrier density) recombination rate outside the active region. Because of 1), the carrier density outside the active region rises with injection current, even above threshold, and because of 2), the useful fraction of current (that ends up as output light) decreases. We derive a universal closed-form expression for the internal differential quantum efficiency η_{int} that holds true for QD, QWR, and QW lasers. This expression directly relates the power and threshold characteristics. The key parameter, controlling η_{int} and limiting both the output power and the LCC linearity, is the ratio of the threshold values of the recombination current outside the active region to the carrier capture current into the

active region. Analysis of the LCC shape is shown to provide a method for revealing the dominant recombination channel outside the active region. A critical dependence of the power characteristics on the laser structure parameters is revealed. While the new mechanism and our formal expressions describing it are universal, we illustrate it by detailed exemplary calculations specific to QD lasers. These calculations suggest a clear path for improvement of their power characteristics. In properly optimized QD lasers, the LCC is linear and the internal quantum efficiency is close to unity up to very high injection-current densities (15 kA/cm^2). Output powers in excess of 10 W at η_{int} higher than 95% are shown to be attainable in broad-area devices. Our results indicate that QD lasers may possess an advantage for high-power applications.

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Solid-State Electron.
vol. 47, no. 2, pp. 205-212, 2003

Temperature-insensitive semiconductor quantum dot laser

L.V. Asryan, S. Luryi

Different approaches to the design of a genuinely temperature-insensitive quantum dot (QD) laser are proposed. Suppression of the parasitic recombination outside the QDs, which is the dominant source of the temperature dependence of the threshold current in the conventional design of a QD laser, is accomplished either by tunneling injection of carriers into the QDs or by band-gap engineering. Elimination of this recombination channel alone enhances the characteristic temperatures T_0 above 1000 K. Remaining sources of temperature dependence (recombination from higher QD levels, inhomogeneous line broadening, and violation of charge neutrality in QDs) are studied. Tunneling-injection structures are shown to offer an additional advantage of suppressed effects of inhomogeneous broadening and neutrality violation.

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Appl. Phys. Lett.
vol. 81, no. 12, pp. 2154-2156, 2002

Intrinsic nonlinearity of the light-current characteristic of semiconductor lasers with a quantum-confined active region

L. V. Asryan, S. Luryi, R. A. Suris

We describe a mechanism of nonlinearity of the light–current characteristic common to heterostructure lasers with a reduced-dimensionality active region. It arises from (i) noninstantaneous carrier capture into the active region and (ii) nonlinear (in the carrier density) recombination rate outside the active region. Because of (i), the carrier density outside the active region rises with injection current above threshold, and because of (ii), the useful fraction of current (that ends up as output light) decreases. We derive a universal closed-form expression for the internal differential quantum efficiency that holds true for quantum well, quantum wire, and quantum dot lasers.

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Proc. SPIE
vol. 4656, pp. 59-68, 2002

Tunneling-injection quantum dot laser

L. V. Asryan, S. Luryi

Different approaches to the design of a genuinely temperature-insensitive quantum dot (QD) laser are proposed. Suppression of the parasitic recombination outside the QDs, which is the dominant source of the temperature dependence of the threshold current in the conventional design of a QD laser, is accomplished either by tunneling injection of carriers into the QDs or by bandgap engineering. Elimination of this recombination channel alone enhances the characteristic temperature T_0 above 1000 K. Remaining sources of temperature dependence

(recombination from higher QD levels, inhomogeneous line broadening, and violation of charge neutrality in QDs) are studied. Tunneling injection structures are shown to offer an additional advantage of suppressed effects of inhomogeneous broadening and neutrality violation.

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International J. High Speed Electron. Syst.,
Special Issue on "Quantum Dot Heterostructures
- Fabrication, Application, Theory"
vol. 12, no. 1, pp. 111-176, 2002

Theory of threshold characteristics of quantum dot lasers: Effect of quantum dot parameter dispersion

L. V. Asryan, R. A. Suris

Gain and threshold current of a quantum dot (QD) laser are analyzed theoretically taking into account the inhomogeneous line broadening caused by fluctuations in QD parameters. Two regimes of QD filling by carriers, nonequilibrium and equilibrium, are identified, depending on temperature, barrier heights and QD size. Critical tolerable parameters of the QD structure, at which lasing becomes impossible to attain, are shown to exist. The minimum threshold current density and optimum parameters are calculated. Violation of charge neutrality in QDs is revealed, which affects significantly the threshold current and its temperature dependence. The gain-current dependence is calculated. The voltage dependences of the electron and hole level occupancies in QDs, gain and current are obtained. The observed temperature dependence of threshold current (constant at low temperatures and rapid increase above a certain temperature) is predicted and explained. Violation of charge neutrality is shown to give rise to the slight temperature dependence of the current component associated with the recombination in QDs. The characteristic temperature T_0 is calculated considering carrier recombination in the optical confinement layer and violation of charge neutrality in QDs. The inclusion of violation of charge

neutrality is shown to be critical for the correct calculation of T_0 at low T. T_0 is shown to fall off profoundly with increasing T. Theoretical estimations confirm the possibility of a significant reduction of the threshold currents and enhancement of T_0 of QD lasers as compared with the conventional quantum well (QW) lasers. Longitudinal spatial hole burning is analyzed. Unlike QW lasers, thermally excited escapes of carriers from QDs, rather than diffusion, are shown to control the smoothing-out of the spatially nonuniform population inversion and multimode generation in QD lasers. A decrease in the QD size dispersion is shown not only to decrease the threshold current but to increase considerably the relative multimode generation threshold as well. Concurrent with the increase of threshold current, an increase of the multimode generation threshold is shown to occur with a rise in temperature. Ways to optimize the QD laser, aimed at maximizing the multimode generation threshold, are outlined.

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J. Appl. Phys.
vol. 90, no. 3, pp. 1666-1668, 2001

Maximum modal gain of a self-assembled InAs/GaAs quantum-dot laser

L. V. Asryan, M. Grundmann, N. N. Ledentsov, O. Stier, R. A. Suris, D. Bimberg

Gain and threshold current of a self-assembled InAs/GaAs quantum-dot (QD) laser are simulated. A small overlap integral of the electron and hole wave functions in pyramidal QDs is shown to be a possible reason for the low single-layer modal gain, which limits lasing via the ground-state transition at short (under a millimeter) cavity lengths.

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IEEE J. Quantum Electron.
vol. 37, no. 7, pp. 905-910, 2001

Tunneling-injection quantum-dot laser: Ultrahigh temperature stability

L. V. Asryan, S. Luryi

We propose a genuinely temperature-insensitive quantum dot (QD) laser. Our approach is based on direct injection of carriers into the QDs, resulting in a strong depletion of minority carriers in the regions outside the QDs. Recombination in these regions, which is the dominant source of the temperature dependence, is thereby suppressed, raising the characteristic temperature T_0 above 1500 K. Still further enhancement of T_0 results from the resonant nature of tunneling injection, which reduces the inhomogeneous line broadening by selectively cutting off the nonlasing QDs.

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IEEE J. Quantum Electron.
vol. 37, no. 5, pp. 676-683, 2001

Gain and threshold characteristics of long wavelength lasers based on InAs/GaAs quantum dots formed by activated alloy phase separation

M. V. Maximov, L. V. Asryan, Yu. M. Shernyakov, A. F. Tsatsul'nikov, I. N. Kaiander, V. V. Nikolaev, A. R. Kovsh, S. S. Mikhrin, V. M. Ustinov, A. E. Zhukov, Zh. I. Alferov, N. N. Ledentsov, D. Bimberg

Experimental and theoretical study was made of injection lasers based on InAs/GaAs quantum dots (QDs) formed by the activated alloy phase separation and emitting at about 1.3 m. Electroluminescence and gain spectra were investigated. The maximum modal gain is measured experimentally using two different techniques. Threshold current densities as low as 22 A cm^{-2} per QD sheet were achieved. A step-like switch from ground- to excited-state transition lasing was observed with an increasing cavity loss. The characteristic temperatures for a sample

with four cleaved sides and a 2-mm long stripe device at 300 K were 140 and 83 K, respectively. Single lateral-mode continuous-wave (CW) operation with the maximum output power of 210 mW was realized. Threshold characteristics of a laser were simulated taking into account radiative recombination in QDs, the wetting layer, and the optical confinement layer. The dependence of the threshold current density on the cavity length was shown to be extremely sensitive to the QD-array parameters determining the maximum gain for ground- and excited-state transitions and to the waveguide design. Our analysis reveals that nonradiative recombination channels may play an important role in the laser operation.

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IEEE J. Quantum Electron.
vol. 37, no. 3, pp. 418-425, 2001

Effect of excited-state transitions on the threshold characteristics of a quantum dot laser

L. V. Asryan, M. Grundmann, N. N. Ledentsov, O. Stier, R. A. Suris, D. Bimberg

The general relationship between the gain and spontaneous emission spectra of a quantum dot (QD) laser is shown to hold for an arbitrary number of radiative transitions and an arbitrary QD-size distribution. The effect of microscopic parameters (the degeneracy factor and the overlap integral for a transition) on the gain is discussed. We calculate the threshold current density and lasing wavelength as a function of losses. The conditions for a smooth or step-like change in the lasing wavelength are described. We have simulated the threshold characteristics of a laser based on self-assembled pyramidal InAs QDs in the GaAs matrix and obtained a small overlap integral for transitions in the QDs and a large spontaneous radiative lifetime. These are shown to be a possible reason for the low single-layer modal gain, which limits lasing via the ground-state transition for short (several hundreds of micrometers) cavity lengths.

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Semiconductors
vol. 35, no. 3, pp. 343-346, 2001

Carrier photoexcitation from levels in quantum dots to states of the continuum in lasing

L. V. Asryan, R. A. Suris

Carrier photoexcitation from levels in quantum dots to continuous-spectrum states during lasing is analyzed theoretically. The simplest approach is used to provide upper estimates of the absorption coefficient and the photoexcitation cross section. Light absorption in carrier photoexcitation is shown to be essential for quantum dot laser operation only at very low total losses, e.g., in the case of long cavities.

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Semicond. Sci. Technol.
vol. 15, no. 12, pp. 1131-1140, 2000

Threshold characteristics of InGaAsP/InP multiple quantum well lasers

L. V. Asryan, N. A. Gun'ko, A. S. Polkovnikov, G. G. Zegrya, R. A. Suris, P.-K. Lau, T. Makino

A theoretical analysis and computer simulation of the threshold current density j_{th} and characteristic temperature T_0 of multiple quantum well lasers (MQWLs) are presented. Together with the spontaneous radiative recombination, the Auger recombination and the lateral diffusive leakage of carriers from the active region are included into the model. A first-principle calculation of the Auger recombination current is performed. It is shown that the lateral diffusive leakage current is controlled by the radiative and Auger currents. When calculating the carrier densities, the electrons in the barrier regions are properly taken into account.

Redistribution of electrons over the active region is shown to increase the threshold current considerably. The dependences of j_{th} and T_0 on temperature, number of QWs, cavity length and lateral size are discussed in detail. The effect of lattice and carrier heating on j_{th} and T_0 is investigated and shown to be essential at high temperature.

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IEEE J. Quantum Electron.
vol. 36, no. 10, pp. 1151-1160, 2000.

Longitudinal spatial hole burning in a quantum-dot laser

L. V. Asryan, R. A. Suris

Detailed theoretical analysis of longitudinal spatial hole burning in quantum-dot (QD) lasers is given. Unlike conventional semiconductor lasers, escape of thermally excited carriers from QDs, rather than diffusion, is shown to control the smoothing-out of the spatially nonuniform population inversion and multimode generation in QD lasers. The multimode generation threshold is calculated as a function of structure parameters (surface density of QDs, QD size dispersion, and cavity length) and temperature. A decrease in the QD size dispersion is shown to increase considerably the relative multimode generation threshold. The maximum tolerable QD size dispersion and the minimum tolerable cavity length, at which lasing is possible to attain, are shown to exist. Concurrent with the increase of threshold current, an increase of the multimode generation threshold is shown to occur with a rise in temperature. Ways to optimize the QD laser, aimed at maximizing the multimode generation threshold, are outlined.

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Proc. SPIE
vol. 3944, pp. 823-834, 2000

Effect of excited-state transitions on the threshold characteristics of a quantum dot laser

*L. V. Asryan, M. Grundmann, N. N. Ledentsov,
O. Stier, R. A. Suris, D. Bimberg*

Theoretical study of threshold characteristics of a quantum dot (QD) laser in the presence of excited-state transitions is given. The effect of microscopic parameters (degeneracy factor and overlap integral for a transition) on the gain is discussed. An analytical equation for the gain spectrum is derived in an explicit form. Transformation of the gain spectrum with the injection current is analyzed. The threshold current density is calculated as a function of the total losses. The conditions for a smooth or step-like change in the lasing wavelength with the losses are formulated. Threshold characteristics of a laser based on self-assembled pyramidal InAs QDs in GaAs matrix are simulated. A small overlap integral for transitions in such QDs (and hence large spontaneous radiative lifetime) is shown to be a main possible reason for a low value of the maximum single-layer modal gain of the respective structure which is deficient to attain lasing at moderately short (several hundreds of micrometers) cavity lengths.

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Semicond. Sci. Technol.
vol. 14, no. 12, pp. 1069-1075, 1999

High power and high temperature operation of InGaAsP/InP multiple quantum well lasers

*L. V. Asryan, N. A. Gun'ko, A. S. Polkovnikov, R. A. Suris, G. G. Zegrya,
B. B. Elenkrig, S. Smetona, J. G. Simmons, P.-K. Lau, T. Makino*

An analytical model of the effect of heating on the high-power and high-temperature operation of semiconductor multiple quantum well lasers (MQWLs) is developed. Both the lattice heating and the carrier heating in

the active region are shown to play an important role. The lattice heating predominates at high injection currents, while the carrier heating prevails at low currents. The maximum output power and the corresponding injection current are shown to be decreasing functions of temperature. The ways to increase the maximum output power of MQWLs are discussed. The effect of the series resistance on the maximum output power is investigated. Optimization of MQWLs with respect to the QW number and the cavity length is carried out. The results are illustrated by the example of a ridge MQW structure lasing at 1.3 μm. The theoretical and experimental dependences are compared.

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Semiconductors
vol. 33, no. 9, pp. 981-984, 1999

Role of thermal ejection of carriers in the burning of spatial holes in quantum dot lasers

L.V. Asryan, R.A. Suris

The role of thermal carrier ejection from quantum dots and free carrier diffusion in the burning of spatial holes in semiconductor quantum dot lasers is analyzed. The balance of the spatially inhomogeneous population inversion in the longitudinal direction of the cavity is shown to be controlled by thermal ejection from quantum dots. Because of this circumstance, hole burning in quantum dot lasers can show up more strongly and the threshold for multimode lasing can be lower than in semiconductor lasers with three-dimensional active regions or quantum-well lasers. The threshold for multimode lasing is determined as a function of the dispersion in the quantum dot size, cavity length, and temperature for structures that have been optimized to minimize the threshold current density of the fundamental mode.

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Appl. Phys. Lett.
vol. 74, no. 9, pp. 1215-1217, 1999

Spatial hole burning and multimode generation threshold in quantum-dot lasers

L. V. Asryan, R. A. Suris

The multimode generation threshold in quantum-dot (QD) lasers is calculated as a function of the parameters of structure and temperature. Thermally excited escapes of carriers away from QDs are shown to control the multimode generation threshold. A decrease in the QD size dispersion is shown to increase considerably the relative multimode generation threshold. The maximum tolerable QD size dispersion and the minimum tolerable cavity length, at which the lasing is possible to attain, are shown to exist. Concurrent with the decrease of threshold current, the reduction of multimode generation threshold is shown to occur with decrease of temperature.

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Proc. SPIE
vol. 3625, pp. 293-301, 1999

Spatial hole burning in a quantum dot laser

L. V. Asryan, R. A. Suris

Detailed theoretical analysis of the longitudinal spatial hole burning in quantum dot (QD) lasers is given. The multimode generation threshold is calculated as a function of the parameters of structure (surface density of QDs, Q D size dispersion, and cavity length) and temperature. Unlike conventional semiconductor lasers, thermally excited escapes of carriers away from QDs, rather than diffusion, are shown to control smoothing-out spatially nonuniform population inversion and hence the multimode generation threshold in QD lasers. A decrease in the QD size dispersion

is shown to increase considerably the relative multimode generation threshold. The maximum tolerable QD size dispersion and the minimum tolerable cavity length, at which the lasing is possible to attain, are shown to exist. Concurrent with the decrease of threshold current, the reduction of multimode generation threshold is shown to occur with decreased temperature. For the structures optimized to minimize the threshold current density for the main longitudinal mode, the dependences of the multimode generation threshold on the QD size dispersion, cavity length, and temperature are obtained. The ways to optimizing the QD laser structure, aimed at maximizing the multimode generation threshold, are outlined.

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Nanophotonics and metamaterials

Semiconductors
vol. 52, no. 4, pp. 442-446, 2018

Experimental observation of Dyakonov plasmons in the mid-infrared

O. Takayama, P. Dmitriev, E. Shkondin, O. Yermakov, M. Panah, K. Golenitskii, F. Jensen, A. Bogdanov, A. Lavrinenko

In this work, we report on observation of Dyakonov plasmons at an interface with a hyperbolic metamaterial in the mid-IR. The hyperbolic metamaterial is implemented as a CMOS-compatible high aspect ratio grating structure with aluminium-doped ZnO (AZO) ridges grown by atomic layer deposition in deep trench silicon matrix. The dispersion of Dyakonov plasmons is characterized by the attenuated total reflection method in the Otto configuration. We demonstrate that Dyakonov plasmons propagate in a broad range of directions (a few tens of degrees) in contrast to the classical Dyakonov surface waves (about one tenth of degree). The obtained results provide useful guidelines for practical implementations of structures supporting Dyakonov plasmons in the mid-IR.

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J. Mod. Opt.
vol. 64, no. 15, pp. 1501-1509, 2017

A study of a phase formalism for calculating the cumulative density of states of one-dimensional photonic crystals

R. A. Abram, A. A. Greshnov, S. Brand, M. A. Kaliteevski

We explore a phase formalism that underpins a method of calculation of the cumulative density of states of one-dimensional photonic crystals based on the node counting theorem. Node counting is achieved by considering the spatial dependence of a phase variable proportional to the logarithmic derivative of the electric field in the structure. The properties of the phase variable are considered for photonic crystals in general, and illustrative algebraic and numerical results are presented for

the phase variable and cumulative density of states of a model crystal. It is also shown how a simple extension of the theory can facilitate the calculation of the reflectivity of finite samples. For a disordered model crystal, a differential equation for the distribution function of the phase variable is derived and then used to obtain a closed-form expression for the ensemble-averaged cumulative density of states and numerical results to illustrate band tailing in the photonic bandgap.

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Proc. PIERS 2017
(Progress In Electromagnetics Research
Symposium - Spring, St.Petrsburg, Russia, 2017)
pp. 2817-2824, 2017

Optical bound state in the continuum in the one-dimensional photonic structures: Transition into a resonant state

Z. F. Sadrieva, I. S. Sinev, A. K. Samusev, I. V. Iorsh, A. A. Bogdanov, K. L. Koshelev, O. Takayama, R. Malureanu, A. V. Lavrinenko

Optical bound states in the continuum (BIC) are localized states with energy lying above the light line and having infinite lifetime. Any losses taking place in real systems result in transformation of the bound states into resonant states with finite lifetime. In this work, we analyze properties of BIC in CMOS-compatible one-dimensional photonic structure based on silicon-on-insulator wafer at telecommunication wavelengths, where the absorption of silicon is negligible. We reveal that a high-index substrate could destroy both off-Γ BIC and in-plane symmetry protected at-Γ BIC turning them into resonant states due to leakage into the diffraction channels opening in the substrate. We show how two concurrent loss mechanisms — scattering due to surface roughness and leakage into substrate — contribute to the suppression of the resonance lifetime and specify the condition when one of the mechanisms becomes dominant. The obtained results provide useful guidelines for practical implementations of structures supporting optical bound states in the continuum.

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Proc. PIERS 2017
(Progress In Electromagnetics Research
Symposium - Spring, St.Petrsburg, Russia, 2017)
pp. 3842-3846, 2017

Plasmonic nanoantenna for enhancement of vertical emission from whispering gallery mode laser

A. A. Bogdanov, E. I. Moiseev, N. Kryzhanovskaya, Yu. S. Polubavkina, M. V. Maximov, M. M. Kulagina, Yu. M. Zadiranov, A. A. Lipovskii, I. S. Mukhin, A. M. Mozharov, F. E. Komissarenko, Z. F. Sadrieva, A. E. Krasnok, A. V. Lavrinenko, A. E. Zhukov

We analyze the optical forces acting on a nanoparticle placed in the vicinity of a plasmonic interface. We show that the under oblique plane wave excitation the nanoparticle excites surface plasmon polariton propagating along the plasmonic interface. The momentum conservation law in the plane of the interface results in appearance of optical recoil force attracting the particle to the source of light. The analyzed recoil force could increase the radiation pressure force by an order of magnitude.

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Proc. PIERS 2017
(Progress In Electromagnetics Research
Symposium - Spring, St.Petrsburg, Russia, 2017)
pp. 581-582, 2017

Optical binding near a planar interface

N. A. Kostina, M. I. Petrov, A. N. Ivinskaya, A. A. Bogdanov, A. S. Shalin, P. B. Ginzburg

Light carries momentum which can influence the matter through optical forces. Nowadays, studying of optical forces became a promising field due to widespread usage of single and organized molecular and atomic structures in chemical and biological research, nanophotonics, different miniaturized electronic devices. Optical binding is an optical force

appearing in the ensemble of particles that controls their motion and can lead to self-organization of structural elements. If an array of nanoparticles is illuminated by light, each element of the array scatters incident wave and a set of potential wells is created which defines stable positions of particles.

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Phys. Rev. Lett.
vol. 119, no. 24, 243901, 2017

High-Q supercavity modes in subwavelength dielectric resonators

M. V. Rybin, K. L. Koshelev, Z. F. Sadrieva, K. B. Samusev,
A. A. Bogdanov, M. F. Limonov, Yu. S. Kivshar

Recent progress in nanoscale optical physics is associated with the development of a new branch of nanophotonics exploring strong Mie resonances in dielectric nanoparticles with a high refractive index. The high-index resonant dielectric nanostructures form building blocks for novel photonic metadevices with low losses and advanced functionalities. However, unlike extensively studied cavities in photonic crystals, such dielectric resonators demonstrate low quality factors (*Q* factors). Here, we uncover a novel mechanism for achieving giant *Q* factors of subwavelength nanoscale resonators by realizing the regime of bound states in the continuum. In contrast to the previously suggested multilayer structures with zero permittivity, we reveal strong mode coupling and Fano resonances in homogeneous high-index dielectric finite-length nanorods resulting in high-*Q* factors at the nanoscale. Thus, high-index dielectric resonators represent the simplest example of nanophotonic supercavities, expanding substantially the range of applications of all-dielectric resonant nanophotonics and meta-optics.

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Tech. Phys.
vol. 62, no. 7, pp. 1082-1086, 2017

Lasing in microdisks with an active region based on lattice-matched InP/AlInAs nanostructures

D. V. Lebedev, A. M. Mintairov, A. S. Vlasov, V. Yu. Davydov, M. M. Kulagina, S. I. Troshkov , A. A. Bogdanov, A. N. Smirnov, A. Gocalinska, G. Juska, E. Pelucchi, J. Kapaldo, S. Rouvimov, J. L. Merz

The emissivity of unstrained quantum-dimensional InP/AlInAs nanostructures and their lasing properties in microdisk cavities prepared by wet etching have been studied. For as-prepared structures, it has been found that they radiate owing to quantum-dimensional InP islands 50–300 nm in diameter. At temperatures below 160 K, whispering gallery modes have been observed in the microdisks. Experimental data on the PL intensity for microcavity modes versus the pump power, which were obtained at liquid helium temperature, have made it possible to find the lasing threshold, 50 W/cm^2. The half-width of the laser line at abovethreshold powers equals 0.06 nm, which corresponds to a *Q* factor of 15 000.

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ACS Photonics
vol. 4, no. 2, pp. 275-281, 2017

Light outcoupling from quantum dot-based microdisk laser via plasmonic nanoantenna

E. I. Moiseev, N. Kryzhanovskaya, Yu. S. Polubavkina, M. V. Maximov, M. M. Kulagina, Yu. M. Zadiranov, A. A. Lipovskii, I. S. Mukhin, A. M. Mozharov, F. E. Komissarenko, Z. F. Sadrieva, A. E. Krasnok, A. A. Bogdanov, A. V. Lavrinenko, A. E Zhukov

Microdisk lasers demonstrate high performance and low threshold characteristics due to supporting of whispering gallery modes with a high quality factor. One of the challenging problems impeding some practical

applications of whispering gallery mode lasers is that they have isotropic emission predominantly lying in the plane of the cavity. In this work, we present a novel method that provides both enhancement of the laser emission and modifies its directivity, making the vertical direction favorable. Electromagnetic energy outcouples from the cavity through the platinum−carbon plasmonic wire nanoantenna grown by electron-beam assisted deposition right up the side wall of the cavity. Evanescent field of whispering gallery mode excites surface plasmon polariton which propagates along the nanoantenna and scatters at its tip. We demonstrate 20× enhancement of the dominant mode intensity with 24 dB of side mode suppression increment without essential worsening of the Q-factor which remains over 3×10^4 . The proposed approach of the efficient control over the spectrum, directivity, and emission efficiency from microdisk lasers could be very promising for many practical applications from telecommunication technologies to biosensing.

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Proc. SPIE
vol. 10343, 103430F, 2017

High-Q resonances with low azimuthal indices in all-dielectric high-index nanoparticles

K. L. Koshelev, A. A. Bogdanov, Z. F. Sadrieva, K. B. Samusev, M. V. Rybin, M. F. Limonov, Yu. S. Kivshar

Recently, a novel class of high-Q optical resonators based on all-dielectric subwavelength nanoparticles with high refractive index has been proposed [M. V. Rybin, et al, arXiv:1706.02099, 2017]. Here we study a complex spectrum of such nanoscale resonators by means of the resonant-state expansion, treating the problem as a non-Hermitian eigenproblem. We show that the high-Q features can be described within the mechanism of external coupling of open channels via the continuum. For ceramic resonators with permittivity $\varepsilon = 40$, we demonstrate that the quality factor of a trapped mode with a low azimuthal index could reach the value $Q = 10^4$.

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Phys. Rev. B
vol. 94, no. 11, 115439, 2016

Interplay between anisotropy and spatial dispersion in metamaterial waveguides

K. L. Koshelev, A. A. Bogdanov

We analyze the spectrum of waveguide modes of an arbitrary uniaxial anisotropic metamaterial slab with nonlocal electromagnetic response whose permittivity tensor could be described within the Drude approximation. Spatial dispersion was introduced within the hydrodynamical model. By considering both anisotropy and spatial dispersion as perturbations, we distinguish their effect on the spectrum of the slab and analyze lifting of the degeneracy of eigenmodes at plasma frequency in detail. Spatial dispersion is shown to result in a break of the singularity in the density of optical states in the hyperbolic regime and in suppression of negative dispersion induced by anisotropy. We demonstrate that the interplay of spatial dispersion and anisotropy can bring light to a complete stop at certain frequencies.

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Phys. Rev. A
vol. 94, no. 4, 043815, 2016

Tamm-Langmuir surface waves

K. Yu. Golenitskii, K. L. Koshelev, A. A. Bogdanov

In this work we develop a theory of surface electromagnetic waves localized at the interface of periodic metal-dielectric structures. We have shown that the anisotropy of plasma frequency in metal layers lifts the degeneracy of plasma oscillations and opens a series of photonic band gaps. This results in appearance of surface waves with singular density of states—we refer to them as Tamm-Langmuir waves. Such naming is natural since we have found that their properties are very similar to the properties of both bulk Langmuir and surface Tamm waves. Depending on the anisotropy parameters, Tamm-Langmuir waves can be either

forward or backward waves. Singular density of states and high sensitivity of the dispersion to the anisotropy of the structure makes Tamm-Langmuir waves very promising for potential applications in nanophotonics and biosensing.

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2016 Conference on Lasers and
Electro-Optics (CLEO), San Jose, USA
7788328, 2016

Attraction optical forces inside hyperbolic metamaterials

S.V. Sukhov, A.S. Shalin, A.A. Bogdanov; P.A. Belov, P. Ginzburg

Hyperbolic metamaterials provide a platform for a new type of optical manipulation using highly confined extraordinary modes. Here we predict and analyze optical attracting forces acting on a small particle inside a hyperbolic slab.

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2016 Conference on Lasers and
Electro-Optics (CLEO), San Jose, USA
7787576, 2016

Optical pulling force in the vicinity of plasmonic interfaces

A. A. Bogdanov, M. I. Petrov, S. V. Sukhov, A. S. Shalin, A. Dogariu

We demonstrate both analytically and numerically the existence of optical pulling forces acting on particles located near plasmonic interfaces. This effect can be utilized for effective optomechanical control of nanoobjects over metallic surface.

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Opt. Lett.
vol. 41, no. 4, pp. 749-752, 2016

Dark-field imaging as a noninvasive method for characterization of whispering gallery modes in microdisk cavities

D. A. Baranov, K. B. Samusev, I. I. Shishkin, A. K. Samusev, P. A. Belov, A. A. Bogdanov

Whispering gallery mode microdisk cavities fabricated by direct laser writing are studied using dark-field imaging and spectroscopy in the visible spectral range. Dark-field imaging allows us to directly visualize the spatial intensity distribution of whispering gallery modes. We extract their azimuthal and radial mode indices from dark-field images, and find the axial mode number from the dispersion relation. The scattering spectrum obtained in the confocal arrangement provides information on the density of optical states in the resonator. The proposed technique is a simple noninvasive way to characterize the optical properties of microdisk cavities.

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Phys. Rev. A
vol. 91, no. 6, 063830, 2015

Optical pulling forces in hyperbolic metamaterials

A. S. Shalin, S. V. Sukhov, A. A. Bogdanov, P. A. Belov, P. Ginzburg

Control over mechanical motion of nanoscale particles is a valuable functionality desired in a variety of multidisciplinary applications, e.g., biophysics, and it is usually achieved by employing optical forces. Hyperbolic metamaterials enable tailoring and enhancing electromagnetic scattering and, as the result, provide a platform for a new type of optical manipulation. Here optical pulling forces acting on a small particle placed inside a hyperbolic metamaterial slab were predicted and analyzed. In order to attract particles to a light source, highly confined extraordinary modes of hyperbolic metamaterial were excited via scattering from an imperfection situated at the slab's interface. This type of structured illumination together with remarkable

scattering properties, inspired by the hyperbolic dispersion in the metamaterial, creates optical attraction. Forces acting on high-, low-index dielectric, and gold particles were investigated and it was shown that the pulling effect emerges in all of the cases. The ability to control mechanical motion at nanoscale using auxiliary photonic structures paves the way for investigation of various phenomena, e.g., biochemical reactions, molecular dynamics, and more.

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Sci. Rep.
vol. 5, 15846, 2015

Optical forces in nanorod metamaterial

A. A. Bogdanov, A. S. Shalin, P. Ginzburg

Optomechanical manipulation of micro and nano-scale objects with laser beams finds use in a large span of multidisciplinary applications. Auxiliary nanostructuring could substantially improve performances of classical optical tweezers by means of spatial localization of objects and intensity required for trapping. Here we investigate a three-dimensional nanorod metamaterial platform, serving as an auxiliary tool for the optical manipulation, able to support and control near-field interactions and generate both steep and flat optical potential profiles. It was shown that the ‘topological transition’ from the elliptic to hyperbolic dispersion regime of the metamaterial, usually having a significant impact on various light-matter interaction processes, does not strongly affect the distribution of optical forces in the metamaterial. This effect is explained by the predominant near-fields contributions of the nanostructure to optomechanical interactions. Semi-analytical model, approximating the finite size nanoparticle by a point dipole and neglecting the mutual re-scattering between the particle and nanorod array, was found to be in a good agreement with full-wave numerical simulation. In-plane (perpendicular to the rods) trapping regime, saddle equilibrium points and optical puling forces (directed along the rods towards the light source), acting on a particle situated inside or at the nearby the metamaterial, were found.

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Opt. Lett.
vol. 40, no. 17, pp. 4022-4025, 2015

Mode selection in InAs quantum dot microdisk lasers using focused ion beam technique

A. A. Bogdanov, I. S. Mukhin, N. Kryzhanovskaya, M. V. Maximov, Z. F. Sadrieva, M. M. Kulagina, Zadiranov, A. A. Lipovskii, E. I. Moiseev, Y. V. Kudashova, A E Zhukov

Optically pumped InAs quantum dot microdisk lasers with grooves etched on their surface by a focused ion beam are studied. It is shown that the radial grooves, depending on their length, suppress the lasing of specific radial modes of the microdisk. Total suppression of all radial modes, except for the fundamental radial one, is also demonstrated. The comparison of laser spectra measured at 78 K before and after ion beam etching for a microdisk of 8 μm in diameter shows a sixfold increase of mode spacing, from 2.5 to 15.5 nm, without a significant decrease of the dominant mode quality factor. Numerical simulations are in good agreement with experimental results.

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Phys. Rev. B
vol. 92, no. 8, 085305, 2015

Temperature-tunable semiconductor metamaterial

K. L. Koshelev, A. A. Bogdanov

We propose a class of temperature-tunable semiconductor metamaterials for terahertz applications. These metamaterials are based on doped semiconductor superlattices with ultrathin barriers of about 1 nm thickness. Due to the tunnel transparency of the barriers, layers of the superlattice cannot be considered as isolated and, therefore, the classical homogenization approach is inapplicable. We develop a theory

of quantum homogenization which is based on the Kubo formula for conductivity. The proposed approach takes into account the wave functions of the carriers, their distribution function, and energy spectrum. We show that the components of the dielectric tensor of the semiconductor metamaterial can be efficiently manipulated by external temperature and a topological transition from the dielectric to hyperbolic regime of metamaterial can be observed at room temperature. Using a GaAs/Al0.3Ga0.7As superlattice slab as an example, we provide a numerical simulation of an experiment which shows that the topological transition can be observed in the reflectance spectrum from the slab.

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Proc. DD 2015
(Int. Conf. Days on Diffraction 2015)
pp. 371-375, 2015

New types of surface waves on hyperbolic metasurface

O. Y. Yermakov, A. I. Ovcharenko, I. V. Iorsh,
A. A. Bogdanov, Yu. S. Kivshar

We reveal the existence of a new types of surface electromagnetic waves supported by hyperbolic metasurface, described by a local diagonal anisotropic conductivity tensor. We present a comprehensive analysis of the dispersion and the equal frequency contours of surface waves propagating along hyperbolic metasurface. We demonstrate that the spectrum of the hyperbolic metasurface waves consists of two branches corresponding to hybrid transverse electric – transverse magnetic waves with a polarization that varies from linear to elliptic or circular depending on the wave frequency and propagation direction.

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Proc. DD 2015
(Int. Conf. Days on Diffraction 2015)
pp. 250-254, 2015

Optical forces induced at the metal surface

M. I. Petrov, A. A. Bogdanov, S. V. Sukhov, A. Dogariu, A.S. Shalin

In this paper we discuss the optical forces acting on a small nanoparticle in the vicinity of a plane metallic surface. We show that illuminating the nanoparticle by a plane wave leads to the excitation of a surface plasmon polariton wave at the metallic interface, which governs the opto-mechanical response of nanoparticle. The presented calculations show that for a nanoparticle in the Rayleigh approximation one can achieve lateral force acting in the direction opposite to incident field.

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Proc. DD 2015
(Int. Conf. Days on Diffraction 2015)
pp. 154-157, 2015

Homogenization of quantum metamaterial

K. L. Koshelev, A. A. Bogdanov

The classical effective medium theory is usually applied to calculate a permittivity tensor of a multilayered structure. The main assumption of this theory is that the thickness of a single layer should be less that the light wavelength. However, when the thicknesses of the layers are comparable with the electron wavelength we should take into account the tunnel transparency of the layers and the quantum confinement effects. Due to the tunnel transparency of the barriers, layers of the superlattice cannot be considered as isolated and, therefore, the classical homogenization approach should be modified. We develop a theory of quantum homogenization which is based on the Kubo formula for conductivity. The proposed approach takes into account the wave functions of the carriers, their distribution function and energy spectrum.

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Proc. DD 2015
(Int. Conf. Days on Diffraction 2015)
pp. 36-41, 2015

Dark-field spectroscopy of whispering gallery mode cavities

D. A. Baranov, I. I. Shishkin, D. S. Permyakov, K. B. Samusev, A. K. Samusev, A. A. Bogdanov

Cylindrical resonators fabricated by direct laser writing and supporting whispering gallery modes are analyzed numerically and experimentally using dark-field spectroscopy. Electric field intensity distribution corresponding to the whispering gallery modes is observed directly in scattered radiation in the visible spectrum range. In the the dark-field spectroscopy experiments, we observed beating of photon density of states, which is explained by the excitation of the eigenmodes of higher radial order. Numerical simulation of both spectrum and mode intensity distribution is provided and good agreement with the experiment is achieved.

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Proc. METAMATERIALS 2015
(9th Int. Congress on Advanced Electromagnetic
Materials in Microwaves and Optics, Oxford, UK)
pp. 154-156, 2015

Temperature induced topological transition in semiconductor metamaterial

K. L. Koshelev, A. A. Bogdanov

We propose new type of temaperature tunable metamaterial based on semiconductor superlattice for THz applications. We have shown that temperature activation of donors in semiconductor metamaterial results in drastic changes of the dielectric function in terahertz region. We have analyzed that the shape and topology of equal frequency contours depending on the external temperature. It was shown that transition from

elliptical to hyperbolic regime, so called ”topological transition”, can be observed at room temperature.

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Opt. Express
vol. 22, no. 21, pp. 25782-25787, 2014

Control of emission spectra in quantum dot microdisk/microring lasers

N. V. Kryzhanovskaya, I. S. Mukhin, E. I. Moiseev, I. I. Shostak, A. A. Bogdanov, A. M. Nadtochiy, M. V. Maximov, A. E. Zhukov, M. M. Kulagina, K. A. Vashanova, Yu. M. Zadiranov, S. I. Troshkov, A. A. Lipovskii, A. Mintairov

Focused ion beam is applied to quantum dot based microresonators to form pits or groove on their surface. The emission spectra of the resonators based lasers are significantly thinned out after the ion beam milling, and one or two modes become dominant instead of a group of modes having comparable intensities. The linewidth of the lasing mode is kept unchanged, whereas the lasing threshold demonstrates an insignificant growth.

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Semiconductors
vol. 48, no. 12, pp. 1626-1630, 2014

Lasing in microdisks of ultrasmall diameter

A. E. Zhukov, N. V. Kryzhanovskaya, M. V. Maximov, A. A. Lipovskii, A. V. Savelyev, A. A. Bogdanov, I. I. Shostak, E. I. Moiseev, D. V. Karpov, J. Laukkanen, J. Tommila

It is demonstrated by calculations and experimental results that roomtemperature lasing can be obtained at the groundstate optical transition of InAs/InGaAs/GaAs quantum dots in optical microcavities

with a recordsmall diameter of 1.5 μm. In 1μm cavities, lasing occurs at the wavelength of one of the whis peringgallery modes within the band corresponding to the first excitedstate optical transition.

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Solid State Commun.
vol. 158, pp. 38-45, 2013

Analytical theory of light localization in one-dimensional disordered photonic crystals

A. A. Greshnov, M. A. Kaliteevski, R. A. Abram

Influence of the various types of disorder on propagation of light in one-dimensional periodic structures is studied analytically using statistical approach based on a Fokker–Planck type equation. It is shown that light localization length behaves non-monotonically as a function of disorder amplitude in all the examined models except for purely geometric disorder. This feature is explained by crossover between weak disorder regime corresponding to gradual destruction of the reflecting properties of a photonic crystal and strong disorder regime, when periodic component of the refractive index can be treated as a perturbation. The region of small disorder is shown to be universal provided that a disorder parameter is properly introduced.

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Solid State Commun.
vol. 146, no. 3-4, pp. 157-160, 2008

Density of states in 1D disordered photonic crystals: Analytical solution

A. A. Greshnov, M. A. Kaliteevski, R. A. Abram, S. Brand, G. G. Zegrya

A novel analytical approach to the calculation of the density of states of one-dimensional disordered photonic crystals has been developed. It is

shown that the problem can be reduced to the solution of a stationary Fokker–Planck equation for the distribution function of a reduced phase variable Ψ which is directly related to the quantity $(dE/dz)/E$ where $E(z)$ is the electric field of the electromagnetic wave and z the position in the structure. We have obtained an analytical expression for the density of states within and close to the first photonic band gap and have examined various approximations. Our analytical expressions for the density of states are in good agreement with the results of direct numerical calculations.

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Phys. Solid State
vol. 49, no. 10, pp. 1999-2003, 2007

Density of states of a one-dimensional disordered photonic crystal

A. A. Greshnov, M. A. Kaliteevski, R. A. Abram, S. Brand, G. G. Zegrya

An analytic theory of the density of states in one-dimensional disordered photonic crystals is proposed. It is shown that the problem of the density of optical modes can be reduced in the small dielectric contrast approximation to solving a generalized Fokker–Planck equation for the distribution function of the logarithmic derivative of the electric field (the wave phase). The exact analytic solution and density-of-states asymptotics deep in the band gap of the photonic crystal and close to the band gap edge are derived. The results obtained agree well with the empirical relations derived earlier from numerical experiments.

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Nanomaterials and composites

Tech. Phys. Lett.
vol. 44, no. 6, pp. 479-482, 2018

The mechanism of generation of singlet oxygen in the presence of excited nanoporous silicon

D. M. Samosvat, O. P. Chikalova-Luzina, V. S. Khromov, A. G. Zegrya, G. G. Zegrya

A theoretical analysis of the mechanism of generation of singlet oxygen in the presence of photoexcited nanoporous silicon is presented. It is demonstrated that the mechanism of generation of singlet oxygen is based on nonradiative energy transfer from nanoporous silicon to an oxygen molecule by the exchange mechanism. An analytical expression of the probability of energy transfer from nanoporous silicon to an oxygen molecule is obtained, and a numerical estimate of this process is given. The numerical estimation is of the order of 10^3–10^4 s^{-1}, a value that agrees rather well with the experiment.

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Tech. Phys. Lett.
vol. 43, no. 10, pp. 896-898, 2017

Initiation of explosive conversions in energy-saturated nanoporous silicon-based compounds with fast semiconductor switches and energy-releasing elements

G. G. Savenkov, A. F. Kardo-Sysoev, A. G. Zegrya, I. A. Os’kin, V. A. Bragin, G. G. Zegrya

The first findings concerning the initiation of explosive conversions in energy-saturated nanoporous silicon-based compounds via the electrical explosion of a semiconductor bridge are presented. The obtained results indicate that the energy parameters of an explosive conversion depend on the mass of a combustible agent—namely, nanoporous silicon—and the silicon-doping type.

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Semiconductors
vol. 51, no. 4, pp. 477-482, 2017

Sensitivity of energy-packed compounds based on superfine and nanoporous silicon to pulsed electrical treatments

G. G. Zegrya, G. G. Savenkov, V. A. Morozov, A. G. Zegrya, N. V. Ulin, V. P. Ulin, A. A. Lukin, V. A. Bragin, I. A. Oskin, Yu. M. Mikhailov

The sensitivity of an energy-packed compound based on nanoporous silicon and calcium perchlorate to a high-current electron beam is studied. The initiation of explosive transformations in a mixture of potassium picrate with a highly dispersed powder of boron-doped silicon by means of a high-voltage discharge is examined. It is shown that explosive transformation modes (combustion and explosion) appear in the energy-packed compound under study upon its treatment with an electron beam. A relationship is established between the explosive transformation modes and the density of the energy-packed compound and between the breakdown (initiation) voltage and the mass fraction of the silicon powder.

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Russ. Chem. Bull.
vol. 65, no. 10, pp. 2400-2404, 2016

Impact sensitivity of energy systems based on nanoporous silicon and oxidant: influence of the hydrogen content and specific surface

Yu. M. Mikhailov, V. A. Garanin, Yu. V. Ganin, T. K. Goncharov, L. V. Ganina, G. G. Zegrya

The impact sensitivity of the energy systems based on nanoporous silicon, obtained by electro chemical etching of monocrystalline silicon wafers in an HFcontaining electrolyte, and calcium perchlorate was studied using a modified Weller—Ventselberg technique (estimation of

the impact sensitivity of initiating explosives). The impact sensitivity of these systems is shown to be determined by both the presence of hydrogen, which is stored on the porous silicon surface during the preparation of the latter, and also the influence of other factors, including the specific surface of porous silicon. The composition, amount of the generated gas, and gas evolution rate during non isothermal and isothermal calcination of porous silicon in a temperature range of 60—120 °C were determined using methods of thermal gravimetry (TG), measurement of the gas volume, and mass spectrometry. The generated gas almost completely consists of hydrogen, and its content in the studied samples of porous silicon achieved ~3.8 wt.%. The calculated activation energy of the hydrogen evolution process in vacuo was 103.7±3.3 kJ mol^{-1}. The dependences of the impact sensitivity of the energy composition based on porous silicon and heat of combustion of porous silicon on oxygen on the hydrogen content were established. The impact sensitivity of the energy system decreases with a decrease in the hydrogen content in porous silicon and its specific surface.

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Ukr. J. Phys.
vol. 57, no. 7, pp. 695-699, 2012

Interaction of DNA with silver nanoparticles

*G.M. Glibitskiy, V. V. Jelali, M. O. Semenov, A.D. Roshal,
D.M. Glibitskiy, O.Y. Volyanskiy, G.G. Zegrya*

The dehydrational self-organization of DNA with Na^+ and Ag^+ ions and silver nanoparticles has been studied. It has been shown that the character of the formation of dendritic textures (the size of the area occupied on the film surface) is governed by the conformational state of DNA.

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Proc. of the 221st ECS Meeting
Seattle, Washington, USA
Abs. 1367, 2012

Qed kapitza conductance of graphene

A. G. Petrov, S. V. Rotkin

The theory for the QED Kapitza conductance of nano-carbons on a polar substance is developed. A universal formula is found describing the magnitude of the effect via the fundamental constants and material parameters. Calculated values of the QED interface conductance show that the nano-carbon thermal interconnects may be interesting for industrial applications.

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Proc. Of WINDS 2012
(Workshop on Innovative Nanoscale
Devices and Systems, Hawaii, USA, 2012)

Qed interfacial heat conductance in nanocarbon thermal interconnects

V. Rotkin, A. G. Petrov, A. M. Nemilentsau

Heat management solutions are critical nowadays in multiple fields and applications, from nanoelectronics to spacecrafts. Interfacial thermal barrier is known to be one of the largest problems that modern nanomaterials were aimed to overcome. Nanocarbons in various forms have been suggested to serve as a cheap and excellent thermal interconnect material, though their interface heat conductance has not been completely understood so far. We show that the bulk heat conductance of the nanocarbons (graphene and nanotubes are studied in details) is unlikely to be a bottleneck for thermal applications. It is rather the thermal interfacial conductance mechanism which will be of critical importance. On the basis of atomistic quantum models and fluctuational electrodynamics we studied the QED thermal conductance across the interface between a nanocarbon material and a dielectric/semiconductor/metal substrate. Extremely high and potentially

controllable thermal conductance was found and the physics of the effect was explained in terms of the near-field radiative heat transport. Both analytical models and useful empirical fits will be presented to guide the design of well-tempered nanocarbon thermal interconnects.

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Bull. Am. Phys. Soc.
(APS March Meeting 2012)
vol. 57, no. 1, P7.014, 2012

Qed Kapitza conductance of nano-carbon thermal interconnects

S. V. Rotkin, A. G. Petrov

The theory for the near-field Kapitza conductance across the interface of a nano-carbon material and the quartz is thoroughly investigated. The near-field photon tunneling is shown to contribute to the total heat flux between the hot and cold sides of the interface on the order of or even larger than the normal thermal conductance. Quartz is chosen as the most common example of non-conductive and strongly polar substrate material with the well known polarization properties, though the theory is not restricted to quartz only. Our approach allowed us to derive a unified expression for QED Kapitza conductance of the nanocarbon thermal interconnect material, such as graphene, a nanotube, or a nanotube forest and predict thermal phenomena, such as the heat rectification, as a function of the materials properties of the interface.

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Proc. of the 217th ECS Meeting,
Vancouver, Canada
Abs. 1563, 2010

Thermal management in heterogeneous carbon nanoelectronics

S. V. Rotkin, A. G. Petrov

The talk focuses on the thermal coupling between a substrate and a channel of a graphene/nanotube electronic device (such as a transistor, a RF switch or a LED), operating at a high driving voltage. We proposed recently that a novel thermal conductance mechanism may exist in such structures. This theory has been confirmed experimentally in recent papers for NTs and graphene. Here we elucidate the physics of nanotube (NT) and layered graphene (LG) electronic coupling to the surface electromagnetic modes that exist at the interface with the SiO2, Al2O3 or a high-k oxide, the material of the choice for modern nano-technology.

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Proc. of 10th IEEE Conference
on Nanotechnology Joint Symposium with
Nano Korea 2010, KINTEX, Korea
pp. 66-71, 2010

Surface polariton scattering for charge transport and heat management in carbon-based heterogeneous electronics: Problem or solution?

S. V. Rotkin, A. G. Petrov

With increasing importance of non-Si electronics for the future generations of digital and analog devices the questions of ultimate performance limits and reliability of new electronic materials become critical. In the paper we review a particular case of heterogeneous carbon-based electronics. We assume that the nanotube material is combined with the materials of the standard Si-technology. Interface of the nanotubes or graphene with oxides presents, as we demonstrate below, a significant source of inelastic surface scattering. Hot electrons release the energy by emitting surface polaritons with the scattering rate of the order of ten fs. Such a fast mechanism, dominating scattering in the heterogeneous electronics devices, should determine (i) low-field mobility at room temperature, (ii) saturation currents in the high-power regime and (iii) thermal coupling to the substrate, discussed here in details. Such thermal coupling is explained below in terms of large QED

Kapitsa conductance. Good thermal properties of carbon hetero-interfaces with Si and high-k oxides are promising for efficient heat dissipation and thermal management.

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Bull. Am. Phys. Soc.
(APS March Meeting 2010)
vol. 55, no. 2, J12.006, 2010

Graphene and nanotubes on the polar insulator: Near-field thermal conductance across the interface

S. V. Rotkin, A. G. Petrov

Our ability to apply carbon-based materials for electronic devices requires detailed knowledge of their electronic properties as well as thermal ones in the real environment (rather than in vacuum). We present a microscopic theory of the electromagnetic coupling of the charge carriers in graphene and single-wall carbon nanotube to the surface electromagnetic modes of the SiO_2 substrate, which allows a new interpretation of experimental data. Such coupling changes the physics of both inelastic hot charge carrier scattering in carbon-based electronic devices and thermal conductance across the interface with the substrate. Our modeling predicts that the near-field scattering by the surface modes results in (A) a dominating inelastic scattering channel (with a typical 30 nm m.f.p.) [Nano Lett 9, 1850, (2009)] and (B) the most significant interface thermal conductance mechanism (0.1 W/m^2K) [SPIE Proc. 7399, 7399-0F (2009)]. Both effects have to be taken into account to study the high-electric field transport and to compute the Joule losses and channel steady-state temperature. This talk focuses on the novel thermal coupling mechanism which is a QED (near-field) counterpart of the Kapitza conductance. We discuss possibilities to tweak it for graphene and nanotube materials on the polar substrates.

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Nano Lett.
vol. 9, no.5, pp.1850-1855, 2009

An essential mechanism of heat dissipation in carbon nanotube electronics.

A. G. Petrov, S. V. Rotkin, V. Perebeinos, P. Avouris

Excess heat generated in integrated circuits is one of the major problems of modern electronics. Surface phonon−polariton scattering is shown here to be the dominant mechanism for hot charge carrier energy dissipation in a nanotube device fabricated on a polar substrate, such as SiO_2. By use of microscopic quantum models, the Joule losses were calculated for the various energy dissipation channels as a function of the electric field, doping, and temperature. The polariton mechanism must be taken into account to obtain an accurate estimate of the effective thermal coupling of the nonsuspended nanotube to the substrate, which was found to be 0.1−0.2 W/(m·K) even in the absence of the bare phononic thermal coupling.

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Nano Lett.
vol. 9, no. 1, pp. 312–316, 2009

The effects of substrate phonon mode scattering on transport in carbon nanotubes

V. Perebeinos, S. V. Rotkin, A. G. Petrov, Ph. Avouris

Carbon nanotubes (CNTs) have large intrinsic carrier mobility due to weak acoustic phonon scattering. However, unlike two-dimensional metal−oxide−semiconductor field effect transistors (MOSFETs), substrate surface polar phonon (SPP) scattering has a dramatic effect on the CNTFET mobility, due to the reduced vertical dimensions of the latter. We find that for the van der Waals distance between CNT and an

SiO_2 substrate, the low-field mobility at room temperature is reduced by almost an order of magnitude depending on the tube diameter. We predict additional experimental signatures of the SPP mechanism in dependence of the mobility on density, temperature, tube diameter, and CNT−substrate separation

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Bull. Am. Phys. Soc.
(APS March Meeting 2008)
vol. 53, no. 2, Y29.001, 2008

Anisotropic casimir interactions between a one-dimensional object (nanotube) and a polar substrate

S. V. Rotkin, A. G. Petrov, J. A. Rogers

The energy of Casimir interaction of a polarizable one-dimensional object (1DO), e.g. a nanotube, and a polar substrate was estimated. Within our model the energy of the dipole moment induced in the 1DO by the external electric field of the fluctuations of the quantized surface optical phonon modes is evaluated. Such polariton modes are known to exist in polar insulators and have the electric field with an exponentially decreasing wing in vacuum. If the polarization tensor of the 1DO is not isotropic, an orientation dependent Casimir force may arise. To the best of our knowledge, such anisotropic Casimir interaction has not been considered before and may lead to an orientation of long flexible objects, like nanotubes, at polar substrates. The interaction energy is derived analytically for the case of a single-wall nanotube on the ST-cut quartz. Besides a material dependent energy constant, it is proportional to the ratio of the volume of interacting segment of the nanotube and cube of the distance to the substrate.

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Bull. Am. Phys. Soc.
(APS March Meeting 2007)
vol. 52, no. 1, S28.013, 2007

Remote phonon scattering in NT field effect transistors

S. V. Rotkin, A. G. Petrov

We developed a theory of the remote phonon (RP) scattering for the hot charge carriers in nanotube (NT) field effect devices that use polar dielectric substrates, such as SiO2 or high-kappa materials [JETP Lett 84, 156, 2006]. We calculated the effect of this novel scattering mechanism on the NT conductivity. We stress that in contrast to any other scattering mechanisms studied earlier the RP scattering allows to transfer the excess energy of the hot carriers directly to the substrate (not through the NT lattice). The macroscopic substrate has no limitation of a finite thermal capacity as a single NT has. Therefore, our RP scattering mechanism is advantageous for the high power NT devices, especially when aggressively scaling down the size and scaling up the operational frequency. We obtained a scattering time within a self-consistent quantum mechanical approach for inter- and intra-subband transitions in semiconductor and metallic NTs. The intra-subband transitions with forward scattering are shown to prevail over the inter-subband transitions as well as the backward scattering. We obtained the polaronic effects by solving for the electron energy and life-time self-consistently. We found the upper limit of the spacing between the NT and the polar dielectric for the RP scattering to become ineffective, which is approximately 40 nm for the quartz substrate.

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Bull. Am. Phys. Soc.
(APS March Meeting 2006)
vol. 51, no. 1, G18.007, 2006

Nanotube exciton spectrum: Triangular quantum well model

S. V. Rotkin, A. G. Petrov.

The analytical solution for the problem of NT-exciton is found using the approximation for the screened Coulomb potential between the electron and hole. We derive the screening via calculating a self-consistent dielectric function with both spatial and time dispersion taken into account, $\epsilon(q,\varphi)$, which characterizes the response to the q component of the Coulomb potential at the frequency φ. The latter corresponds to the energy of the exciton and is to be sought. We calculated the RPA dielectric function of the SWNT in the orthogonal tight-binding approach. Then, the inverse Fourier transform of the screened Coulomb potential gives the shape of the potential well for the electron-hole pair (direct Coulomb interaction term). We show that this screened potential can be approximated by a triangular quantum well, which model allows analytical solutions for the exciton wave function and the binding energy. The exchange term is short-ranged and can be added as the delta-function barrier in the middle of the well. The exciton binding energy is calculated to be a universal function of E_g, the one-particle band gap, R, the NT radius and λ, the electric length in the triangular quantum well potential. The effective Bohr radius is also a universal function of R and λ. The analytical expression for the oscillator strength of the optical transition is presented.

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JETP letters
vol. 84, no.3, pp. 156-160, 2006

Energy relaxation of hot carriers in single-wall carbon nanotubes by surface optical phonons of the substrate

A. G. Petrov, S.V. Rotkin

A new mechanism is proposed for the energy relaxation of hot carriers in single-wall carbon nanotubes: scattering with the emission of surface optical phonons into the semiconductor substrate. The theory involves intrasubband and intersubband forward and backward scattering. The analytical result and numerical data indicate that intrasubband forward scattering is the main process: the corresponding lifetime comprises several femtoseconds for a quartz substrate, which allows this mechanism of energy relaxation to be considered dominating for a nanotube on the surface of a polar semiconductor or a dielectric.

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Phys. Rev. B
vol. 70(3), 035408, 2004

Transport in nanotubes: Effect of remote impurity scattering

A. G. Petrov, S.V. Rotkin

Theory of the remote Coulomb impurity scattering in single-wall carbon nanotubes is developed within one-electron approximation. Boltzmann equation is solved within drift-diffusion model to obtain the tube conductivity. The conductivity depends on the type of the nanotube band structure (metal or semiconductor) and on the electron Fermi level. We found exponential dependence of the conductivity on the Fermi energy due to the Coulomb scattering rate has a strong dependence on the momentum transfer. We calculate intrasubband and intersubband scattering rates and present general expressions for the conductivity. Numerical results, as well as obtained analytical expressions, show that the degenerately doped semiconductor tubes may have very high

mobility unless the doping level becomes too high and the intersubband transitions impede the electron transport.

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Nano Lett.
vol. 3, no. 6, pp. 701–705, 2003

Breaking of nanotube symmetry by substrate polarization

A. G. Petrov, S.V. Rotkin

Substrate and nanotube polarization are shown to change qualitatively a nanotube bandstructure. The effect is studied in a linear approximation in an external potential which causes the changes. A work function difference between the nanotube and gold surface is estimated to be large enough to break the band symmetry and lift a degeneracy of a lowest but one subband of a metallic nanotube. This subband splitting for [10,10] nanotube is about 50 meV in absence of other external potential.

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J. Comput. Electron.
vol. 1, no. 3, pp. 323-326, 2002

Many-body terms in van der Waals cohesion energy of nanotubes

S. V. Rotkin, K. Hess

We have developed a model for the calculation of van der Waals force for layered systems with axial symmetry. Our result can be applied to compute the cohesion of a carbon nanotube to a substrate, the cohesion between nanotubes, and between shells of multiwall nanotubes. We have obtained unusual power laws for the distance dependence of the many-body van der Waals potential.

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JETP Lett.
vol. 75, no 4, pp. 205-209, 2002

Nanotube devices: Microscopic model

K. A. Bulashevich, S. V. Rotkin

A microscopic model is developed for calculating electrostatic properties of nanotube devices. It is shown that the quantum-mechanical approach yields the same results as the statistical calculation in the limit of a thin tube suspended over a conducting gate at a distance exceeding the nanotube radius. A closed analytic expression is obtained for the atomistic capacitance of a straight nanotube and for a nanotube with a modest curvature. This method allows the fast and exact calculation of device parameters for the nanotube electromechanical systems and nanotube electronic devices.

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Mat. Res. Soc. Symp. Proc.
(Symposium W - Nanotubes, Fullerenes,
Nanostructured and Disordered Carbon.
Warrendale, PA, USA, September 2001.)
vol. 675, pp. W2.9.1-W2.9.5, 2001

SWNT nucleation: Energetics of Zipping-edge mechanism

S. V. Rotkin

A novel mechanism of SWNT nucleation is considered in oppose to an existing model. The latter model based on the formation of a hemispherical carbon bowl nucleus has no correct description within the thermodynamics and kinetics of the nucleation process. The new mechanism can explain the prevalent formation of [10,10] armchair nanotube on the base of the continuum graphene energetics.

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AIP Conf. Proc.
vol. 591, pp. 454-457, 2001

Zipping of graphene edge as a mechanism for NT nucleation

S. V. Rotkin, I. Zharov, K. Hess

The energetics of the nanotube formation was studied by the continuum analytical theory and the atomistic simulation within the novel mechanism of the nucleation from the graphite edge. The optimum shape of the nucleus was calculated to be close to that of a [10,10] nanotube.

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Nanotechnology
vol. 11, pp. 332-335, 2000

Renormalization of electron energy in 0D systems due to depolarization shift

S. V. Rotkin

A giant level shift, resulting from the interaction of an electron in a spherical quantum dot with zero-point oscillations of confined modes of the electric field, is divulged. This electron potential energy renormalization depends on the dot radius which has to show up in experiment. The size scaling of the depolarization effect is computed semiclassically. A change of the optical properties of the matrix surrounding the dot also provides a method with which to study the shift experimentally.

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Phys. Lett. A
vol. 261, pp. 98-101, 1999

Bond passivation model: Diagram of carbon nanoparticle stability

S. V. Rotkin, R. A. Suris

A new heuristic model for the calculation of the formation energy of the carbon nanoclusters was proposed. The model uses only three parameters: two energies, E_c and ε_5, are determined from the comparison with the experimental data, the results of computer simulations for various carbon nanoclusters, and the last one is the dangling carbon bond energy, E_b. The knowledge of the energies of the formation of the carbon cluster series, obtained in the frame of the unified phenomenological approach, allows one to judge the relative energetic stability of these clusters. The dangling bond passivation is shown to change drastically the phase diagram of the co-existence of the clusters of the different type.

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Opt. Mater.
vol. 12, pp. 391-394, 1999

Polymer-C60 exciton mixing

S. V. Rotkin, N. A. Gunko

The one-electron spectrum of C_{60} cluster which is coupled to PPV chain is calculated. It shows that non-rigid band scheme has to be considered for this composite system. The splitting of states in the closest valence and conduction bands is discussed.

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Phys. Solid State
vol. 41, no. 5, pp. 729-732, 1999

Energy characteristics of carbon clusters with passivated bonds

V.V. Rotkin, R.A. Suris

A modified phenomenological model is proposed for calculating the formation energy of carbon nanoclusters which makes it possible to analyze the regions of existence of clusters of various forms. A new parameter of the model, which corresponds to passivation of broken carbon bonds, affects the shape of the equilibrium optimum clusters, i.e., those having a minimum energy for a fixed number of atoms. Analytic dependences of equilibrium-configuration states determining the existence of spheroidal closed clusters, nanopipes, and fragments of a graphite plane, on the broken-bond energy parameter obtained in this model are presented.

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Carbon
vol. 37, no. 5, pp. 847-850, 1999

Frenkel excitations of CN (N=12,60) clusters

S. F. Harlapenko, S. V. Rotkin

The simple Frenkel-exciton model Hamiltonian is applied for calculation of spectrum of electron-hole excitations in carbon nanoclusters. The group-theoretical approach allows to find analytically mode frequencies as well as wavevectors of excitations.

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Mat. Res. Soc. Symp. Proc.
(Symposia BB - Computational and Mathematical
Models of Microstructural Evolution,
Warrendale, PA, USA, 1998)
vol. 529, pp. 175-180, 1998

Energetics of fullerene clusters

S. V. Rotkin, R. A. Suris

A new phenomenological model for calculation of formation energy of carbon nanoclusters of definite shape is proposed. The model uses only three energetic parameters: two first, E_c and ε_5, being determined from comparison with experimental data, results of computer simulation for various carbon nanoclusters, and the last one is the dangling carbon bond energy, E_b. Energies of formation of carbon clusters shaped as a cylinder, a sphere, an icosahedral polyhedron, a capsule were calculated in frame of the unified phenomenological approach, which allows to judge the relative energetic stability of these clusters.

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Mat. Res. Soc. Symp. Proc.
(Symposia BB - Computational and Mathematical
Models of Microstructural Evolution,
Warrendale, PA, USA, 1998)
vol. 529, pp. 169-172, 1998

Self-organization of fullerene clusters

S. V. Rotkin

The paper introduces a plasmon-Frenkel-exciton model [1] for fullerene solids and explains a possible reason for the formation of van-der-Waals C_{60} cluster complexes. The interaction of the cluster and an organic (non-polar) liquid solvent will be considered. The motivation of this interest is related also to experiments on the photoclusterization in the water solution [2] and cluster formation in beams [3].

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Growth of materials and nanostructures

Opt. Express
vol. 23, no. 8, pp. 1703-1713, 2015

Analysis of mirror soft-x-ray–EUV scattering using generalized continuous growth model of multiscale reliefs

L. Goray, M. Lubov

Combined computer simulations of the growth of multilayer mirrors and their exact differential reflection coefficients in the soft-x-ray–EUV range have been conducted. The proposed model describes the variation of the surface roughness of the multilayer Al/Zr mirror boundary profiles taking into account a random noise source. Theoretically calculated Al/Zr boundary profiles allow one to know real rough boundary statistics including rms roughnesses and correlation lengths and, to obtain rigorously EUV specular and diffuse reflection coefficients. The proposed integrated approach opens up a way to performing exact theoretical studies similar in accuracy to results obtained by quantitative microscopy investigations of nanoreliefs and synchrotron radiation measurements.

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Tech. Phys. Lett.
vol. 41, no. 10, pp. 961–963, 2015

Kinetic modeling of the growth of copper clusters of various heights in subsurface layers of lead

D. V. Kulikov, M. N. Lubov, Yu. V. Trushin, V. S. Kharlamov

The growth of subsurface copper clusters of various shapes and heights during the deposition of copper onto lead has been studied by kinetic modeling. The heights and radii of clusters have been calculated. Based on a comparison with experimental data, it is established that significant differences in the heights of clusters possessing different shapes are determined by the specific elastic energy of the copper cluster–lead interface.

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Bull. Russ. Acad. Sci. Phys.
vol. 78, no. 6, pp. 481–484, 2014

Kinetic simulation of the 3D growth of subsurface impurity nanoclusters during cobalt deposition onto a copper surface

M. N. Lubov, D. V. Kulikov, O. Kurnosikov, Yu. V. Trushin

A physical model of the 3D growth of a subsurface cobalt cluster during the epitaxy of cobalt atoms on a copper substrate is developed. Time dependences are established for the cobalt cluster radius and height.

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J. Surf. Invest.: X-Ray, Synchrotron Neutron Tech.
vol. 8, no. 3, pp. 444-455, 2014

Nonlinear continual growth model of nonuniformly scaled reliefs as applied to the rigorous analysis of the X-ray scattering intensity of multilayer mirrors and gratings

L. Goray, M. Lubov

It is revealed that certain terms entering into the nonlinear continual equation describing thin-film growth enable its application to the simulation of the surfaces of multilayer mirrors and gratings with a large height and/or jumps of boundary-profile gradients. The proposed model characterizes both variations in the power spectral-density function of the surface of Al/Zr multilayer mirrors and the smoothing and shift of the boundaries of Mo/Si and Al/Zr gratings grown on Si substrates with triangular groove profiles by means of magnetron and ion-beam deposition. Rigorous calculations indicate that the intensities of diffuse X-ray scattering by Au mirrors, which have similar boundary profiles with Gaussian and exponential autocorrelation functions, differ substantially from each other. Computer simulation of the growth of Mo/Si and Al/Zr multilayer gratings is performed. On the basis of the calculated boundary profiles, the absolute diffraction efficiencies of the Mo/Si and Al/Zr

gratings are found via the integral equation method in the extreme UV region. It is demonstrated that the proposed comprehensive approach to calculations of the boundary profiles and the intensities of short-wavelength scattering from multilayer mirrors and gratings makes it possible to carry out studies comparable in accuracy to measurements based on synchrotron radiation.

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J. Appl. Cryst.
vol. 46, pp. 926-932, 2013

Nonlinear continuum growth model of multiscale reliefs as applied to rigorous analysis of multilayer short-wave scattering intensity. I. Gratings

L. Goray, M. Lubov

It is shown that taking into proper account certain terms in the nonlinear continuum equation of thin-film growth makes it applicable to the simulation of the surface of multilayer gratings with large boundary profile heights and/or gradient jumps. The proposed model describes smoothing and displacement of Mo/Si and Al/Zr boundaries of gratings grown on Si substrates with a blazed groove profile by magnetron sputtering and ion-beam deposition. Computer simulation of the growth of multilayer Mo/Si and Al/Zr gratings has been conducted. Absolute diffraction efficiencies of Mo/Si and Al/Zr gratings in the extreme UV range have been found within the framework of boundary integral equations applied to the calculated boundary profiles. It has been demonstrated that the integrated approach to the calculation of boundary profiles and of the intensity of short-wave scattering by multilayer gratings developed here opens up a way to perform studies comparable in accuracy to measurements with synchrotron radiation, at least for known materials and growth techniques.

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Tech. Phys.
vol. 58, no. 3, pp. 26-30, 2013

Theoretical analysis of impurity precipitation in nanopores in crystals. II: Kinetics of impurity cluster growth in pores

M. N. Lubov, D. V. Kulikov, Yu. V. Trushin, O. Kurnosikov

The kinetics of the formation of impurity clusters in subsurface nanopores in crystals is studied theoretically. A physical model of precipitation of the impurity phase in nanopores in a sample with sinks of various types is developed. This model forms the basis for the calculation of the annealing kinetics of copper containing subsurface pores and cobalt impurity atoms. The optimal annealing conditions are determined in which cobalt atoms diffuse predominantly into pores and form impurity clusters in them.

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Mater. Sci. Forum
vol. 740-742, pp. 393-396, 2013

Kinetic Monte Carlo simulation of impurity effects on nucleation and growth of SiC clusters on Si(100)

M. N. Lubov, J. Pezoldt, Yu. V. Trushin

The influence of attractive and repulsive impurities on the nucleation process of the SiC clusters on Si(100) surface was investigated. Kinetic Monte Carlo simulations of the SiC clusters growth show that that increase of the impurity concentration (both attractive and repulsive) leads to decrease of the mean cluster size and rise of the nucleation density of the clusters.

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Tech. Phys.
vol. 58, no. 1, pp. 46-53, 2013

Theoretical analysis of the formation of impurity precipitates in nanocavities. I. thermodynamic analysis

M. N. Lubov, D. V. Kulikov, Yu. V. Trushin, O. Kurnosikov

The kinetics of the formation of impurity clusters in subsurface nanopores in crystals is studied theoretically. A physical model of precipitation of the impurity phase in nanopores in a sample with sinks of various types is developed. This model forms the basis for the calculation of the annealing kinetics of copper containing subsurface pores and cobalt impurity atoms. The optimal annealing conditions are determined in which cobalt atoms diffuse predominantly into pores and form impurity clusters in them.

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J. Comput. Theor. Nanosci.
vol. 9, pp. 1941–1966, 2012

Multi-scale simulation of nucleation and growth of nanoscale SiC on Si

J. Pezoldt, D. V. Kulikov, V. S. Kharlamov, M. N. Lubov, Yu. V. Trushin

The main obstacle of implementing numerical simulations for the prediction of nucleation and epitaxial growth is the variety of physical processes with a considerable difference in time and spatial scales. During the growth of nanostructures and epitaxy deposition of atoms, surface and bulk diffusion, nucleation of two-dimensional and three-dimensional clusters, transitions from two dimensional to three dimensional growth, stress relaxation occur. Thus, it is challenging to describe all of them in the framework of a single physical model. In the present work a multi-scale simulation of the epitaxial growth of silicon carbide nanostructures on silicon using three numerical methods, namely Molecular Dynamics, kinetic Monte Carlo, and the Rate Equations was implemented. Molecular Dynamics was used for the estimation of kinetic parameters of atoms and stress fields at the surface, which are input

parameters for the other simulation methods. Kinetic Monte Carlo simulations allowed investigating basic nucleation processes and the transition from two dimensional nucleation to three dimensional cluster growth as well as the ordering of nanoclusters. Furthermore the influence of impurities on the nucleation of nanoscale SiC was studied. The energy barriers values obtained in Molecular Dynamics and the physical model used in the rate equation simulations was validated by Kinetic Monte Carlo. The Rate Equation simulation allowed studying the growth process at larger time scales taking into account the surface stress fields. As a result, a full time scale description spanning over a large substrate area of the morphological and structural surface evolution during SiC formation on Si was developed.

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Cryst. Growth Des.
vol. 10, no. 9, pp. 3949-3955, 2010

Stress-driven nucleation of three-dimensional crystal islands: from quantum dots to nanoneedles

V. G. Dubrovskii, N. V. Sibirev, X. Zhang, R. A. Suris

We study theoretically new effects during the stress-driven nucleation of three-dimensional (3D) crystal islands in lattice mismatched material systems. It is shown that the formation enthalpy of a coherent strained 3D island is a function of two independent variables: the base dimension and the aspect ratio. The minimum nucleation barrier relates to a saddle point of formation enthalpy. If the 3D barrier is smaller than the two-dimensional (2D) one, the islands tend to adopt a 3D form with the energetically preferred aspect ratio, which is a function of the lattice mismatch ε0, material constants, and supersaturation. With different approximations for the elastic energy relaxation, we map out the growth diagrams separating the domains of 2D, 3D, and the Stranski−Krastanow (SK) growth. The preferred aspect ratio increases with the lattice mismatch from modest values typical for quantum dots (QDs) at ε_0 ~ 4−12% to very large values of the order of ten at ε_0 = 46%, corresponding to the case of GaAs nanoneedles (NNs) on sapphire. It is shown that the NNs grown in the 111 direction at sufficiently high

supersaturation should adopt the hexagonal wurtzite phase. Overall, the stress-driven nucleation of highly anisotropic islands may offer a new growth mechanism for the fabrication of catalyst-free NNs and nanowires (NWs).

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Phys. Status Solidi C
vol. 7, no. 2, pp. 378–381, 2010

Influence of wurtzite–zinc-blende interfacial energy on growth and crystal phase of the III-V nanowires

M. Lubov, D. Kulikov, Yu. Trushin

Influence of wurtzite–zinc-blende energy on nucleation rate and growth kinetics is studied. The physical model of III-V nanowires growth is proposed. We show that wurtzite–zinc-blende interfacial energy caused formation of the zinc-blende structure on the initial stage of nanowires growth. Role of the fluctuations in quasiperiodic crystal structure formation representing alternating layers of wurtzite and zinc-blende phase is revealed. Calculations of the growth of the nanowire growth accounting fluctuations in the droplet alloy are carried out. The results of the calculations are in a good agreement with available experimental data.

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Phys. Status Solidi C
vol. 7, no. 2, pp. 141– 144, 2010

Designing the Si(100) conversion into SiC(100) by Ge

R. Nader, F. Niebelschütz, D. V. Kulikov, V. S. Kharlamov, Yu. V. Trushin, P. Masri, J. Pezoldt

The deposition of Germanium (Ge) prior to the conversion of Si(100) into 3C-SiC(100) results in changes of the structure and surface morphology of the formed silicon carbide layer. First of all it reduces the thickness of

the 3C-SiC layer grown during the conversion process and therefore the probability of voids formation. Secondly, it increases the nucleation density of the formed 3C-SiC nuclei and therefore, decreases the grain size at Ge coverages below two monolayers. These affect the roughness of the SiC surface positively by modifying the width of the SiC-Si interface. If the Ge coverages exceed two monolayers the structural and morphological properties begin to degrade. Simulated and measured Si, Ge and C SIMS depth profiles in case of depositing 2 ML Ge prior to the conversion of Si(100) into 3C-SiC(100).

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Tech. Phys.
vol. 55, no. 1, pp. 85–91, 2010

Kinetic model of growth of GaAs nanowires

M. N. Lubov, D. V. Kulikov, Yu. V. Trushin

A kinetic model of growth and formation of the crystal structure of gallium arsenide nanowires by molecular beam epitaxy on surfaces activated by Au drops is developed. The thicknesses of alternating layers of cubic and hexagonal phases formed due to fluctuations of the solution composition in the drop are calculated and compared with experimental data.

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Tech. Phys. Lett.
vol. 35, no. 4, pp. 377–379, 2009

Quasi-periodic structures formed in GaAs nanowires activated by gold drops

M. N. Lubov, D. V. Kulikov, Yu. V. Trushin

A physical model that describes the formation of quasi-periodic structures in GaAs nanowires (NWs) growing under gold drops is proposed. Calculations of the growth of these NWs under the molecular

beam epitaxy conditions have been performed with allowance for the fluctuations of gallium concentration in the catalyst drop. The temporal variation of the NW height is determined and the thicknesses of cubic and hexagonal phase layers are calculated, which show good agreement with the available experimental data.

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Tech. Phys. Lett.
vol. 35, no. 2, pp. 99–102, 2009

Computer simulation of the growth of GaAs nanowhiskers with inhomogeneous crystal structures

M. N. Lubov, D. V. Kulikov, Yu. V. Trushin

A physical model is proposed for the growth of GaAs nanowhiskers (NWs) with inhomogeneous crystal structures during the molecular beam epitaxy. Numerical calculations performed using this model give the temporal variation of the growth rate and the height of NWs and indicate the moments of switching from one crystal phase to another. The results of calculations coincide with the available experimental data.

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Tech. Phys. Lett.
vol. 35, no. 1, pp. 57–59, 2009

Computer simulation of the vertical growth of subsurface cobalt nanoclusters in gold

D. V. Kulikov, O. Kurnosikov, M. Sicot, Yu. V. Trushin

The vertical growth of nanodimensional cobalt clusters buried under the surface of a gold substrate has been studied using computer simulation methods with allowance for the interdiffusion of Au and Co atoms and

the fields of elastic stresses generated by cobalt clusters in the gold matrix. The temporal variation of the concentrations of Co and Au atoms in the near-surface layers is described and the characteristic times of gold replacement by cobalt in layers above the buried clusters are determined. The results of simulations are compared to the available experimental data.

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Tech. Phys.
vol. 53, no. 11, pp. 1490–1503, 2008

Study of Si and C adatoms and SiC clusters on the silicon surface by the molecular dynamics method

V. S. Kharlamov, Yu. V. Trushin, E. E. Zhurkin, M. N. Lubov, J. Pezoldt

Individual Si and C adatoms, as well as SiC clusters, on a Si surface are simulated by the molecular dynamics method in the course of investigation of the initial stages of formation of a SiC layer on silicon with the help of molecular beam epitaxy. The potential energy surfaces for Si and C adatoms on the (2×1) reconstructed Si(001) surface and on the nonreconstructed Si(111) surface, as well as on the Si(111) surface with a SiC cluster, are calculated and analyzed. The values of migration barriers for adatoms on these surfaces are calculated. The effect of the SiC cluster on deformation of the surface region of Si(111) and on the migration of adatoms is investigated. The deep minima observed on the potential energy surfaces immediately above a cluster and at its boundaries can trap diffusing adatoms. The distributions of stresses and strains in the silicon lattice under a cluster on the surface are studied and described.

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J. Appl. Phys.
vol. 103, 114904, 2008

**Atomic assembly during ion-beam assisted growth:
Kinetic modeling**

*Yu. V. Trushin, D. V. Kulikov, K. L. Safonov, J. W. Gerlach,
Th. Höche, B. Rauschenbach*

The influence of an additional bombardment with low-energy ions during conventional molecular beam epitaxy deposition is studied. A model is proposed describing the initial growth stages during conventional molecular beam epitaxy and ion-beam assisted molecular beam epitaxy. The additional bombardment with low-energy ions leads to a transformation of the growth mode from island growth to layer-by-layer growth. In the first stages of film growth, the hyperthermal ion bombardment causes an increasing detachment of atoms from the tops of the growing islands. Based on the model, using simulation by the kinetic-equation method, the size distribution function of growing clusters is calculated. The theoretical results are in good agreement with experimental results obtained upon the deposition of GaN films.

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Bull. Russ. Acad. Sci. Phys.
vol. 72, no. 7, pp. 937–940, 2008

**Kinetic equations and nanocrystal growth
in molecular beam epitaxy methods**

Yu. V. Trushin, D. V. Kulikov, K. L. Safonov, B. Rauschenbach

The processes of nucleation and growth of GaN, Ge, and InAs nanoclusters in molecular beam epitaxy (conventional and nitrogen-ion-assisted) have been investigated by computer simulation methods. Physical models are proposed to explain the regularities of nanostructure evolution, depending on the epitaxy conditions. The role of nitrogen-ion irradiation, leading to radical changes in the epitaxial growth regime, is revealed.

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Surf. Sci.
vol. 601, no. 18, pp. 4395–4401, 2007

Diffusion-controlled growth of semiconductor nanowires: Vapor pressure versus high vacuum deposition

V. G. Dubrovskii, N. V. Sibirev, R. A. Suris, G.E. Cirlin, J. C. Harmand, V. M. Ustinov

Theoretical model of nanowire formation is presented, that accounts for the adatom diffusion from the sidewalls and from the substrate surface to the wire top. Exact solution for the adatom diffusion flux from the surface to the wires is analyzed in different growth regimes. It is shown theoretically that, within the range of growth conditions, the growth rate depends on wire radius R approximately as $1/R^2$, which is principally different from the conventional $1/R$ performance. The effect is verified experimentally for the MBE grown GaAs and AlGaAs wires. The dependences of wire length on the drop density, surface temperature and deposition flux during vapor pressure deposition and high vacuum deposition are analyzed and the differences between these two growth techniques are discussed.

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Tech. Phys.
vol. 53, no. 11, pp. 1490–1503, 2008

Computer simulation of coherent island growth in Ge/Si and InAs/GaAs systems

K. L. Safonov, V. G. Dubrovskii, N. V. Sibirev, Yu. V. Trushin

The nucleation and growth of coherent nanodimensional island arrays in the course of molecular beam epitaxy in Ge/Si and InAs/GaAs semiconductor systems have been studied using computer simulation methods. The parameters of nanoisland arrays are determined as functions of the growth conditions (substrate temperature and deposition rate). The results of calculations are compared to the available experimental data.

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Nucl. Instrum. Methods Phys. Res. B
vol. 253, pp. 241–245, 2006

Carbon surface diffusion and SiC nanocluster self-ordering

*J. Pezoldt, Yu. V. Trushin, V. S. Kharlamov, A. A. Schmidt,
V. Cimalla, O. Ambacher*

The process of the spatial ordering of SiC nanoclusters on the step edges on Si surfaces was studied by means of multi-scale computer simulation. The evolution of cluster arrays on an ideal flat surface and surfaces with terraces of various widths was performed by kinetic Monte Carlo (KMC) simulations based on quantitative studies of potential energy surfaces (PES) by molecular dynamics (MD). PES analysis revealed that certain types of steps act as strong trapping centres for both Si and C adatoms stimulating clusters nucleation. Spatial ordering of the SiC nanoclusters at the terrace edges can be achieved if the parameters of the growth process (substrate temperature, carbon flux) and substrate (steps direction and terrace widths) are adjusted to the surface morphology. Temperature ranges for growth regimes with and without formation of cluster chains were determined. Cluster size distributions and the dependence of optimal terrace width for self ordering on the deposition parameters were obtained.

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Semiconductors
vol. 40, no. 9, pp. 1075-1082, 2006

The role of surface diffusion of adatoms in the formation of nanowire crystals

*V. G. Dubrovski, N. V. Sibirev, R. A. Suris, G. E. Cirlin,
V. M. Ustinov, M. Tchernysheva, J. C. Harmand*

A model of the formation of nanowire crystals on surfaces activated by droplets of the catalyst of growth is developed. In the model, the diffusion of adatoms from the surface of the substrate to the lateral surface of the

crystals is taken into account. The exact solution of the diffusion problem for the flow of adatoms from the surface to the nanowire crystals is obtained, and the particular cases of the solution for the short and long diffusion lengths of adatoms, λ_s, are analyzed. A general expression for the length of the nanowire crystals, *L*, in relation to their radius R and to the conditions of growth is derived. The expression is applicable to a large variety of technologies of growth. The theoretical results are compared with the experimental dependences *L(R)* in the range of *R* = 20–250 nm for GaAs nanowire crystals grown by molecular-beam epitaxy on the GaAs (111) V Ga surface activated by Au. It is shown that, in some range of the parameters, the dependence *L(R)* follows the function $1/R^2 ln(\lambda_s/R)$, which is radically different from the classical diffusion dependence *1/R*.

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Mater. Sci. Forum
vol. 527-529, pp. 315-318, 2006

Multi-scale simulation of MBE-grown SiC/Si nanostructures

A. A. Schmidt, Yu. V. Trushin, K. L. Safonov, V. S. Kharlamov, D. V. Kulikov, O. Ambacher, J. Pezoldt

The main obstacle for the implementation of numerical simulation for the prediction of the epitaxial growth is the variety of physical processes with considerable differences in time and spatial scales taking place during epitaxy: deposition of atoms, surface and bulk diffusion, nucleation of two-dimensional and three-dimensional clusters, etc. Thus, it is not possible to describe all of them in the framework of a single physical model. In this work there was developed a multi-scale simulation method for molecular beam epitaxy (MBE) of silicon carbide nanostructures on silicon. Three numerical methods were used in a complex: Molecular Dynamics (MD), kinetic Monte Carlo (KMC), and the Rate Equations (RE). MD was used for the estimation of kinetic parameters of atoms at the surface, which are input parameters for other simulation methods. The KMC allowed the atomic-scale simulation of the cluster formation, which is the initial stage of the SiC growth, while the RE method gave the ability to study the growth process on a longer time scale. As a result, a full-scale description of the surface evolution during SiC formation on Si substrates was developed.

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Materialwiss. Werkstofftech.
vol. 37, no. 11, pp. 929-932, 2006

Simulation of quality of SiC/Si interface during MBE deposition of C on Si

D. V. Kulikov, A. A. Schmidt, S. A. Korolev, F. M. Morales, Th. Stauden, Yu. V. Trushin, J. Pezoldt

In the present paper we simulate the processes accompanying the SiC/Si epitaxial growth. The model suggested describes the formation and growth of voids at SiC/Si interface. These voids are sources of Si atoms for SiC growth. According to the model the size distribution function was obtained being in good agreement with experimental data. The influence of surfactants on the nucleation and growth of SiC nanoislands on Si was studied as well.

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Tech. Phys. Lett.
vol. 32, no. 8, pp. 687–690, 2006

Molecular dynamics study of the diffusion barriers for silicon and carbon adatoms on a Si(111) surface

V. S. Kharlamov, M. N. Lubov, E. E. Zhurkin, Yu. V. Trushin

Barriers for the diffusion of silicon and carbon adatoms on an ideal (nonreconstructed) Si(111) surface and at silicon carbide (SiC) clusters of various sizes occurring on this surface have been determined using molecular dynamics simulations with a many-body Tersoff potential.

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Semiconductors
vol. 40, no. 3, pp. 372-379, 2006

The role of one-dimensional diffusion in a growth model of the surface of a Kossel's crystal

A. M. Boiko, R. A. Suris

The kinetic mechanism of defect formation on a vicinal surface misoriented in two directions, in the case of molecular-beam epitaxy, is studied. These defects are two adatoms stuck together in a potential trench near the step edge. The effects of the surface parameters, as well as growth rate on the probability of defect formation are studied. It is shown that an increase in the misorientation angle of the surface is conducive to a drastic decrease in the number of defects during growth.

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Comput. Mater. Sci.
vol. 33, pp. 375–381, 2005

Growth of three-dimensional SiC clusters on Si modelled by KMC

A. A. Schmidt, V. S. Kharlamov, K. L. Safonov, Yu. V. Trushin, E. E. Zhurkin, V. Cimalla, O. Ambacher, J. Pezoldt

The formation of silicon carbide nanoclusters on silicon substrates by MBE deposition of carbon provides a variety of applications, such as antidot structures, nanowire heterostructures, wave guides and arrays of tips for cold cathode emission. The SiC growth on Si is unusual for semiconductor systems with large lattice mismatch due to the formation of a $Si_{1-x}C_x$ solid solution along with the formation of two-dimensional 3C–SiC, and a subsequent step transforming the two-dimensional (2D) clusters into three-dimensional (3D) clusters for overall stress minimization. At the same time there are strong experimental evidences that under some experimental conditions 2D clusters could exist even at relatively high coverages. To study the transition from the 2D to the 3D cluster during SiC nucleation and growth the kinetic Monte Carlo method was used. Silicon and carbon atoms are allowed to exchange between

the fixed sites of the 3D lattice with the symmetry of the diamond lattice (to simulate the growth of the 3C–SiC polytype mainly observed in growth experiments). The fitting parameters were estimated by means of molecular dynamics simulation as well as by comparing the data obtained with the experimental TEM results. Formation of a three-dimensional clusters and pits in the surface is demonstrated.

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Mater. Sci. Forum
vol. 483-485, pp. 169-172, 2005

Computer simulation of the early stages of nano scale SiC growth on Si

K. L. Safonov, Yu. V. Trushin, O. Ambacher, J. Pezoldt

Solid source molecular beam epitaxy was applied to create silicon carbide nanoclusters on silicon. The island size distribution can be controlled by an appropriate substrate temperature, carbon fluxes and process times. Rate equation computer simulation was applied to simulate the experimental obtained nano scale nuclei properties.

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Tech. Phys. Lett.
vol. 30, no. 8, pp. 641–643, 2004

Initial stages of the MBE growth of silicon carbide nanoclusters on a silicon substrate

Yu. V. Trushin, E. E. Zhurkin, K. L. Safonov, A. A. Schmidt,
V. S. Kharlamov, S. A. Korolev, M. N. Lubov, J. Pezoldt

The growth of silicon carbide (SiC) nanoclusters by molecular beam epitaxy on silicon substrates has been studied using a combination of experimental and theoretical methods. The first results concerning the initial stages of this growth are presented.

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Proc. SPIE
vol. 5131, pp. 51-55, 2004

Molecular dynamics study of diffusion barriers of Si and C adatoms on Si surfaces

V. S. Kharlamov, M. N. Lubov, J. Pezoldt, Yu. V. Trushin, E. E. Zhurkin

Diffusion of Si and C adatoms on Si surface play very important role in the process of SiC film formation by Molecular Beam Epitaxy with deposition of carbon atoms on silicon substrate. Nowadays the reliable measurements of surface diffusion and initial stages of nanofilm growth on the Si substrates are rare. Theoretical studies in frames of various ab initio techniques are restricted and cover only limited set of simple phenomena like single adatom absorption and diffusion on perfect surfaces. In the present work we used atomic scale modeling in frame of classical molecular dynamics (MD) method in order to calculate diffusion barriers of Si and C adatoms on Si(100) 2x1 reconstructed and Si(111) surfaces. Tersoff potential was used in the MD code for interatomic interactions description in the Si-C system. Diffusion barriers were studied by means of Potential Energy Surface calculation for Si and Cadatoms. Calculated diffusion barriers values were compared with available experimental data and data of ab initio simulations.

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Int. J. Nanosci.
vol. 03, no. 1-2, pp. 29-37, 2004

Second nearest neighbors interaction and equilibrium shape of steps on Kossel crystal vicinal surface

V. B. Korsakov, R. A. Suris

The structure of monoatomic steps on (001)-vicinal surface of Kossel crystal is investigated theoretically. We consider all step directions except for relatively small vicinities of <10>-directions. The structure of such steps at sufficiently low temperature is shown to be controlled only by interaction between second nearest neighbors. If this interaction is repulsive, steps have saw-like shape, while attractive interaction leads to straightening of steps. More general case of nonpairwise interactions is also considered.

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Russ. J. Phys. Chem.
vol. 77, pp. S149-S153, 2003

Kinetics of nucleation at low supersaturations

V. B. Korsakov, R. A. Suris

The kinetics of the nucleation of a weakly supersaturated vapor into a condensed phase in two and three-dimensional space was studied. At low supersaturations, the decrease in the supersaturation around nuclei becomes low enough to make the nucleation rate vanishingly small, thereby rendering the average-concentration model incorrect. A depletion zone model was used to derive analytical expressions for the main characteristics of the nucleation process.

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Proc. SPIE
vol. 5127, pp. 128-131, 2003

Influence of the growth temperature on SiC nanocluster nucleation on Si(111) surface during MBE process

K. L. Safonov, D. V. Kulikov, Yu. V. Trushin, J. Pezold

Rate equations approach of computer simulation has been applied to investigate the SiC clusters nucleation and growth on Si surface during molecular beam epitaxy. Cluster surface densities have been obtained for a range of temperatures. The temperature influence on the consequent clusters density, including the surface phase transition (which occurs with simultaneous structure reconstruction), has been determined. The results obtained by the application of the suggested physical model have appeared to be in the reasonable agreement with experimental data.

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Mater. Sci. Forum
vol. 433-436, pp. 591-594, 2003

Modelling the formation of nano-sized SiC on Si

*K. L. Safonov, A. A. Schmidt, Yu. V. Trushin, D. V. Kulikov,
V. Cimalla, J. Pezoldt*

Silicon carbide nano-clusters have some promising specific properties for micro- and optoelectronics. In this work the SiC clusters formation and the growth on the silicon (111) surface during molecular beam epitaxy (MBE) have been investigated theoretically with implementation of the rate equations simulation model. The model was successfully applied to obtain the temperature dependence of the cluster concentration. The results were compared with the experimental data. Furthermore, influence of the surface reconstruction transition (7×7) → (1×1) on the temperature concentration dependence was investigated.

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Proc. SPIE
vol. 5023, pp. 23-26, 2003

Nanostructures in porous substrate for mismatched film technology and lateral growth model

*A.V. Bobyl, S.G. Konnikov, D.V. Shantsev,
A.A. Sitnikova, R.A. Suris, V.P. Ulin*

A porous GaAs (100) substrate was prepared with nanoscale (5 - 20 nm) surface roughness, 108 cm^{-2} density of nanoscale inlet holes at the surface, and a network of pores (20 - 100 nm) along [111] on the 50 - 100 nm depth. The lattice misfit of the heterostructure GaSb/GaAs with the porous substrate was 22% less than that for the same rigid substrate. The structure of pores is discussed in connection with possible electrochemical processes of pore formation in A_3B_5 materials. The initial stage of growth has been analyzed assuming a strain dependence of the lateral growth rate at the side film/pore interface. This dependence accounts for the formation of bridges over the pores followed by a

smooth growth of continuous film. Using a strain distribution calculated for a model heterostructure of two mismatched layers with pores we estimated the dynamics of bridging and evolution of the crystallization front.

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Phys. Rev. B
Vol. 66, 195408, 2002

Atomic-scale modeling of cluster-assembled Ni_xAl_{1-x} thin films

M. Hou, V. S. Kharlamov, E. E. Zhurkin

Thermodynamic and structural properties of Ni-Al cluster assembled materials are investigated at the atomic scale. Model predictions are available for elemental systems but the field of bimetallic nanostructured systems remains close to unexplored. The aim of the present work is to model at the atomic scale the structural and segregation properties in the Ni_xAl_{1-x} bimetallic cluster assembled materials that are synthesized in two different ways. In the first, isolated clusters are compacted at high pressure. We consider the $L1_2$ and B2 phases of the initial free clusters. Compaction of clusters at thermodynamic equilibrium is modeled by classical molecular dynamics combining isobaric and isothermal schemes. After compaction, interface segregation is computed by Metropolis Monte Carlo importance sampling in the semigrand canonical ensemble. After this model treatment, clusters are found to keep their identity, and their structural and segregation states do not differ much from those in the initial free clusters. The cluster cores keep the stable bulk phases while segregation may take place at the interfaces. The second method is low-energy cluster beam deposition. Cluster impact is found to influence chemical and structural order in the films formed. This is shown and discussed on the example of $L1_2$ cluster deposition. Molecular dynamics is used therefore, which accounts for electron-phonon coupling in the equations of motion. The slowing down of a single cluster is examined in detail. It is found that the epitaxial accommodation of the cluster with the substrate and chemical order in the cluster depend on the mechanical properties of the substrate material. Competition between chemical order and epitaxy is observed.

The harder the material, the higher the epitaxy and the lower the chemical order. The cluster impact induces significant chemical disorder but the clusters forming the cluster assembled film keep their initial identities. Similarly to the sample obtained by compaction, this one displays partial structural and chemical order at its interfaces. The film density is particularly low and the open volumes form a fully interconnected network of pores.

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Nucl. Instrum. Methods Phys. Res. B
vol. 193, pp. 538–543, 2002

Atomic scale modelling of nanosize Ni3Al cluster beam deposition on Al, Ni and Ni3Al (111) surfaces

V. S. Kharlamov, E. E. Zhurkin, M. Hou

The slowing down of Ni_3Al clusters on a Al, Ni and Ni_3Al (111) surfaces is studied by atomic scale modelling. The semi-grand canonical metropolis Monte Carlo is used for the preparation of isolated clusters at thermodynamic equilibrium. The cluster deposition on the surface is studied in detail by classical Molecular Dynamics simulations that include a model to account for electron–phonon coupling. Long- and short-range orders in the cluster are evaluated as functions of temperature in an impact energy range between 0 and 1.5 eV/atom.
The interaction between the Ni_3Al cluster and an Al surface is characterised low short range (chemical) disorder. No sizeable epitaxy is found, subsequent to the impact. In contrast, in the case of Ni and Ni_3Al substrates, which are harder materials than aluminium, the chemical disorder is higher and epitaxial accommodation is possible. With these substrates, chemical disorder in the cluster is an increasing function of the impact energy, as well as of temperature when the impact energy is low enough. The cluster epitaxy is enhanced by both the temperature and the impact energy. A direct correlation between epitaxy and chemical disordering is found during the accommodation of the cluster with the surface.

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Semicond. Sci. Technol.
vol. 17, no. 6, pp. 545-550, 2002

Control of density, size and size uniformity of MBE-grown InAs quantum dots by means of substrate misorientation

V. P. Evtikhiev, A. M. Boiko, I. V. Kudryashov, R. A. Suris, A. N. Titkov, V. E. Tokranov

The influence of (001) GaAs substrate misorientation in the [001] direction on the parameters of InAs quantum dot (QD) ensembles has been studied by means of atomic force microscopy. It is shown that terrace patterning on vicinal surfaces permits control over the density, size and size uniformity of InAs QDs during their growth in the Stranski–Krastanow mode. By using the Monte Carlo approach for simulating the surface annealing, it was shown that surface misorientation exhibits a stable tendency towards self-organization of undulate structure.

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Proc. SPIE
vol. 4627, pp. 165-169, 2002

Nucleation of SiC on Si and their relationship to nano-dot formation: II. Theoretical investigation

K. L. Safonov, D. V. Kulikov, Yu. V. Trushin, J. Pezoldt

The processes of SiC clusters growth on Si(111) surface has been investigated theoretically. The SiC cluster formation and growth on Si surface stimulated by deposition of elemental carbon onto Si(111) with molecular beams have been studied by applying the kinetic equations (so-called rate equations) method. The simulated cluster size distribution function obtained within this method appeared to be in reasonable agreement with the experimental data. Obtained cluster capture rates agree with KMC investigations.

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J. Cryst. Growth
vol. 201/202, pp. 1154-1157, 1999

Characteristics of the InAs quantum dots MBE grown on the vicinal GaAs(0 0 1) surfaces misoriented to the [0 1 0] direction

*V. P. Evtikhiev, V. E. Tokranov, A. K. Kryganovskii,
A. M. Boiko, R. A. Suris, A. N. Titkov*

Atomic-force microscopy is used to study InAs quantum dot arrays grown by molecular beam epitaxy on vicinal GaAs(0 0 1) surfaces misoriented to the [0 1 0] direction by 1°, 2°, 4°, and 6°. For a chosen misorientatoin direction, it is shown that the vicinal GaAs(0 0 1) surface is covered with a net of stepped terraces. The condensation of the network of terraces upon increasing of the misorientation angle leads to the suppression of adatom surface diffusion and makes it possible to achieve higher densities and better uniformity of quantum dots arrays.

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Semiconductors
vol. 32, no. 7, pp. 765-769, 1998

Growth of InAs quantum dots on vicinal GaAs(001) surfaces misoriented in the [010] direction

*V. P. Evtikhiev, V. E. Tokranov, A. K. Kryzhanovski,
A. M. Boiko, R. A. Suris, A. N. Titkov*

Atomic-force microscopy (AFM) is used to study InAs quantum-dot structures grown by molecular-beam epitaxy (MBE) on vicinal GaAs(001) surfaces misoriented in the [010] direction by 1, 2, 4, and 6°. It is shown for a chosen misorientation direction that a vicinal GaAs(010) surface is covered with a network of stepped terraces. The thickening of the network of terraces with increasing misorientation angle leads to the suppression of adatom surface diffusion and makes it possible to achieve higher densities and more uniform ensembles of quantum dots, while simultaneously decreasing the probability of their coalescence.

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High-temperature superconductivity

JETP
vol. 105, no. 1, pp. 246-249, 2007

Nonlinear microwave properties of $YBa_2Cu_3O_{7-x}$ block epitaxial films near the superconducting transition temperature

S. V Baryshev, A. V. Bobyl, V. V. Kurin, R. A. Suris

The structure and local properties of a nonlinear microwave response of $YBa_2Cu_3O_{7-x}$ block films, as well as microbridges of these films, are studied using low-temperature scanning microscopy. Correlation between the halfwidth of the temperature dependence of the third harmonic power W TH and the curve of the electron-beam induced voltage W EBIV is observed for the medium size of the block. A theoretical model is proposed, which demonstrates that the nonlinear microwave response for large blocks is determined by intrablock pinning of Abrikosov vortices; for blocks of smaller size, the response acquires an additional contribution associated with pinning of hypervortices on the Josephson network of the boundaries between the blocks.

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Phys. Rev. B
vol. 74, 220511(R), 2006

Collapse of the critical state in superconducting niobium

R. Prozorov, D. V. Shantsev, R. G. Mints

Giant abrupt changes in the magnetic-flux distribution in niobium foils were studied by using magnetooptical visualization, thermal, and magnetic measurements. Uniform flux jumps and sometimes almost total catastrophic collapse of the critical state are reported. Results are discussed in terms of thermomagnetic instability mechanism with different development scenarios.

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Phys. Rev. Lett.
vol. 97, 077002, 2006

Onset of dendritic flux avalanches in superconducting films

D. V. Denisov, D. V. Shantsev, Y. M. Galperin, E.-M. Choi, H.-S. Lee, S.-I. Lee, A. V. Bobyl, P. E. Goa, A. A. F. Olsen, T. H. Johansen

We report a detailed comparison of experimental data and theoretical predictions for the dendritic flux instability, believed to be a generic behavior of type-II superconducting films. It is shown that a thermomagnetic model published very recently [Phys. Rev. B 73, 014512 (2006)] gives an excellent quantitative description of key features like the stability onset (first dendrite appearance) magnetic field, and how the onset field depends on both temperature and sample size. The measurements were made using magneto-optical imaging on a series of different strip-shaped samples of MgB_2. Excellent agreement is also obtained by reanalyzing data previously published for Nb.

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Phys. Solid State
vol. 48, no. 12, pp. 2260-2269, 2006

Effect of the microstructure of epitaxial $YBa_2Cu_3O_{7-x}$ films on their electrophysical and nonlinear microwave properties

Yu. N. Nozdrin, E. E. Pestov, V. V. Kurin, S. V. Baryshev, A. V. Bobyl', S. F. Karmanenko, D. A. Sakseev, R. A. Suris

The local nonlinear microwave response of $YBa_2Cu_3O_{7-x}$ films was measured by near-zone field microscopy with a spatial resolution of 50 μm, and $YBa_2Cu_3O_{7-x}$ film microbridges were locally studied by low-temperature scanning microscopy with a spatial resolution of 4 μm. The microstructure of epitaxial $YBa_2Cu_3O_{7-x}$ films was examined using x-ray diffraction and electron microscopy. A correlation is detected between the average crystallite size and the half-widths of the temperature

dependences of the third-harmonic power (W_{TH}) and the electron-beam-induced voltage (W_{EBIV}). The experimental results are described in terms of a model of a two-phase medium taking into account the nonlinear *I-V* characteristic of the superconductor. For large crystallites, the nonlinear microwave response is shown to be caused by intracrystallite vortex pinning. As the average crystallite size decreases, an additional contribution to the nonlinear response appears due to the pinning of a magnetic flux by the Josephson network of crystallite boundaries. Calculations show that a three-fold increase in the crystallite size decreases the nonlinearity coefficient of $YBa_2Cu_3O_{7-x}$ films by two orders of magnitude.

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Phys. Rev. Lett.
vol. 96, 097009, 2006

Non-Gaussian low-frequency noise as a source of qubit decoherence

Y. M. Galperin, B. L. Altshuler, J. Bergli, D. V. Shantsev

We study decoherence in a qubit with the distance between the two levels affected by random flips of bistable fluctuators. For the case of a single fluctuator we evaluate explicitly an exact expression for the phase-memory decay in the echo experiment with a resonant ac excitation. The echo signal as a function of time shows a sequence of plateaus. The position and the height of the plateaus can be used to extract the fluctuator switching rate γ and its coupling strength v. At small times the logarithm of the echo signal is ~ t^3. The plateaus disappear when the decoherence is induced by many fluctuators. In this case the echo signal depends on the distribution of the fluctuators parameters. According to our analysis, the results significantly deviate from those obtained in the Gaussian model as soon as $v \geq \gamma$.

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Phys. Rev. B
vol. 73, 014512, 2006

Dendritic and uniform flux jumps in superconducting films

D. V. Denisov, A. L. Rakhmanov, D. V. Shantsev,
Y. M. Galperin, T. H. Johansen

Recent theoretical analysis of spatially-nonuniform modes of the thermomagnetic instability in superconductors [Phys. Rev. B 70, 224502 (2004)] is generalized to the case of a thin film in a perpendicular applied field. We solve the thermal diffusion and Maxwell equations taking into account nonlocal electrodynamics in the film and its thermal coupling to the substrate. The instability is found to develop in a nonuniform, fingering pattern if the background electric field, E, is high and the heat transfer coefficient to the substrate, h_0, is small. Otherwise, the instability develops in a uniform manner. We find the threshold magnetic field, $H_{fing}(E,h_0)$, the characteristic finger width, and the instability buildup time. Thin films are found to be much more unstable than bulk superconductors, and have a stronger tendency for formation of fingering (dendritic) pattern.

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Phys. Rev. B
vol. 72, 024541, 2005

Size of flux jumps in superconducting films

D. V. Shantsev, A. V. Bobyl, Y. M. Galperin, T. H. Johansen, S. I. Lee

Magneto-optical imaging is used to visualize vortex avalanches in MgB_2 films at 4 K. Avalanches ranging from 50 to 50 000 vortices were detected. The size distribution function has a clear peak whose position moves towards larger sizes as the applied field increases. This field dependence as well as variation of flux density profile during an avalanche is well described by a proposed model assuming a thermal origin of the avalanches. The model is based on the adiabatic approach and takes into account nonlocal electrodynamics in thin

superconductors. The threshold field for thermal avalanches is predicted to be much smaller than that for thick superconductors, in agreement with the experiment.

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Europhys. Lett.
vol. 71, pp. 21-27, 2005

Rabi oscillations of a qubit coupled to a two-level system

Y. M. Galperin, D. V. Shantsev, J. Bergli, B. L. Altshuler

The problem of Rabi oscillations in a qubit coupled to a fluctuator and in contact with a heath bath is considered. A scheme is developed for taking into account both phase and energy relaxation in a phenomenological way, while taking full account of the quantum dynamics of the four-level system subject to a driving AC field. Significant suppression of the Rabi oscillations is found when the qubit and fluctuator are close to resonance. The effect of the fluctuator state on the read-out signal is discussed. This effect is shown to modify the observed signal significantly. This may be relevant to recent experiments by Simmonds et al. (Phys. Rev. Lett., 93 (2004) 077003).

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Appl. Phys. Lett.
vol. 87, 042502, 2005

**Avalanche-driven fractal flux distributions
in NbN superconducting films**

I. A. Rudnev, D. V. Shantsev, T. H. Johansen, A. E. Primenko

Flux distributions in thin superconducting NbN films placed in a perpendicular magnetic field have been studied using magneto-optical imaging. Below 5.5 K the flux penetrates in the form of abrupt avalanches resulting in dendritic structures. Magnetization curves in this

regime exhibit extremely noisy behavior. Stability is restored both above a threshold temperature *T** and applied field *H** , where *H** is smaller for increasing field than during descent. The dendrite size and morphology are strongly *T* dependent, and fractal analysis of the first dendrites entering into a virgin film shows that dendrites formed at higher *T* have larger fractal dimension.

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Phys. Rev. B
vol. 70, 224502, 2004

Finger patterns produced by thermomagnetic instability in superconductors

A. L. Rakhmanov, D. V. Shantsev, Y. M. Galperin, T. H. Johansen

A linear analysis of thermal diffusion and Maxwell equations is applied to study the thermomagnetic instability in a type-II superconducting slab. It is shown that the instability can lead to formation of spatially nonuniform distributions of magnetic field and temperature. The distributions acquire a finger structure with fingers perpendicular to the screening current direction. We derive the criterion for the instability, and estimate its build-up time and characteristic finger width. The fingering instability emerges when the background electric field is larger than a threshold field, $E>E_c$, and the applied magnetic field exceeds a value $H_{fing} \sim 1/\sqrt{E}$. Numerical simulations support the analytical results, and allow us to follow the development of the fingering instability beyond the linear regime. The fingering instability may be responsible for the nucleation of dendritic flux patterns observed in superconducting films using magneto-optical imaging.

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NATO Science Series II
v.142 (Magneto-Optical Imaging)
pp. 223-228, 2004

Flux jumps in magnesium diboride

D. V. Shantsev, P. E. Goa, F. L. Barkov, A. V. Bobyl,
T. H. Johansen, W. N. Kang, S. I. Lee, M. Kühberger,
G. Gritzner, M. Roussel, S. X. Dou

Magneto-optical imaging was used to study flux penetration into MgB_2 films in a slowly increasing perpendicular applied field. A variety of flux jumps and avalanches have been observed at temperatures below 10 K. At small fields, jumps with typical size of 20 μm and regular shape occur at random locations along the flux front. Above some threshold field of 2–10 mT, big dendritic jumps with dimensions comparable to the sample size (mm scale) take place. The jumps are developing extremely fast, result in highly-branching irreproducible flux patterns, and effectively suppress the apparent critical current. Both types of jumps are believed to result from thermo-magnetic instability.

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NATO Science Series II
v.142 (Magneto-Optical Imaging)
pp. 205-214, 2004

Flux dynamics in current-carrying superconductors

A. V. Bobyl, T. H. Johansen, D. V. Shantsev

PC controlled setup for magneto- optical (MO) investigations of current-carrying superconducting films was developed. It included a current pulse circuit synchronized with the microscope and PC software for image processing allowing us to determine field distributions across superconducting strip using spatially-dependent calibration and iterative inversion to find current distributions. We study these distributions during and after a current pulse, with and without applied magnetic field, current re-distribution during the pulse, precursors to strip burn-out at high

currents, and dendritic instability triggered by the pulse. We find critical-state behaviour accompanied by slow creep of magnetic flux at moderate currents in YBCO films, and fast avalanches related to heating effects at higher currents in YBCO and MgB_2.

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Cryogenics
vol. 43, pp. 663-666, 2003

Dendritic flux avalanches in superconducting Nb_3Sn films

I. A. Rudnev, S. V. Antonenko, D. V. Shantsev,
T. H. Johansen, A. E. Primenko

The penetration of magnetic flux into a thin superconducting film of Nb_3Sn with critical temperature 17.8 K and critical current density 6 MA/cm^2 was visualized using magneto-optical imaging. Below 8 K an avalanche-like flux penetration in form of big and branching dendritic structures was observed in response to increasing perpendicular applied field. When a growing dendritic branch meets a linear defect in the film, several scenarios were observed: the branch can turn and propagate along the defect, continue propagation right through it, or ‘‘tunnel’’ along a flux-filled defect and continue growth from its other end. The avalanches manifest themselves in numerous small and random jumps found in the magnetization curve.

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Supercond. Sci. Technol.
Vol. 16, pp. 1109-1114, 2003

Magnetostrictive behaviour of thin superconducting disks

T. H. Johansen, D. V. Shantsev

Flux-pinning-induced stress and strain distributions in a thin disk superconductor in a perpendicular magnetic field are analysed. We

calculate the body forces, solve the magneto-elastic problem and derive formulae for all stress and strain components, including the magnetostriction $\Delta R/R$. The flux and current density profiles in the disk are assumed to follow the Bean model. During a cycle of the applied field the maximum tensile stress is found to occur approximately midway between the maximum field and the remanent state. An effective relationship between this overall maximum stress and the peak field is found.

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Supercond. Sci. Technol.
Vol. 16, pp. 566-570, 2003

Interplay of dendritic avalanches and gradual flux penetration in superconducting MgB2 films

D. V. Shantsev, P. E. Goa, F. L. Barkov, T. H. Johansen, W. N. Kang, S. I. Lee

Magneto-optical imaging was used to study a zero-field-cooled MgB_2 film at 9.6 K where in a slowly increasing field the flux penetrates by an abrupt formation of large dendritic structures. Simultaneously, a gradual flux penetration takes place, eventually covering the dendrites, and a detailed analysis of this process is reported. We find an anomalously high gradient of the flux density across a dendrite branch, and a peak value that decreases as the applied field increases. This unexpected behaviour is reproduced by flux creep simulations based on the non-local field–current relation in the perpendicular geometry. The simulations also provide indirect evidence that flux dendrites are formed at an elevated local temperature, consistent with a thermo-magnetic mechanism of the instability.

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Phys. Rev. B
vol. 67, 064513, 2003

Local threshold field for dendritic instability in superconducting MgB_2 films

F. L. Barkov, D. V. Shantsev, T. H. Johansen, P. E. Goa, W. N. Kang, H. J. Kim, E. M. Choi, S. I. Lee

Using magneto-optical imaging the phenomenon of dendritic flux penetration in superconducting films was studied. Flux dendrites were abruptly formed in a 300-nm-thick film of MgB_2 by applying a perpendicular magnetic field. Detailed measurements of flux density distributions show that there exists a local threshold field controlling the nucleation and termination of the dendritic growth. At 4 K the local threshold field is close to 12 mT in this sample, where the critical current density is 10^7 A/cm^2. The dendritic instability in thin films is believed to be of thermomagnetic origin, but the existence of a *local* threshold field and its small value are features that distinctly contrast with the thermomagnetic instability (flux jumps) in bulk superconductors

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Europhys. Lett.
vol. 59, no. 4, pp. 599-605, 2002

Dendritic magnetic instability in superconducting MgB_2 films

T. H. Johansen, M. Baziljevich, D. V. Shantsev, P. E. Goa, Y. M. Galperin, W. N. Kang, H. J. Kim, E. M. Choi, M.-S. Kim, S. I. Lee

Magneto-optical imaging reveal that below 10 K the penetration of magnetic flux in MgB_2 films is dominated by dendritic structures abruptly formed in response to an applied field. The dendrites show a temperature-dependent morphology ranging from quasi-1D at 4 K to large tree-like structures near 10 K. This behaviour is responsible for the

anomalous noise found in magnetization curves, and strongly suppresses the apparent critical current. The instability is of thermomagnetic origin, as supported by our simulations of vortex dynamics reproducing the variety of dendritic flux patterns.

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Appl. Phys. Lett.
vol. 80, pp. 4588-4590, 2002

Current-induced dendritic magnetic instability in superconducting MgB_2 films

A. V. Bobyl, D. V. Shantsev, T. H. Johansen, W. N. Kang, H. J. Kim, E. M. Choi, S. I. Lee

Magneto-optical imaging reveals that in superconducting films of MgB_2 a pulse of transport current creates avalanche-like flux dynamics where highly branching dendritic patterns are formed. The instability is triggered when the current exceeds a threshold value, and the superconductor, shaped as a long strip, is initially in the critical state. The instability exists up to 19 K, which is a much wider temperature range than in previous experiments, where dendrites were formed by a slowly varying magnetic field. The instability is believed to be of thermomagnetic origin indicating that thermal stabilization may become crucial in applications of MgB_2 .

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Phys. Rev. B
vol. 65, 184512, 2002

Scaling and exact solutions for the flux creep problem in a slab superconductor

D. V. Shantsev, Y. M. Galperin, T. H. Johansen

The flux creep problem for a superconductor slab placed in a constant or time-dependent magnetic field is considered. Logarithmic dependence of

the activation energy on the current density is assumed, $U=U_0 ln(J/J_c)$, with a field dependent J_c . The density B of the magnetic flux penetrating into the superconductor is shown to obey a scaling law, i.e., the profiles *B(x)* at different times *t* can be scaled to a function of a single variable x/t^b . We found exact solution for the scaling function in some specific cases, and an approximate solution for a general case. The scaling also holds for a slab carrying transport current *I* resulting in a voltage $V\sim I^p$, where *p~1*. When the flux fronts moving from two sides of the slab collapse at the center, the scaling is broken and *V(I)* crosses over to $V\sim I^{U0/kT}$.

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Supercond. Sci. Technol.
vol. 15, pp. 82-89, 2002

Relaxation of transport current distribution in a YBaCuO strip studied by magneto-optical imaging

A. V. Bobyl, D. V. Shantsev, Y. M. Galperin, T. H. Johansen, M. Baziljevich, S. F. Karmanenko

The dynamics of magnetic flux distributions across a $YBa_2Cu_3O_{7-\delta}$ strip carrying transport current is measured using magneto-optical imaging at 20 K. The current is applied in pulses of 40–5000 ms duration and of magnitude close to the critical one, 5.5 A. During the pulse some extra flux usually penetrates the strip, so the local field increases in magnitude. When the strip is initially penetrated by flux, the local field either increases or decreases depending on both the spatial coordinate and the current magnitude. Meanwhile, the current density always tends to redistribute more uniformly. Despite the relaxation, all distributions remain qualitatively similar to the Bean-model predictions.

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Physica C
vol. 372-376, pp. 508-510, 2002

The ferrite/superconductor layered structure for tunable microwave device

*A. Bobyl, R. Suris, S. Karmanenko, A. Semenov,
A. Melkov, S. Konuhov, A. Olshevski*

The ferrite/superconductor (FS) structure composed from the separate ferrite garnet $Y_3Fe_5O_{12}$ epitaxial layers and superconducting films was used for development of such microwave devices as tunable pass-band filter, phase-shifter and delay line. Application of superconducting layer decreases the microwave losses and it provides new functions of magnetostatic waveguide FS structures. The central frequency of band-pass filter is tuned from 1.5 up to 3 GHz; bandwidth can be regulated by the geometry of antenna transducers (from 30 up to 300 MHz); band insertion loss is about 1.5–3 dB.

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Tech. Phys.
vol .46, no. 10, pp. 1218-1224, 2001

The propagation of magnetostatic surface waves in ferrite/superconductor structures

*A. A Semenov, S. F. Karmanenko, A. A. Melkov, A. V. Bobyl,
R. A. Suris, Y. M. Gal`perin, T. H. Johansen*

An electrodynamic model that describes the dispersion of magnetostatic surface waves in ferrite/superconductor structures is suggested. On its basis, a new approach to determining the microwave sheet resistance R_S of superconducting films in a magnetic field is elaborated. The values calculated (R_S =0.20–0.96 mΩ) agree with results obtained by the Tauber method. For YIG/YBCO structures, the controllable phase shift is about 1.5π when the depth of magnetostatic wave penetration into the YBCO film varies from 2.0 to 0.8 μm.

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Phys. Rev. B
vol. 63, 184510, 2001

Symmetry of the remanent state flux distribution in superconducting thin strips: Probing the critical state

A. V. Bobyl, D. V. Shantsev, Y. M. Galperin, T. H. Johansen

The critical-state in a thin strip of $YBa_2Cu_3O_{7-\delta}$ is studied by magneto-optical imaging. The distribution of magnetic flux density is shown to have a specific symmetry in the remanent state after a large applied field. The symmetry was predicted [Phys. Rev. Lett. 82, 2947 (1999)] for any $j_c(B)$, and is therefore suggested as a simple tool to verify the applicability of the critical-state model. At large temperatures we find deviations from this symmetry, which demonstrates a departure from the critical-state behavior. The observed deviations can be attributed to an explicit coordinate dependence of j_c since both a surface barrier and flux creep would break the symmetry in a different way.

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Phys. Rev. B
vol. 61, pp. 9699-9706, 2000

Thin superconducting disk with field-dependent critical current: Magnetization and ac susceptibilities

D. V. Shantsev, Y. M. Galperin, T. H. Johansen

Magnetization hysteresis loops and the ac susceptibility $\chi=\chi'+i\chi''$ of a superconducting thin disk are calculated in the critical-state model assuming a field-dependent critical current density $J_c(B)$. The results are obtained by solving numerically the set of coupled integral equations for the flux and current distributions [Phys. Rev. B 60, 13112 (1999)] for a disk placed in a perpendicular applied field B_a . From the magnetization curves the range of fields where the vertical width of the loop $\Delta M(B_a)$ relates directly to $J_c(B_a)$ is determined. The susceptibility is analyzed in the limits of small and large ac-field amplitudes B_{am}, and also as a parametric relation $\chi''(\chi')$. Comparing our results with experimental data

for $\chi''(\chi')$ shows that by taking the B dependence of J_c into account the agreement improves dramatically, in particular at small $|\chi|$ (large field amplitudes). We show that the asymptotic behavior for large B_{am} changes from $\chi' \sim B_{am}^{-3/2}$ and $\chi'' \sim B_{am}^{-1}$ for the Bean model, to $\chi' \sim B_{am}^{-3}$ and $\chi'' \sim B_{am}^{-2}$ for J_c decreasing with $|B|$ as $|B|^{-1}$ or faster. For small B_{am} the behavior can always be described by an effective Bean model with a renormalized J_c . We also find that in the $\chi''(\chi')$ plot the peak of χ'' increases in magnitude and shifts towards $\chi'=0$ when J_c decreases with $|B|$. This allows an easy experimental discrimination between a Bean model behavior, one with $J_c(B)$, and one where flux creep is an ingredient.

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Supercond. Sci. Technol.
vol. 13, no. 3, pp. 273-286, 2000

Fabrication process and noise properties of antenna-coupled microbolometers based on superconducting YBCO films

S. F. Karmanenko, A. A. Semenov, I. A. Khrebtov, V. N. Leonov, T. H. Johansen, Yu. M. Galperin, A. V. Bobyl, A. I. Dedoboretz, M. E. Gaevski, A. V. Lunev, R. A. Suris

An analysis of how the detectivity and lifetime depend on the fabrication process of superconducting antenna-coupled microbolometers has been carried out. The temperature dependences of responsivity and noise equivalent power (NEP) have been estimated in terms of the thermal model. To reveal the main degradation mechanism, *1/f*-noise characterization has been used. Monte-Carlo simulation of the annealing procedure of $YBa_2Cu_3O_7$ (YBCO) films for the operating ranges of frequency and temperature has shown that prevailing sources of flicker noise in superconducting microstrips are associated with transitions of oxygen atoms situated close to low-angle boundaries of the film blocks. The magnetron sputtering technique has been optimized to reduce the Hooge parameter for flicker noise to a record-breaking low value for YBCO films of about 10^{-4} at 93 K. Comparative analysis of chemical, ion and laser etching techniques by low-temperature scanning electron microscopy and magneto-optics allowed the fabrication of microstrips

with uniform current distribution characterized by critical current density higher than 10^6 A cm^{-2} at 77 K and long-time stability. The process of low-energy ion milling of YBCO films with an Ar^+ beam generated in a duopigatron ion source was used to reach a width resolution at the topology edge better than 0.2 μm. The antenna-coupled bolometers fabricated from the superconducting microstrips were used to register microwave radiation at a frequency of 70.3 GHz and temperature of 93 K. It is demonstrated that the developed technology makes possible the fabrication of long-lived YBCO-based antenna microbolometers with electrical $NEP_e = 1.5 \times 10^{-12}$ $W\ Hz^{-1/2}$. The calculated response time of the antenna is about 30-150 ns. Further development is associated with fabrication of coupling microbolometers with immersed lens, with predicted optical detectivity $D^* = (4 \times 10^9 - 4 \times 10^{10}$) cm $Hz^{1/2}\ W^{-1}$ in the wavelength range 100-1000 μm.

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Physica C
vol. 341-348, pp. 1145-1146, 2000

Comparison of two methods for analysis of vortex motion: flux creep versus nonlinear current-voltage curve approach

D. V. Shantsev, A. V. Bobyl, Y. M. Galperin, T. H. Johansen

We compare two commonly accepted approaches for simulations of thermally-activated vortex motion in superconductors. The flux creep approach is based on the expression $E=vB$ for the electric field via the local flux density and the velocity of the thermally-activated flux motion. The other approach employs a phenomenological nonlinear current-voltage curve, $E(j)$. Our numerical simulations show that the two approaches give similar but clearly different results, the difference being most pronounced in the areas of low B. We find that the flux creep approach provides a better description of the experimental current distributions in a YBaCuO current-carrying strip determined by magneto-optical imaging.

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Physica C
vol. 341-348, pp. 1443-1444, 2000

The low-field peak in magnetization loops of uniform and granular superconductors in perpendicular magnetic fields

T. H. Johansen, D. V. Shantsev, M. R. Koblischka,
Y. M. Galperin, P. Nalevka, and M. Jirsa

The present work aims to explain the anomalous position of the low-field peak in magnetization loops in Bi-2223 tapes, where the peak is often seen shifted to a positive field on the descending field branch. We prove theoretically that for an infinitely thin and long strip placed in a perdendicular field, the central peak occurs exactly at 0 *T*, for any function $J_c(B)$. This general result is shown to be in excellent agreement with experimental data. After introducing granularity in such a film into a lattice of small weakly-overlapping disks, the peak becomes shifted to positive values. We conclude that this anomalous behaviour in the magnetization is a definite signature of granularity.

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Supercond. Sci. Technol.
vol. 13, no. 2, pp. 183-186, 2000

Temperature dependence of filament coupling in Bi-2223 tapes: Magneto-optical study

A. V. Bobyl, D. V. Shantsev, T. H. Johansen, M. Baziljevich,
Y. M. Galperin, M. E. Gaevski

Coupling through random superconducting bridges between filaments in a multifilamentary Ag-sheathed $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$ tape has been investigated by magneto-optical imaging at temperatures from 20 K up to T_c. Magnetic flux distributions have been measured on the surface of an intact tape in the remanent state on applying a strong perpendicular

magnetic field. The flux distributions observed at low temperatures reflect the arrangement of individual filaments. At high temperatures, the distribution becomes more similar to that for a uniform monocore tape, indicating that superconducting connections appear between the filaments. To discuss the relative contributions of the intra- and inter-filament currents, a simple model based on the Bean critical state was proposed and applied to analyse the temperature dependent behaviour. The inter-filament coupling, increasing with temperature, reaches at 77 K a point where the currents flowing in large inter-filament loops are roughly equal to the intra-filament currents.

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Tech. Phys.
vol. 45, no. 4, pp. 443-452, 2000

Sources of flicker noise and the technology of superconducting microstripes based on yttrium barium cuprate films

S. F. Karmanenko, A. A. Semenov, V. N. Leonov, A. V. Bobyl',
A. I. Dedoborets, A. V. Lunev, A. V. Nashchekin, R. A. Suris

It has been shown by annealing simulations of $YBa_2Cu_3O_7$ epitaxial films that the predominant sources of flicker noise in superconducting microstripes in operating ranges of frequency and temperature are related to oxygen transitions in the vicinity of boundaries of the small-angle blocks. To make superconducting microstripes with a dimension of ~1 μm the techniques of magnetron sputtering, as well as chemical and ion beam etching, were applied.

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Phys. Solid State
vol. 41, no. 11, pp. 1771-1774, 1999

Excess noise in $YBa_2Cu_3O_7$ epitaxial films and antenna-type microbolometers based on them

A. V. Bobyl', M. E. Gaevski, A. V. Lunev, R. A. Suris, A. I. Dedoborets, S. F. Karmanenko, A. A. Semenov, V. N. Leonov, I. A. Khrebtov

Monte Carlo modelled anneals of $YBa_2Cu_3O_7$ epitaxial films have been carried out, and the excess flicker noise in the operating frequency and temperature ranges were shown to be dominated by oxygen migration near small-angle block boundaries. Optimization of film and planar-microstructure fabrication permitted reaching a record-low Hooge noise parameter ($1.83{\cdot}10^{24}$ at 93 K) for test structures, which can be used to prepare high-performance antenna-type strip microbolometers. Calculations show that the reduction of the microstrip size to $1{\cdot}0.7\ \mu m^2$ and of the flicker noise made possible detection of radiation within the spectral range from 3 mm to 300 μm (100–1000 GHz) at 90 K, with a nanosecond response and a noise-equivalent power of $1.5{\cdot}10^{-12}$ $W/Hz^{1/2}$ at frequencies from 30 to 10^7 Hz, which is close to the limitations imposed by phonon noise.

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Phys. Rev. B
vol. 60, pp. 12485-12494, 1999

Temperature and magnetic field dependence of conductivity of YBaCuO films in the vicinity of superconducting transition: Effect of Tc-inhomogeneity

D. V. Shantsev, M. E. Gaevski, R. A. Suris, A. V. Bobyl, V. E. Gasumyants, O. L. Shalaev

Temperature and magnetic field dependences of the conductivity of $YBa_2Cu_3O_{7-\delta}$ films in the transition region are analyzed taking into account spatial inhomogeneity in transition temperature T_c. (i) An expression for the superconducting contribution to conductivity $\sigma_s(T,H,T_c)$

of a homogeneous superconductor for low magnetic fields $H \ll H_{c2}(0)$ is obtained using the solution of the Ginzburg-Landau equation in form of perturbation expansions [S. Ullah and A. T. Dorsey, Phys. Rev. B 44, 262 (1991)]. (ii) The error in $\sigma_s(T,H,T_c)$ occurring due to the presence of T_c inhomogeneity is calculated and plotted on an H-T plane diagram. These calculations use an effective medium approximation and a Gaussian distribution of T_c. (iii) Measuring the temff mperature dependences of a voltage, induced by a focused electron beam, we determine spatial distributions of the critical temperature for $YBa_2Cu_3O_{7-\delta}$ microbridges with a 2 μm resolution. A typical T_c-distribution dispersion is found to be ≈ 1 K. For such dispersion, error in $\sigma_s(T,H,T_c)$ due to T_c inhomogeneity exceeds 30% for magnetic fields $H<1$ T and temperatures $|T-T_c|<0.5$ K. (iv) Experimental $R(T,H)$ dependences of resistance are well described by a numerical solution of a set of Kirchoff equations for the resistor network based on the measured spatial distributions of T_c and the expression for $\sigma_s(T,H,T_c)$.

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Phys. Rev. Lett.
vol. 82, no. 14, pp. 2947-2950, 1999

Central peak position in magnetization loops of high-Tc superconductors

D. V. Shantsev, M. R. Koblischka, Y. M. Galperin, T. H. Johansen, P. Nalevka, M. Jirsa

Exact analytical results are obtained for the magnetization of a superconducting thin strip with a general behavior $J_c(B)$ of the critical current density. We show that within the critical-state model the magnetization as a function of applied field, B_a, has an extremum located exactly at $B_a = 0$. This result is in excellent agreement with presented experimental data for a $YBa_2Cu_3O_{7-\delta}$ thin film. After introducing granularity by patterning the film, the central peak becomes shifted to positive fields, $B_{cp} > 0$, on the descending field branch of the loop. Our results show that a positive B_{cp} is a definite signature of granularity in superconductors.

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Phys. Solid State
vol. 41, no. 6, pp. 877-880, 1999

Magneto-optic study of spatial magnetic-field distribution relaxation in an HTSC film strip after transport current turn-on

M. E. Gaevski, D. V. Shantsev, Y. M. Galperin, A. V. Bobyl, T. H. Johansen, H. Hauglin

The paper provides the first demonstration of the efficiency of applying the magneto-optic method to studies of the spatial and temporal magnetic-field relaxation in an $YBa_2Cu_3O_7$ film strip after the transport current is switched on. It is shown that the evolution of magnetic flux distribution is adequately described in terms of a modified Bean model with time-dependent critical current. At a time 50 ms after the current is switched on, the critical current of the samples studied decreases by ≈ 15%. This proves the significance of thermally activated magnetic flux motion (creep) in the regime investigated. The magnetic vortex pinning energy has been estimated as $U_0 \approx 20\ kT$.

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Phys. Solid State
vol. 41, no. 6, pp. 870-876, 1999

Simulation of 1/f noise spectra in $YBa_2Cu_3O_7$ epitaxial films

A. A. Berzin, A. I. Morozov, A. V. Bobyl’, R. A. Suris, A. I. Dedoborets

A Monte Carlo simulation of the *1/f* noise spectra in the normal phase of YBa2Cu3O7 epitaxial films is reported. It is conjectured that the main contribution to the noise is from oxygen transitions to vacant sites in the CuO plane. It is shown that the annealing regime and the mismatch strains between the film and the substrate are the main factors governing the domain and defect structure of the film and, hence, the *1/f* noise spectrum.

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Inorg. Mater.
vol. 35, no. 8, pp. 852-856, 1999

Twins and fluctuator defects in $YBa_2Cu_3O_7$ epitaxial films: Monte Carlo simulation of annealing and detwinning

A. V. Bobyl', R. A. Suris, A. I. Dedoborets, A. I. Morozov

Monte Carlo simulations were used to model the spatial distributions of oxygen atoms in CuO planes and those of barrier heights for the transition of oxygen to a nearest neighbor lattice site in films close in composition to $YBa_2Cu_3O_7$ for various annealing conditions in the presence of uniaxial strain P. Three regions can be distinguished, depending on annealing temperature: in region I, equilibrium phase fluctuations occur and metastable defects are missing after annealing; in regions II and III, quasi-isothermal annealing (rapid relaxation) results in the formation of metastable point defects ($P \neq 0$) and twins ($P = 0$), respectively. A two-step activation micromodel is proposed for movement of 90° domain boundaries: the interaction energy rises in the first step of the transition of an atom to a neighboring site and decreases in the second step. For 45° boundaries, a single-step model is proposed: the interaction energy decreases upon the transition of an atom to a nearest neighbor site.

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Phys. Rev. B
vol. 59, no. 14, pp. 9655-9664, 1999

Magneto-optical study of magnetic flux penetration into a current-carrying high-temperature superconductor strip

M. E. Gaevski, A. V. Bobyl, D. V. Shantsev, S. F. Karmanenko, Y. M. Galperin, T. H. Johansen, M. Baziljevich, H. Bratsberg

The magnetic-flux distribution across a high-temperature superconductor strip is measured using magnetooptical imaging at 15 K. Both the current-carrying state and the remanent state after transport current are studied up to currents of $0.97I_c$ where I_c is the critical current. To avoid

overheating of the sample current pulses with a duration of 50 ms were employed. The results are compared with predictions of the Bean model for the thin strip geometry. In the current-carrying state, reasonable agreement is found. However, there is a systematic deviation—the flux penetration is deeper than theoretically predicted. A much better agreement is achieved by accounting for flux creep as shown by our computer simulations. In the remanent state, the Bean model fails to explain the experimental results. The results for the currents $I \leq 0.7 I_c$ can be understood within the framework of our flux creep simulations. However, after the currents $I > 0.7 I_c$ the total flux trapped in a strip is substantially less than predicted by the simulations. Furthermore, it *decreases* with *increasing* current. Excessive dissipation of power in the annihilation zone formed in the remanent state is believed to be the source of this unexpected behavior.

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J. Appl. Phys.
vol. 84, no. 9, pp.5089-5096, 1998

Spatially-resolved studies of chemical composition, critical temperature, and critical current density of YBaCuO thin film

M. E. Gaevski, A. V. Bobyl, D. V. Shantsev, Y. M. Galperin, V. V. Tret'yakov, T. H. Johansen, R. A. Suris

Spatially resolved studies of a $YBa_2Cu_3O_{7-\delta}$ thin film bridge using electron probe microanalysis (EPMA), low-temperature scanning electron microscopy (LTSEM), and magneto-optical flux visualization have been carried out. Variations in chemical composition along the bridge were measured by EPMA with 3 μm resolution. Using LTSEM the spatial distributions of the critical temperature, T_c, and of the local transition width, ΔT_c, were determined with 5 μm resolution. Distributions of magnetic flux over the bridge in an applied magnetic field have been measured at 15 and 50 K by the magneto-optical technique. The critical current density j_c as a function of coordinate along the bridge was extracted from the measured distributions by a new specially developed method. Significant correlations between j_c, T_c, ΔT_c and cation composition have been revealed. It is shown that in low magnetic fields

deviation from the stoichiometric composition leads to a decrease in both T_c and j_c. The profile of j_c follows the T_c profile on large length scales and has an additional fine structure on short scales. The profile of j_c along the bridge normalized to its value at any point is almost independent of temperature.

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Physics of radiation processes in solids

J. Appl. Phys.
vol. 123, 215302, 2018

Reconstruction of concentration profiles in heterostructures with chemically modified interfaces

V. S. Kharlamov, D. V. Kulikov, M. N. Lubov, Ch. Zgheib, H. Romanus, Yu. V. Trushin, J. Pezoldt

An approach for the reconstruction of the composition profiles of heterostructures with chemically modified interfaces is presented. It is based on the comprehensive simulation of the heterostructure growth stages and the compositional changes occurring at the depth profiling stage during sputtering by secondary ion mass spectrometry. Combining simulation of the growth and the concentration measurement process allows the calculation of the real concentration depth profiles of the heterostructure components. Within the framework of the proposed approach, the composition of the SiC:Ge/Ge/Si:Ge/Si heterostructure is analyzed and the real depth profiles were calculated.

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Mater. Sci. Forum
vol. 858, pp. 501-504, 2016

Concentration profile simulation of SiC/Si heterostructures

J. Pezoldt, V. S. Kharlamov, D. V. Kulikov, M. N. Lubov,Yu. V. Trushin

Computer simulation of the concentration profiles evolution in SiC/Si heterostructures during growth and subsequent ion sputtering is presented. Simulation is based on a complex self consistent approach combining kinetic and ballistic methods. Within the framework of the proposed method concentration depth profiles in SiC/Si heterostructure with pre-deposited Ge impurity are calculated and compared with experimental sputtering profiles obtained by secondary ion mass spectrometry.

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Appl. Surf. Sci.
Vol. 267, pp. 128– 131, 2013

Evolution of subsurface nanocavities in copper under argon bombardment and annealing

D. V. Kulikov, O. Kurnosikov, V. S. Kharlamov, Yu. V. Trushin

The experimental and theoretical studies of evolution of nanocavities in argon-irradiated copper under annealing are presented. The subsurface argon-filled nanocavities are formed during a short annealing at a temperature around 1000 K by migration and interaction of complexes of the simplest defects created by argon irradiation at room temperature. A long-time annealing at a temperature above 1075 K leads to decomposition of nanocavities and desorption of argon from the sample. Using the X-ray photoelectron spectroscopy and scanning tunneling microscopy and spectroscopy, valuable data sets including the density of nanocavities and their size and depth distribution are obtained. A theoretical model describing the nucleation and evolution of nanocavities is developed. Computer simulations based on this model show that the nanocavities grow at elevated temperatures by absorption of argon–vacancy complexes formed during the ion irradiation. By comparison the calculations with experimental results, the migration energy of these complexes is estimated to be around 2.5–2.75 eV. Also, the value of dissociation energy of a complex, consisting of two vacancies and two argon atoms, is found to be equal to approximately 1.10–1.18 eV. The calculation of concentration of nanocavities at different annealing conditions reveals a satisfactory agreement with the experimental observations.

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Phys. Rev. B
Vol. 84, 054109, 2011

Temperature-induced evolution of subsurface nanocavities in argon-implanted copper

O. Kurnosikov, D. V. Kulikov, V. S. Kharlamov, H. J. M. Swagten, Yu. V. Trushin

The evolution of argon-filled nanocavities in a copper crystal under annealing is studied experimentally and theoretically. The subsurface argon-filled nanocavities are formed after a short annealing at a temperature ~1000 K by coalescence of subsurface defects initially created by argon implantation. The further prolonged annealing at a temperature above 1075 K leads to decomposition of the nanocavities and diffusion of implanted argon out of the sample. According to a simple analysis, the mechanism of the nanocavity formation is governed not only by the migration of simplest defects, such as vacancies and argon and copper interstitials, but also to a large extent, by diffusion and interaction of the complexes of these simplest defects. The experimental studies with x-ray photoelectron spectroscopy and scanning tunneling microscopy and spectroscopy provide valuable data sets of the density of nanocavities and their size and depth distribution. Based on the experimental results, a theoretical model is developed. The calculation with the model proves that the growth of the nanocavities is mainly determined by the temperature-induced migration of vacancy-argon complexes. By combining the experimental data with the simulation results, the migration energy of these kinds of complexes is estimated ~2.55–2.75 eV. Moreover, the calculation with our model provides the estimate of the dissociation energy of a multiple complex, consisting of two vacancies and two argon atoms, as 1.10–1.18 eV. These parameters, reported in this article, play a key role in the description of the kinetics of the growth and decomposition of nanocavities.

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Tech. Phys. Lett.
vol. 36, no. 3, pp. 262–264, 2010

Effect of the nitrogen ion energy on the MBE growth of thin gallium nitride films

D. V. Kulikov, Yu. V. Trushin, V. S. Kharlamov

The influence of the energy of bombarding nitrogen ions on the growth of thin gallium nitride (GaN) films under molecular beam epitaxy (MBE) conditions has been simulated using the method of balance kinetic equations. The dependence of the GaN film growth rate on the ion energy is determined and changes in the structure of films grown at different ion energies are explained. Theoretical estimates satisfactorily agree with the available experimental data.

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Bull. Russ. Acad. Sci. Phys.
vol. 74, no. 2, pp. 241–244, 2010

Investigation of Ge and C layer deposition on a Si substrate using SIMS profiling

V. S. Kharlamov, D. V. Kulikov, Yu. V. Trushin, P. Nader, P. Mazri, Th. Stauden, J. Pezoldt

Structures grown using the technique of molecular-beam epitaxy during deposition of carbon and/or germanium atoms on an Si(111) surface were investigated experimentally and theoretically. Experimental profiles of in-depth component distribution were obtained using SIMS-profiling, whereas a complex technique of computer simulation taking into account diffusion and ballistic processes was applied for the calculated profiles.

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Appl. Surf. Sci.
vol. 252, no. 9, pp. 3303–3308, 2006

Vacancy-solute complexes and their clusters in iron

J. Kuriplach, O. Melikhova, C. Domain, C.S. Becquart, D. Kulikov, L. Malerba, M. Hou, A. Almazouzi, C.A. Duque, A. L. Morales

In this contribution, several vacancy-solute complexes in iron are investigated theoretically from the viewpoint of positron annihilation. In particular, V-Si, V-P, V-Cr, V-Mn, V-Ni, V-Cu and V-Mo complexes are examined. In addition, nano-sized vacancy-Cu clusters in the Fe matrix are also studied. We concentrate on positron lifetimes and coincidence Doppler broadening profiles that bring complementary information about the studied complexes and their clusters. Positron calculations are carried out using the atomic superposition method employing realistic atomic configurations obtained recently using an ab initio pseudopotential method (vacancy-solute complexes) and Monte Carlo/molecular dynamics methods (vacancy-Cu clusters). The main aim of this study is to predict as to what extent such defects are detectable and differentiable using positron annihilation techniques. The results obtained are discussed in the context of experimental data available in the literature.

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Bull. Russ. Acad. Sci. Phys.
vol. 70, no. 6, pp. 897–901, 2006

Theory and numerical simulation of ion interaction with surfaces of multicomponent materials

Yu. V. Trushin, D. V. Kulikov, V. S. Kharlamov

Processes due to the interaction of ions with multicomponent semiconductors were studied using numerical simulation methods. Such numerical simulation methods as the molecular dynamics, Monte Carlo, and balance kinetic equations were used. The combination of various

methods allows simulation of physical processes occurring on different time and space scales.

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Philos. Mag.
vol. 86, no. 2, pp. 141–172, 2006

On the binding energies and configurations of vacancy and copper-vacancy clusters in bcc Fe-Cu: A computational study

D. Kulikov, L. Malerba, M. Hou,

Vacancy and copper–vacancy clusters in bcc Fe–Cu alloys have been studied using a combination of metropolis Monte Carlo (MMC) and molecular dynamics (MD) techniques, to investigate their lowest energy configurations and corresponding binding energies, for sizes up to a few hundreds of elements (~2 nm). Two different many-body interatomic potentials were used to perform the calculations, in order to assess the robustness of the results [1, 2]. Empirical expressions for the binding energies, of immediate use in kinetic Monte Carlo (KMC) or rate theory (RT) models, have been obtained. It is observed that vacancy clusters are three-dimensional cavities whose shape is primarily determined by a criterion of maximisation of the number of first and second nearest neighbour pairs. Copper atoms, when present, tend to coat an inner vacancy cluster, while remaining first nearest neighbours to each other. The inner vacancy cluster, when completely coated, tends to be as close as possible to the surface of the hollow precipitate. These findings are consistent with previous experimental and computational work. The binding energy of these complexes is a monotonously growing function of the ratio number of vacancies to number of copper atoms. Pure copper precipitates appear to follow a loose criterion of maximisation of first nearest neighbour pairs. While the two interatomic potentials used in this work provide largely similar values for the binding energies and comparable configurations, some differences are found and discussed. Subtle differences observed in comparison with *ab initio* calculations are also discussed.

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Integr. Ferroelectr.
vol. 72, no. 1, pp. 47–51, 2005

Neutron irradiation effects in PZ and PZT thin films

R. Bittner, K. Humer, H. W. Weber, K. Kundzins, A. Sternberg,
D. A. Lesnyh, D. V. Kulikov, Y. V. Trushin

Neutron irradiation effects on highly oriented antiferroelectric $PbZrO_3$ (PZ) and ferroelectric $PbZr_{0.53}Ti_{0.47}O_3$ (PZT) thin films are investigated in view of their possible application as a temperature sensitive element in a new bolometer system for fusion devices like ITER. All investigated thin films were prepared by a sol-gel technique and by pulsed laser deposition (PLD) respectively. The dielectric properties were investigated in a frequency range from 1 to 250 kHz and at temperatures up to 400◦C, prior to and after irradiation to a neutron fluence of $3{*}10^{22}$ m^{-2} (E > 0.1 MeV). After irradiation, the films were annealed in several steps up to 400^0C in order to remove the radiation-induced defects. The results are discussed in terms of two kinds of radiation-induced defects, i.e. structural defects, such as oxygen-vacancies, and radiation-induced charges. We find that the antiferroelectric PZ heterostructures are radiation harder than the PZT films and that the structural order of the film as well as the interfaces play an important role.

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J. Nucl. Mater.
vol. 342, no. 1, pp. 131–140, 2005

Vacancy dislocation loops in zirconium and their interaction with self-interstitial atoms

D. V. Kulikov, M. Hou

The present work aims at predicting at the atomic scale, binding energies of vacancies to vacancy clusters in zirconium, preparing this way the modelling of their growth. Empirical laws established on the basis of simulation results are suggested, describing the size dependence of

formation and binding energies of small voids (involving up to 1000 atoms) as well as basal, prismatic and pyramidal vacancy loops involving the same number of vacancies. The detailed atomic configurations of the loops are examined and characterized by means of areas where atoms are mis-coordinated and by strain fields. The importance of mis-coordinated areas is emphasized by an examination of self-interstitial atom (SIA) diffusion mechanisms in the vicinity of basal vacancy loops. The loops act as sinks for SIAs that, depending on the temperature, migrate one- or three-dimensionally to the mis-coordinated areas from which they cannot escape. By this mechanism, the annihilation of vacancy loops by SIA absorption is inhibited.

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Nucl. Instrum. Methods Phys. Res. B
vol. 228, pp. 245–249, 2005

Coupling of MC and MD techniques for the calculation of vacancy cluster binding energies

D. Kulikov, L. Malerba, M. Hou

A combination of Metropolis Monte Carlo (MMC) and molecular dynamics (MD) techniques has been used to systematically sample configurations of vacancy clusters (VC) in zirconium and calculate the corresponding binding energies as a function of cluster size. The application of this procedure allowed the interpolation of expressions for the binding energies, which are of immediate use in kinetic Monte Carlo (KMC) or rate theory (RT) models. The results of the application of the procedure are presented, analysed and discussed.

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Nucl. Instrum. Methods Phys. Res. B
vol. 228, pp. 230–234, 2005

Computer simulation of neutron transmutation doping of isotopically engineered heterostructures

D. V. Kulikov, V. S. Kharlamov, A. A. Schmidt, K. L. Safonov, S. A. Korolev, Yu. V. Trushin

Neutron transmutation doping (NTD) of silicon-based isotopically engineered heterostructures is a powerful technique for the creation of the semiconductor devices with the desired spatial distribution of 31P impurities that is defined by the initial distribution of 30Si nuclei.
Computer simulation allows to study dopant distribution changes during NTD process and post-irradiation annealing and to determine appropriate annealing regimes. The initial distribution of the radiation defects was obtained by the dynamic Monte Carlo code DYTRIRS_N, while the subsequent annealing stage was simulated by the rate equations (RE) method. Concentrations of intrinsic defects and depth profiles of phosphorus atoms were obtained.

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J. Nucl. Mater.
vol. 336, no. 1, pp. 125–134, 2005

A model study of displacement cascades distributions in zirconium

M. Hou, D.V. Kulikov

5 to 200 keV displacement cascades in zirconium are studied in the binary collision approximation with the simulation code Marlowe. The cascades are analysed statistically by means of component analysis, fuzzy clustering and isodata analysis. As a consequence of the large recoil ranges and range straggling specific to open hcp lattices like Zr, a large dispersion of the frequencies of Frenkel pair distributions is found, as well as of the spatial extent and morphology of vacancy and interstitial

distributions. In Zr, cascades are formed by a widespread distribution of displacement clusters that can be small. Remarkably, the size and morphology distributions of these clusters are found independent of the primary recoil energy in the energy range investigated.

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J. Appl. Phys.
Vol. 96, 3239, 2004

Oxygen vacancy defects in antiferroelectric $PbZrO_3$ thin film heterostructures after neutron irradiation

R. Bittner, K. Humer, H. W. Weber, K. Kundzins, A. Sternberg, D. A. Lesnyh, D. V. Kulikov, Y. V. Trushin

Neutron irradiation effects on highly oriented antiferroelectric $PbZrO_3$ (PZ) thin films are investigated in view of their possible application as a temperature sensitive element in an alternative bolometer system for fusion devices such as the International Thermonuclear Experimental Reactor (ITER). All films were prepared by a sol-gel technique or by pulsed laser deposition (PLD). The dielectric properties were investigated in a frequency range from 1 to 250 kHz and at temperatures up to 400°C, prior to and after irradiation to neutron fluences of 0.5×10^{22}, 1×10^{22}, 2×10^{22}, and 3×10^{22} m^{-2} (E>0.1 MeV). After irradiation, the films were annealed in several steps up to 400°C in order to remove the radiation-induced defects. The results are discussed in terms of a phenomenological model of radiation effects in PZ films, which takes into account structural defects, such as oxygen vacancies, and radiation-induced charges. We find that the films are most sensitive to neutron irradiation in the vicinity of the phase transistion temperature T_c. In addition, the structural order of the films as well as the interfaces play an important role. We find that the PZ heterostructures prepared by PLD are radiation harder than the sol-gel films. The dielectric properties of the PLD films are more or less unaffected by neutron irradiation up to a fluence of 3×10^{22} m^{-2} (E>0.1 MeV).

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J. Eur. Ceram. Soc.
vol. 24, no. 6, pp. 1653–1657, 2004

Antiferroelectric $PbZrO_3$ thin films: Structure, properties and irradiation effects

A. Sternberg, K. Kundzins, V. Zauls, I. Aulika, L. Čakare, R. Bittner, H. Weber, K. Humer, D. Lesnyh, D. Kulikov, Y. Trushin

Irradiation effects on highly oriented antiferroelectric $PbZrO_3$ and ferroelectric $Pb_{0.92}La_{0.08}(Zr_{0.65}Ti_{0.35})O_3$ thin films are investigated being exposed to neutron irradiation up to fluence $2*10^{22}$ m^{-2}. The higher resistance of antiferroelectric $PbZrO_3$ thin films as compared to ferroelectric heterostructures to large fluences of neutron irradiation is recognized and discussed. Influence of two factors (structural and charge) was taken into account analysing irradiation effects on materials of different polarization states: ferroelectric PLZT (ceramics and thin films) and antiferroelectric PbZrO3 films.

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Proc. SPIE
vol. 5140, pp. 100-102, 2004

Calculations of vacancy binding energies to Cu-V complexes in FeCu alloys

D. V. Kulikov, L. Malerba, O. Ya. Khrushcheva

The binding energies of vacancies to copper-vacany clusters in ferritic alloys containing Cu are of great importance as parameters for Object Kinetic Monte Carlo (OKMC) or Rate Equation (RE) models for the prediction of Cu precipitation under irradiation. Copper-vacancy complexes created after irradiation influence the mechanic properties of irradiated steels since they are obstacles to dislocation motion and lead to hardening and embrittlement of the material. The main purpose of this

work is to find an efficient computational procedure to perform the calculation of copper-vacancy complex formation energies and corresponding vacancy binding energies in bcc Fe-Cu alloys, in order to calculate a whole matrix of values, from small to large complex sizes.

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Ferroelectrics
vol. 308, no. 1, pp. 5-16, 2004

Theoretical study of ferroelectric properties degradation in perovskite ferroelectrics and antiferroelectrics under neutron irradiation

D. V. Kulikov, Yu. V. Trushin

In present study the influence of neutron irradiation on different types of ferroelectric perovskite structures is theoretically investigated. The changes of polarization of PLZT ceramics after irradiation are caused by oxygen vacancies with special reordering of the crystal lattice around a vacancy. This reordering leads to about zero value of local polarization which results in zero polarization of the whole sample when a sufficient number of such vacancies are created. Oxygen vacancies formed by irradiation may also serve as a source of charge carriers in the ferroelectric perovskite materials. In the case of antiferroelectric lead-zirconate thin films the influence of oxygen vacancies on polarization is suppressed and it is possible to clarify the influence of radiation charged defects on the material properties. We associate the decrease of the Curie-Weiss temperature in lead-zirconate thin films under neutron irradiation with the charges located near film surfaces where Schottky junction on the contact between antiferroelectric and metal is formed. In this case the relative decrease of the Curie-Weiss temperature is proportional to the neutron fluence. However the charges possibly remaining in the bulk of the film may change this proportionality to the quadratic law.

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Proc. SPIE
vol. 5127, pp. 124-127, 2003

Computer simulation of the creation of ^{31}P doped layer in $^{28}Si/^{30}Si/^{28}Si$ heterostructure by neutron transmutation doping

Yu. V. Trushin, G. V. Mikhailov, E. E. Zhurkin, V. S. Kharlamov, A. A. Schmidt, F. A. Krusenstern

Recently various physical phenomena involving nuclear spins in semiconductors attract much attention. The problem is to produce an array of impurity atoms with nuclear spin I = 1/2 in the atom matrix with I = 0, i.e. to produce a nuclear-spin engineered semiconductor heterostructure. Both the concentration and the spatial distribution of impurity should be controlled. It is supposed that utilization of ^{31}P atoms as an impurity in ^{28}Si or ^{30}Si matrix possesses significant advantages. Such a structure could be produced by neutron transmutation doping (NTD) of $^{28}Si/^{30}Si/^{28}Si$ isotopic heterostructure, according to the nuclear reaction $^{30}Si+n \rightarrow ^{31}Si(2.6\ hour) \rightarrow ^{31}P$. Computer simulation of the NTD process provides the conditions necessary to create $^{28}Si/^{30}Si{:}^{31}P/^{28}Si$ heterostructure with good crystal structure and well-defined distribution of impurity concentration. Simulation was carried out using parallel computing capabilities of workstation cluster of A.F. Ioffe Physico-Technical Institute of the Russian Academy.

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Proc. SPIE
vol. 5127, pp. 136-139, 2003

Changes in the temperature dependence of the dielectric constant in irradiated antiferroelectric thin films

D. A. Lesnyh, D. V. Kulikov, Yu. V. Trushin, R. Bittner, K. Humer, H. W. Weber, A. R. Sternberg

A model describing the changes of the Curie-Weiss temperature in lead-zirconate thin films under neutron irradiation is proposed. The Curie-Weiss temperature in the irradiated material decreases which is

connected to charges caused by neutron irradiation. The charges located near the surfaces due to Schottky effect and in the bulk of the film results in different rates of the Curie-Weiss temperature decreases with neutron fluence. However the influence of the Schottky layers seems to be more pronounced. Satisfactory agreement between the theoretical results and the experimental data is obtained for different neutron fluences.

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Proc. SPIE
vol. 5122, pp. 341-347, 2003

Irradiation effects in lead zirconate thin films

A. Sternberg, A. Krumins, K. Kundzins, I. Aulika, L. Čakare, R. Bittner, H. Weber, K. Humer, D. Lesnyh, D. Kulikov, Y. Trushin

Lead zirconate $PbZrO_3$ (PZ) and $PbZr_{0.53}Ti_{0.47}O_3$ (PZT) sol-gel films with a thickness of up to 1.5 μm were deposited on TiO_2/Pt/TiO_2/SiO_2/Si substrates by spin coating technique and heterostructures of the same composition as well as on $Pb_{0.92}La_{0.08}$ $(Zr_{0.65}Ti_{0.35})O_3$ (PLZT-8) (with a thickness of 0.4 tm) were pulse laser deposited (PLD) on Pt/Ti/SiO_2/Si. Observation of a typical antiferroelectric (AFE) double hysteresis loop in obtained PZ heterostructures at room temperature was attributed to the superior dielectric strength in case of thin film materials. The thermal behaviour of dielectric permittivity ε of PZ film reveals a maximum near 225°C on heating and 219°C on cooling. The higher resistance of antiferroelectric PZ thin films as compared to ferroelectric (e.g., PZT, PLZT-8) heterostructures to neutron irradiation (up to fluence $2x10^{22}m^{-2}$) is recognized and discussed.

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Nucl. Instrum. Methods Phys. Res. B
vol. 196, pp. 39–50, 2002

The estimation of sputtering yields for SiC and Si

G. Ecke, R. Kosiba, V. Kharlamov, Yu. Trushin, J. Pezoldt

Sputtering yields of crystalline silicon carbide and silicon have been determined experimentally for bombardment by Ne^{+}, Ar^{+} and Xe^{+} ions in the energy range between 0.5 and 5 keV under 60^{0} sputtering with respect to the surface normal. Sputter crater measurements on SiC and Si and Auger depth profiles of SiC on Si have been carried out in order to determine the sputtering yields. The measurements are compared with Monte Carlo simulations which have been computed by the simulation static codes, TRIM and TRIRS and by the dynamic codes DYTRIRS and T-DYN as well as with the sputter theory. The simulation results depend strongly on the input parameters which are not well known especially for SiC. The TRIM simulation fits the experimental results very well and the differences between the results of the simulation programs are sometimes greater than their difference from experimentally measured sputtering yields.

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Tech. Phys. Lett.
vol. 28, no.8, pp. 628-630, 2002

The effect of neutron irradiation on the Curie-Weiss temperature of an antiferroelectric lead zirconate film

*D. V. Kulikov, D. A. Lesnyh, Yu. V. Trushin, H. W. Weber,
K. Humer, R. Bittner, A. R. Sternberg*

A physical model describing variations of the Curie-Weiss temperature of an antiferroelectric lead zirconate ($PbZrO_3$) film under neutron irradiation is proposed. According to model, a relative change in the Curie-Weiss temperature is proportional to the square of the total neutron dose. Theoretical estimates are in good agreement with experimental data.

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Proc. SPIE
vol. 4627, pp. 170-176, 2002

Computational study of the influence of oxygen vacancies on the polarization in irradiated and annealed PLZT ceramics

D. A. Lesnyh, D. V. Kulikov, Yu. V. Trushin, R. Bittner,
K. Humer, H. W. Weber, A. R. Sternberg

A physical model for the oxygen defect evolution in PLZT ceramics under neutron irradiation and annealing is proposed. The influence of the defect system on the polarization of these materials has been investigated. The influence of the La content on the material structure and the oxygen defects has been taken into account. Satisfactory agreement between the theoretically estimated oxygen defect concentration after irradiation and annealing and the experimentally determined polarization has been obtained.

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Proc. SPIE
vol. 4627, pp. 177-180, 2002

Computer simulation and SIMS profiling of Zn implantation in A3B5 semiconductors

B. J. Ber, A. P. Kovarsy, A. A. Schmidt, Yu. V. Trushin,
E. E. Zhurkin, F. A. Krusenstern

The method for the determination of the impurity displacement threshold energy in semiconductor heterostructures is further developed. New experimental samples for this method are proposed. Important parameters for the samples are defined. Also, simulation of the sputtering of wide impurity depth profiles is carried out. Improved values for the penetration lengths of Zn atoms with different impact energies in GaAs were found.

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Integr. Ferroelectr.
vol. 47, no. 1, pp. 143–152, 2002

Dielectric properties of irradiated ferroelectric and antiferroelectric thin films

R. Bittner, K. Humer, H. W. Weber, L. Čakare, A. Sternberg, D. A. Lesnyh, , D. V. Kulikov, Y. V. Trushin

Irradiation effects on highly oriented antiferroelectric (AFE) $PbZrO_3$ (PZ) and on ferroelectric (FE) $Pb_{0.92}La_{0.08}(Zr_{0.65}Ti_{0.35})O_3$ (PLZT-8) films are investigated. The dielectric properties were measured in the frequency range from 20 Hz (hysteresis measurements) to 250 kHz, at temperatures from 400°C to room temperature, as well as before and after irradiation to fast neutron fluences of $1{\cdot}10^{22}$ m^{-2} and $2{\cdot}10^{22}$ m^{-2}. After each irradiation, the films were annealed in several steps up to ~400°C to remove the radiation induced defects. The results are discussed in terms of radiation-induced structural defects and radiation-induced charges. We find that the AFE films show a significantly different behaviour from the FE films.

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Physica C
vol. 355, pp. 245-250, 2001

Changes in the transition temperature after irradiation and annealing in single crystalline $YBa_2Cu_3O_{7-\delta}$

D. V. Kulikov, Yu. V. Trushin, F. M. Sauerzopf, M. Zehetmayer, H. W. Weber

A model for the defect dynamics in $YBa_2Cu_3O_{7-\delta}$ (YBCO) single crystals elucidating the changes in the transition temperature after neutron irradiation and annealing is presented. The influence of neutron irradiation is due to the elastic energy transfer of the incident neutron to the primary recoil atom. Therefore, a full spectrum of defects is obtained, ranging from point defects in all sub-lattices. The data are compared to experimental Tc values on a single crystal after repeated irradiation and

annealing. These changes are found to be closely related to the calculated concentration of vacancies at the Cu-O chain sites.

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Nucl. Instrum. Methods Phys. Res. B
vol. 178, pp. 269–274, 2001

Theoretical and experimental investigations of defect evolution in silicon carbide during N^+ and Al^+ ion implantation taking into account internal stress fields

V. V. Rybin, D. V. Kulikov, Yu. V. Trushin, R. A. Yankov, M. Voelskow, F. Scharmann, J. Pezoldt

A theoretical model is developed which allows to describe the defect evolution in silicon carbide implanted with high doses of nitrogen and aluminium ions and subsequently annealed to form a solid solution. The diffusion of defects, the formation of complexes of defect clusters and the influence of the internal elastic stress fields produced by the implanted ions and the complexes formed are taken into account. Results from the simulations have been correlated with data obtained by Rutherford backscattering spectrometry/ion channelling (RBS/C).

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Tech. Phys. Lett.
vol. 27, no. 4, pp. 316–318, 2001

A physical model of the oxygen subsystem evolution in PLZT ceramics under neutron irradiation and annealing

D. V. Kulikov, D. A. Lesnyh, Yu. V. Trushin, H. W. Weber, K. Humer, R. Bitter, A. Sternberg

A physical model describing the evolution of defects in the oxygen subsystem of ferroelectric PLZT ceramics under neutron irradiation and isochronous annealing conditions is proposed. The model takes into

account the dependence of the material properties on the lanthanum content. The oxygen vacancy concentration variations calculated using this model agree with the experimental data on the polarization behavior in annealed ceramics.

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Integr. Ferroelectr.
vol. 37, no. 1, pp. 275–283, 2001

Dielectric properties of reactor irradiated ferroelectric thin films

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A. Sternberg, D. V. Kulkov, Y. V. Trushin*

Radiation effects in highly oriented $PblZr_{0.53}Ti_{0.47}O_3$ (PZT), $Pb_{0.94}La_{0.06}Zr_{0.65}Ti_{0.35}O_3$ (PLZT-6), and $Pb_1Zr_1O_3$ (PZ) ferroelectric (FE) and antiferroelectric (AF) thin films are investigated in view of their possible application as a temperature sensitive element in a new bolometer system for ITER (International Thermonuclear Experimental Reactor). The dielectric properties (i.e. hysteresis loops, dielectric constants) of the films were investigated in a frequency range from 20 to 10^5 Hz and at temperatures up to 450^0C, before and after neutron irradiation to a neutron fluence of $5x10^{21}$ m^{-2} (E>0.1 MeV). The dielectric constant was measured during cooling with 1.7^0C min^{-1}. The dielectric properties of the films were assessed before and after annealing in several steps up to 490 ^{0}C to remove the radiation induced defects.

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Proc. SPIE
vol. 4348, pp. 275-281, 2001

Estimation of the displacement threshold energies in Si and GaAs by means of the sputtering of structures with thin marker layers.

*V. S. Kharlamov, B. J. Ber, Yu. V. Trushin, E. E. Zhurkin,
A. P. Kovarski, A. A. Schmidt*

The combined experimental and computer simulation technique for the estimation of the displacement threshold energies of impurity atoms in materials has been developed. The technique is based on SIMS sputtering profiling of structures with thin impurity marker layers and computer simulation of this process. Using this technique the displacement threshold energies of Al atoms in GaAs matrix and Sb in Si matrix have been estimated.

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Proc. SPIE
vol. 4348, pp. 264-269, 2001

Computer simulation of ferroelectric property changes in PLZT ceramics under neutron irradiation.

*D. V. Kulikov, Yu. V. Trushin, V. S. Kharlamov, R. Bittner, K. Humer,
H. W. Weber, A. R. Sternberg, D. A. Lesnykh, A. A. Schmidt*

The response of ferroelectric materials to high energy irradiation is of great interest because of their possible application in radiation environments such as thermonuclear reactors. In the present work a physical model for the defect evolution in PLZT ceramics under neutron irradiation and annealing is proposed. The influence of the defect system on the ferroelectric properties of these materials has been investigated. Satisfactory agreement between the theoretically estimated oxygen defect concentration after irradiation and annealing and the experimentally determined polarization has been obtained.

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Proc. SPIE
vol. 4348, pp. 257-263, 2001

Al^+ and N^+ implantation in silicon carbide: A role of point defect clusters in defect evolution

P. V. Rybin, D. V. Kulikov, Yu. V. Trushin, J. Pezoldt

The diffusion processes in silicon carbide under Al^+ and N^+ ion implantation and subsequent annealing have been investigated. The influence of an internal stress field due to point defect clusters has been taken into account. The clusters of interstitials, ions, and impurities have been created during irradiation. The compression stress field due to these complexes has decreased the diffusion of interstitials. The defect profiles have been calculated which have been in good agreement with experimental RBS/C results.

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Proc. SPIE
vol. 4348, pp.254-256, 2001

Computer simulation of the special carbides (WC and MoC) destruction by collision cascades in Fe matrix.

V. S. Kharlamov, Yu. V. Trushin, V. V. Rybin, Ph. Yu. Fedorov

The behaviour of α-Fe alloys with molybdenum and tungsten carbides and oversize substitutional atoms under reactor irradiation has been investigated to study the possibility to substitute the molybdenum atoms for tungsten ones in order to create low activated steels. Computer simulation of collision cascades was used to study the damage of iron targets with Mo and W impurities and carbides under irradiation. It was found that at the ballistic stage of radiation damage the tungsten carbides are damaged to a higher degree and can be destructed more effectively than molybdenum carbides because of differences in interatomic potentials.

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Tech. Phys. Lett.
vol. 26, no. 10, pp. 876–878, 2000

Special features of the effect of oversized impurities on the cascade development in a-iron alloys containing special carbides

V. V. Rybin, Yu. V. Trushin, F. Yu. Fedorov, V. S. Kharlamov

We consider the behavior of an a-iron alloy containing special molybdenum and tungsten carbides (MoC and WC) and oversized impurity atoms (Mo and W) in the solid solution. The effects of molybdenum and tungsten on the development of ballistic (cascade) processes in the alloy under reactor irradiation conditions have been studied by computer simulation methods to assess the possibility of substituting W for Mo in the alloy to obtain low-activated steels.

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Nucl. Instrum. Methods Phys. Res. B
vol. 166, pp. 758–763, 2000

The influence of the implantation sequence on the $(SiC)_{1-x}(AlN)_x$ formation

*J. Pezoldt, P. V. Rybin, D. V. Kulikov, Yu. V. Trushin,
R. A. Yankov, M. Voelskow, U. Kreissig*

The influence of the implantation sequence on the defect and implant distribution during $(SiC)_{1-x}(AlN)_x$ formation was studied by Rutherford backscattering spectrometry/ion channelling (RBS/C) and elastic recoil detection. It is shown that the implantation sequence aluminum followed by nitrogen lead to an improved crystallinity compared to the reverse implantation sequence for implantation temperatures above 400°C. The results obtained are discussed in relation to the defects distributions calculated by using a developed model which includes the effect of stress self-consistently.

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Proc. SPIE
vol. 4064, pp. 288-294, 2000

Copper cluster formation and evolution in amorphous materials grown by co-sputtering of copper with SiO_2

D. V. Kulikov, Yu. V. Trushin, S. A. Gurevich, V. A. Zabelin

The process of copper nanoclusters evolution in amorphous films, formed by co-sputtering of Cu and SiO_2, has been investigated theoretically. Bulk copper diffusion during sample annealing after fabrication have been described by kinetic equation set and cluster size distribution function have been obtained. The reasonable agreement of theoretical and experimental results has been achieved. The values of bulk copper activation migration energy have been estimated. For investigating clusters formation with different copper content method of molecular dynamics have been developed. Both methods have reasonable agreement for low time diffusion.

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Proc. SPIE
vol. 4064, pp. 301-307, 2000

Influence of internal stress fields due to point defect clusters on interstitial diffusion in SiC under irradiation

P. V. Rybin, D. V. Kulikov, Yu. V. Trushin, J. Pezoldt, R. A. Yankov

The fundamental processes that occur when SiC is implanted at elevated substrate temperatures with high doses of N^+ and Al^+ ions to synthesize buried layers of $(SiC)_x(AlN)_{1-x}$ have been investigated. The influence of the mechanical stress induced by formed clusters of interstitials has been taken into account by adding a special term to the expression of current density of defects in the set of differential equations. The satisfactory agreement of simulation results and experimental data is obtained. The theoretical treatment has enabled one to determine the role of internal stress field on the evolution of defect distribution.

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Tech. Phys.
vol. 44, no. 10, pp. 1168-1174, 1999

Physical model for the evolution of the defect system of silicon carbide with allowance for the internal elastic stress fields during implantation of Al^+ and N^+ and subsequent annealing

D. V. Kulikov, Yu. V. Trushin, P. V. Rybin, V. S. Kharlamov

A theoretical analysis is offered for the formation and development of defects in silicon carbide implanted with nitrogen and aluminum ions and then annealed. The diffusion of defects, the formation of complexes, and the influence of the internal elastic stress fields produced by the implanted ions and the created complexes on the migration of interstitials are taken into account. The computed distributions of defects agree satisfactorily with the experimental data. Certain kinetic parameters of silicon carbide are estimated numerically.

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Proc. SPIE
vol. 3687, pp. 290-291, 1999

Physical model of copper clusters formation in hydrogenated amorphous carbon grown by ion cosputtering of graphite and copper

D.V. Kulikov, Yu.V. Trushin, V.S. Kharlamov

Interest of conductive cluster physics is stimulated by its possible applications to nano- and micro-electronics. Modification of Diamond Like Carbon (DLC) properties by introduction of metallic nanoclusters (e.g. copper) is of great interest because of the possibility to vary useful properties of the material and to give deeper insight into its structure. One of the way to make DLC film is to grown it by ion co-sputtering of graphite and copper. The grown films have been investigated by electron microscopy (TEM), Selected Area Electron Diffraction (SAED) and optical absorption. In present work the model is proposed of evolution of copper nanoclusters during DLC film growth. The size distribution

function of these clusters have been obtained with satisfactory agreement with experimental results. The value of surface activation migration energy of copper has been estimated. The main assumptions of the model are the following: (1) Numerical estimations show that during film growth copper and carbon atoms fall on film surface with low energy insufficient to deep penetrate into the sample. Therefore only surface processes are taken into account. (2) Copper atoms may diffuse only on film surface, because copper diffusion in bulk DLC is negligible. So all diffusion processes occur during growth of one or two monolayers of the film. (3) Diffusing copper atoms may create bi-clusters and join to already existing clusters to form clusters with bigger sizes. So copper clusters with different sizes exist in the film.

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Proc. SPIE
vol. 3687, pp. 244-253, 1999

Non-conventional transition layer formation during PLD of nm-period multilayers

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During pulsed laser deposition ions with kinetic energies of the order of 100 eV can already cause intermixing of nm-periodical multilayers followed by non-conventional phase formation in the transition layers. In the present paper experimental studies of concentration profiles in Ni/C, Fe/Al, Co/Cu multilayers prepared by pulsed laser deposition are compared with ballistic simulations of the deposition process. It was found that generally the ballistic simulation provides the right order of magnitude of the real transition layer width. Unusual phase formation in transition layers including supersaturation, amorphization, pseudomorphism, demixing, and interface coarsening are considered to be a result of solid-state processes directed towards minimization of the free energy of the system.

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Proc. SPIE
vol. 3687, pp. 274-275, 1999

Displacement threshold energies of impurity atoms in GaAs heterostructures

B. J. Ber, Yu. A. Kudrjavtsev, V. S. Kharlamov, Yu. V. Trushin, E. E. Zhurkin

The new approach for the determination of displacement threshold energies (E_d) of impurity atoms in multicomponent targets has been proposed. The approach combines an experimental SIMS-profiling technique and a computer simulation by a dynamic DYTRIRS code. The developed approach was applied for the determination of E_d the for Al and In impurity atoms in GaAs targets.

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Proc. SPIE
vol. 3687, pp. 254-257, 1999

Theoretical and experimental studies of $(AlN)_{1-x}(SiC)_x$ layer structures formed by N^+ and Al^+ co-implantation in 6H-SiC

D. V. Kulikov, J. Pezoldt, P. V. Rybin, W. Skorupa, Yu.V. Trushin, R. A. Yankov

The defect formation in silicon carbide implanted with N^+ and Al^+ ions was studied. The model of defect evolution in implanted and annealed silicon carbide was developed taking into account the influence of internal stress field on interstitial diffusion. The parameter of interaction of interstitial with stress field was estimated. Theoretical and experimental results show good agreement.

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Vacuum
Vol. 52, pp. 407-410, 1999

Computer simulation of transition from h-BN TO c-BN during ion beam assisted deposition

V. S. Kharlamov, D. V. Kulikov, Yu. V. Trushin

A model is proposed of c-BN growth during the ion Beam assisted deposition process. This phase appears when N and B atoms in h-BN create inserted *ab*-planes that increase the density of the material, resulting in transition from h-BN to c-BN. The aim is to simulate the processes that occur in growing BN films that lead to the phase transition. The ballistic processes caused by ion beam have been simulated by means of Monte Carlo computer codes TRIRS and DYTRIRS. With the help of computer code GEAR the annealing of the profiles of bombarding particles (Ar, N, B) have been modelled. The sink strengths of dislocation loops and migration energies of Ar, B and N atoms in BN have been estimated. These loops can act as nuclei of inserted ab-planes consisted of B and N, leading to formation of c-BN. It is shown that, according to our model, the transition from h-BN to c-BN is indeed possible, under certain conditions.

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Tech. Phys. Lett.
vol. 25, no. 3, pp. 198-199, 1999

Size distribution of copper nanoclusters in amorphous carbon

D. V. Kulikov, Yu. V. Trushin, V. S. Kharlamov, V. I. Ivanov-Omskii

A theoretical analysis is made of the formation of copper nanoclusters in a growing amorphous carbon film. The calculated size distributions of the copper clusters are compared with the experimental data. A numerical estimate is made of various kinetic parameters of copper in amorphous carbon.

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Nucl. Instrum. Methods Phys. Res. B
vol. 147, pp. 279–285, 1999

Modelling high-temperature co-implantation of N^+ and Al^+ ions in silicon carbide: The effect of stress on the implant and damage distributions

P. V. Rybin, D. V. Kulikov, Yu. V. Trushin, R. A. Yankov,
G. Ecke, W. Fukarek, W. Skorupa, J. Pezoldt

This work is an initial attempt to model the fundamental processes that occur when SiC is implanted at elevated substrate temperatures (200°–800°) with high doses of N^+ and Al^+ ions to synthesise buried layers of $(SiC)_{1-x}(AlN)_x$. The theoretical treatment has involved ballistic calculation of the implant and damage profiles by computer codes specifically developed for modelling multi-elemental targets. The influence of the mechanical stress induced the by implanted ions has been taken into account by a special term in the differential equations describing the evolution of distributions. Results of simulations have been correlated with data obtained by Rutherford backscattering spectrometry/ion channelling (RBS/C). The theoretical approach described has enabled one to determine the interaction energies of the interstitials with the internal stress field as well as the role of stress on the defect distribution.

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Inorg. Mater.
vol. 34, no 10, pp. 1042-1048, 1998

Dynamic simulation of radiation-induced defect formation in multicomponent layered materials in the cascade stage

B. J. Ber, Yu. A. Kudrjavtsev, Yu. V. Trushin,
E. E. Zhurkin, V. S. Kharlamov

A physical model is proposed for ballistic processes under high-fluence ion bombardment, with account of sputtering, ion-bean mixing, and accumulation of radiation-induced defects. Simulated sputtering depth profiles of Al/GaAs heterostructure are compared with experimental data.

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