Optical properties of InN with stoichiometry violation and indium clustering

T. V. Shubina[1], S. V. Ivanov[1], V. N. Jmerik[1], M. M. Glazov[1], A. Vasson[2], J. Leymarie[2], A. Kavokin[2], H. Amano[3], I. Akasaki[3], K. S. A. Butcher[4], Q. Guo[5], B. Monemar[6], and P.S. Kop'ev[1]

[1)]Ioffe Physico-Technical Institute, Russian Academy of Sciences, St.Petersburg 194021, Russia
[2)] LASMEA-UMR 6602 CNRS-UBP, 63177 AUBIERE Cedex, France
[3)] Meijo University, 1-501 Shiogamaguchi, Tempaku-ku, Nagoya 468-8502, Japan
[4)] Physics Department, Macquarie University, Sydney NSW 2109, Australia
[5)] Saga University, Saga 840-8502, Japan
[6)] Linköping University, S581 83 Linköping, Sweden

In spite of careful investigation of InN since the 1980s, using all modern spectroscopic techniques, its band parameters (band gap energy, effective masses) are still under debate. Among the objective reasons for that is the difficulty in the fabrication of high-quality InN epilayers, related to easy deviation from stoichiometric composition.

We report on the dependence of the InN main interband absorption edge on the N/In compositional ratio in a representative set (~25) of InN films grown by different techniques. The composition was determined by an energy dispersive x-ray analysis (EDX), while both conventional optical absorption and thermally detected optical absorption (TDOA) techniques were used to determine the edge. According to our data, the absorption edge in our InN films is near 1.35±0.15 eV, if the composition is close to stoichiometry (N/In~1). Deviation to the lower or higher energies corresponds to N/In<1 and N/In>1. We have proposed that the band gap, being a function of atomic *s* and *p* orbital energies which are strongly different for indium and nitrogen, should vary with both excessive atom incorporation and extraction (vacancies formation). The trends in the energy deviation with the incorporation/extraction of the N and In atoms, as well as the incorporation of oxygen, have been analyzed using the empirical nearest-neighbor tight binding theory.

Infrared (IR) optical properties of InN are also controlled by the interaction of an incident electromagnetic field with plasmon excitations in metallic In nano-clusters, whose formation is thermodynamically favorable in InN. The resonant extinction in the clusters can be successfully described by the Mie theory [1]. Our study reveals that the Mie resonances, being strongly dependent on the dielectric functions of both metal and semiconductor, can be shifted towards the near IR range in InN [2]. The variation of the Mie resonances is considered in regards with the dependence on the cluster shapes and orientations with respect to the field direction at different filling factors.

Comparison of the images collected with back scattered electrons, sensitive to atomic weights, and by micro-cathodoluminescence, recorded at 5 K, both from the surface and across the sample edge, demonstrates a spatial correlation between the 0.7-0.8 eV CL and the extended metallic inclusions. The relevance of the emission to specific transitions taking place near the metal/InN interface is discussed.

[1] G. Mie, Ann. Phys. (Leipzig) **25**, 377 (1908).
[2] T.V. Shubina et al., Phys. Rev. Lett. 92, 117407 (2004).