Optical constants of modified C_{60} determined by Kramers-Kronig analysis of reflection-electron-energy-loss spectroscopy data

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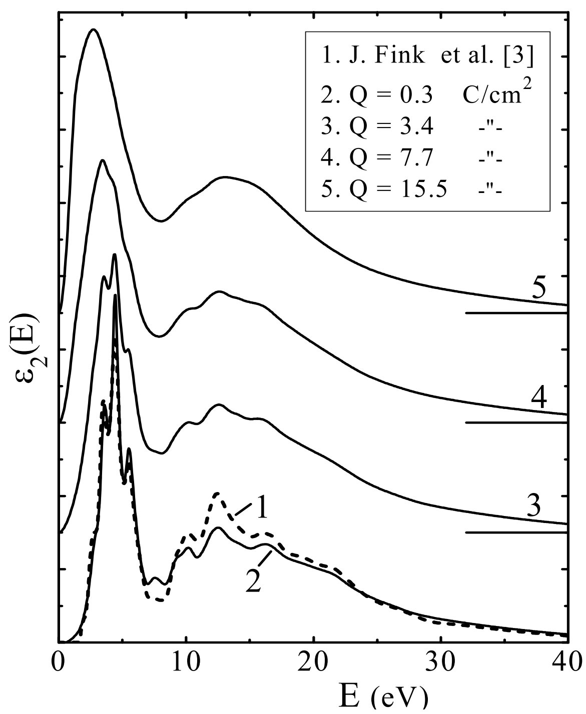
While the optical and electro-physical properties of pristine fullerite C_{60} have already been studied quite well the same properties of modified fullerite [1] are known much more poorly. In this work we present some results which can significantly bridge this gap.

A new calculation technique based on well-known the method of Kramers-Kronig transformation and including some other methods of reflection-electron-energy loss spectra (REELS) processing [2] has been developed. It was successfully applied for processing a set of REEL spectra acquired from C_{60} film modified with different doses (Q) of 1.5 keV electron irradiation and resulted in a set of corresponding dielectric functions $\varepsilon(E,Q)=\varepsilon_1(E,Q)+i\varepsilon_2(E,Q)$. Some of their imaginary parts $\varepsilon_2(E,Q)$ are shown in the figure, they demonstrate dynamics of electron induced transformation of fullerite C_{60} electron structure. The quality and validity of these functions are confirmed by close similarity between function $\varepsilon_2(E)$ obtained for pristine C_{60} using our technique of REELS data processing (curve 2) and the standard one obtained from the data of transmission EELS [3] (curve 2)). Dose dependent real $\varepsilon_1(E,Q)$ and imaginary $\varepsilon_2(E,Q)$ parts of modified C_{60} dielectric function can easily be transformed into any optical function of C_{60} (for instance, refraction and absorption indexes) corresponding to same dose of electron irradiation, thus, they contains an exhaustive information relating to electron and optical properties of this material.



A thorough analysis of obtained data allowed us to specify some details concerning induced transformation of solid C_{60} electron structure. It was found out that in the course of irradiation π-electron state fraction gradually grows from 0.18 in pristine C_{60} to ~0.22 in heavily modified one. The redistribution of electron states density is accompanied with a band gap collapse and noticeable decrease of fullerite C_{60} hybridization extent from $sp^{2.28}$ to $sp^{2.12}$.

The obtained results point out that fabrication of nanoscaled electronic and optical structures by means of electron probe modulating of the spatial structure of pristine C_{60} crystal has real technological prospects.

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[1] V.V.Shnitov, V.M.Mikoushkin, V.V. Bryzgalov and Yu.S.Gordeev, *Phys. Sol. St.* **44**, 428, (2002).
[2] G. Curro, F. Neri, G. Mondio, G. Compagnini, G. Foti, *Phys. Rev.* **B49**, 8411, (1994).
[3] E. Sohmen, J.Fink, and W. Kratschmer, *Z. Phys. (Condenced Matter)* **B86**, 87, (1992).