

## NETWORK STRUCTURE AND ELECTRONIC PROPERTIES OF ANNEALED NANODIAMONDS

**A.V. Okotrub<sup>1</sup>, A.I. Romanenko<sup>1</sup>,  
L.G. Bulusheva<sup>1</sup>, A.V. Gusel'nikov<sup>1</sup>, Ph.A.  
Pruss<sup>1</sup>,  
V.L. Kuznetsov<sup>2</sup>, Yu.V. Butenko<sup>2</sup>**

*Institute of Inorganic Chemistry SB RAS, pr.  
Ak. Lavrent'eva 3, Novosibirsk 630090,  
Russia*

*<sup>2</sup>Borekov Institute of Catalysis SB RAS,  
pr. Ak. Lavrentieva 5, Novosibirsk, 630090  
Russia*

The nanodiamonds (ND) samples were prepared by an explosive method and then were annealed in a high vacuum chamber at temperatures 1000–2100 K. Spherical and polyhedral onion-like carbon (OLC) particles prepared by annealing of nanodiamonds at 1600 and 1900°C were studied by X-ray emission spectroscopy. The  $CK\alpha$  spectra of OLC produced in the temperature range of 1600–1900 K were found to be markedly different from the spectrum of particles formed at 2140 K and characterized by better ordering of graphitic shells. The latter spectrum was shown to be very similar to the  $CK\alpha$  of polycrystalline graphite, while the former ones exhibited a significant increase of high-energy maximum that might be caused by the defect structure of graphitic networks forming at the intermediate temperatures. The experimental spectra were compared to the theoretical ones plotted by the results of quantum-chemical semiempirical AM1 calculation on a few models: fullerene molecule  $C_{240}$  having icosahedral structure,  $C_{240}$  incorporating a greater number of non-hexagonal rings, and a holed structure formed by removing pentagons from the icosahedral molecule. The density of high-energy electronic states in the valence band of graphitic cage was found to be practically invariant to a change in ring statistics but to significantly increase due to localization of electrons on the zigzag sites of a hole boundary.

The occurrence of holes in OLC formed at the lower temperature correlates with the results of magnetoresistance measurement. The electrical resistivity of annealed ND is characteristic of system with localized electrons and can be described in terms of variable hopping-length hopping conductivity. The magnetoresistivity of OLC is negative in range of field  $0 < B < 2$  T, and is positive at  $B > 2$  T. The conduction carrier concentration for OLC samples was estimated in the framework of the theory of

negative magnetoresistance in semiconductors in the hopping conduction region. The free path length for conducting electrons at liquid helium temperature was estimated from the data on positive magnetoresistivity.

An investigation of field emission properties of ND and OLC was performed. The dependence of emission current from the electric field strength for some samples may be interpreted by structure peculiarities of nanoparticles.

This work was supported by INTAS (Project No. 01-237) and the Russian Foundation for Basic Research (Projects Nos. 00-03-32463a, 00-03-32510a, 00-02-17987a).