# ELECTRONIC STRUCTURE AND ION-ELECTRON EMISSION OF NANODIAMONDS AND CARBON NANOTUBES

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Electronic structure of various fractions of the detonation nanodiamonds (ND) and different kinds of carbon nanotubes (NT) were probed using X-ray spectroscopy and X-ray photoelectron spectroscopy. The ND particles have been extracted from the detonation soot using a gradual oxidation procedure and than separated to fractions by centrifugation in the range of G-forces 46-40000 g. X-ray absorption spectra near the K-edges of carbon and oxygen and X-ray photoelectron spectra of the samples were recorded using the Berlin synchrotron radiation facility at the Russian-German laboratory in BESSY-II. The overview X-ray photoelectron spectra of ND fractions detected a presence of nitrogen and oxygen in samples. C1s- and O1s-lines of X-ray photoelectron spectra are split, while N1s-line is presented by a single narrow maximum. The spectral splitting could be caused by the induced charging of ND particles due to oxidized surface layer. Actually, intensity of satellite lines in the C1s- and O1s-spectra was found to correlate with ND agglomerate size and composition of ND surface. The satellite lines drift depending on duration and energy of the exciting synchrotron radiation. With lowering the radiation energy up to 330 eV, the satellite lines were disappeared and C1s-spectra of the samples were interpreted in the terms of chemical shifts under the effect of oxygen-containing functional groups.

Depending on kinetic parameters the products of ND annealing consist of onion-like carbon (OLC) or $sp^2/sp^3$ composites, comprised a diamond core enclosed by graphitic shells. The graphite-like shells were found to begin developing at temperature above 1200 K and almost completely cover a diamond core with ND annealing in the region of 1400–1600 K. When the temperature reaches 1800 K the particles formed have an onion-like structure. The final stage of ND annealing at the temperatures higher than 2000 K yields the hollow graphitic polyhedrons. X-ray fluorescent spectroscopy investigation of the annealing products detected a significant increase of density of high energy occupied states in the OLC compared with the polyhedral particles. The electronic states of interface were separated by subtraction of the ND and graphitic polyhedron X-ray spectra from the composite ones taking into account the true density data on samples. Localization of the electrons near the Fermi level was detected both for the valence and conductance bands of $sp^2/sp^3$ composites. X-ray spectroscopy study on the OLC particles found the strong enhancement of density of occupied states only. To interpret the experimental data the density functional calculations on models were carried out. The fragment of diamond, graphite, diamond/graphite hybrid, and the holed $C_{240}$ fullerene have been computed and the results were used for theoretical spectra plotting. We found the localized electronic states in the composite particles could be attributed to the three-coordinated carbon on the (111) diamond surface, while the origin of electron localization in OLC is non-bonding states of two-coordinated carbon atoms.

We recorded the ion current occurred in the result of d sorption of molecules from ND and NT surface in an electric field. A sawtooth voltage regulated the electric field with certain frequency of 0.01 - 5 Hz. The ion and electron currents and current-voltage characteristics of cathode were measured at a time. The correlations between the potential for ion current appearance and the electron emission threshold were established for different types of carbon nanostructures. The contributions in ion current from residual gas ionization and from ion emission of molecules adsorbed of nanoparticles surface were evaluated. To understand the experimental results in detail the quantum-chemical calculations on models were performed. Effect of electric field on the binding energy of various molecules adsorbed on the top and body of NT and ND was examined.