Chemical state of carbon atoms on nanodiamond surface: growth mechanism of detonation nanodiamond

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Identification of intermediate and final products of a chemical reaction is a key factor in understanding its mechanism. In nanodiamonds the only possible practical way of studying the chemical reactions of carbon atoms is the after synthesis analysis. As a result the identification of different possible chemical states of carbon atoms (such as graphite, diamond, carbon nanotubes, fullerenes, onion-like and adventitious carbon) is required. X-ray photoelectron spectroscopy (XPS) (including electron energy loss at C1s and valence band spectra) and N(E) CKVV Auger spectroscopy are eminently suitable techniques for such an identification since they provide chemical information from the top 2–10 monolayers.

Nanodiamond samples were produced by ALIT (Kiev), SCINTA (Minsk) and Diamond Centre (Saint-Petersburg) and studied before and after chemical cleaning by XPS and Auger spectroscopy.

It was found that the chemical state of carbon atoms is the same before and after chemical cleaning and it can be described as carbon atoms being sp^3-bonded inside nanodiamond particles and having a new unique chemical state on the surfaces. The latter differs significantly from sp^2- and sp^3-bonded carbon and can be figured as the valence band near the Fermi level being occupied by three electrons.

We propose the following mechanism of nanodiamond growth:

1. Formation of CO_2, CO, N_2, NO_X-molecules and C-atoms in the gas phase as a result of the detonation;
2. Recombination of C atoms and NO_X-molecules with the formation of nanodiamond nuclei with the unique chemical state of carbon atoms on its surfaces;
3. Interaction of C atoms and NO_X-molecules with the surface of nanodiamond nuclei which leads to the growth of nanodiamond particles with the formation of sp^3-bonded carbon atoms inside particles but without changing of the chemical state of carbon atoms on their surfaces. The process lasts until no carbon atoms are available for further growth.

These results are contradictive to the generally accepted conception of chemical state of carbon atoms on the nanodiamond surface. The reason of such a contradiction is that XANES and EELS results which are widely used can't provide reliable information on the chemical state of carbon atoms on the surface of nanodiamond particles.