Discussion the Chemistry of Nanodiamond Growth on the Basis of Surface Analysis

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One of the main goals of the surface science is the understanding of the elementary steps occurring in heterogeneous phases reactions. The surface sensitive XPS and XAES techniques were used in this work for identification of chemical states of carbon atoms in nanodiamond particles (NDP) and on their surfaces.

C KVV Auger spectra reflect the occupied valence band states of carbon atoms, with the information depth being about two monolayers. These spectra demonstrate high sensitivity to distinguish different carbon materials: OLC, SWCNT, C_{60}, MWCNT, adventitious carbon (AC), diamond and graphite. Loss spectra of C 1s photoemission are sensitive to the occupied π- and σ-states in valence band. The information depth in this case is about 2 nm.

NDP samples produced by ALIT (Kiev) and SCINTA (Minsk) were studied before and after chemical cleaning. It was found that all samples did not contain any graphite or AC before and after chemical cleaning. The chemical state of carbon atoms (CSCA) on surfaces of NDP was found to be unique and to differ significantly from those of standard sp^2- or sp^3-bonded carbon materials. The same CSCA was observed on surface of natural diamond after hydrogen treatment and on the Si-substrate under diamond CVD nucleation process. NDP is well known to promote diamond CVD growth. So, there is good reason to believe that above discussed CSCA is responsible for diamond nucleation and growth. The bulk chemical state of carbon atoms in NDP were determined to be sp^3.

The cause of the discrepancy between XPS/XAES and XANES/EELS data is discussed.

Our results allow supposing the following mechanism of NDP growth:

1) CO_2, CO, N_2, NO and C-atoms are formed in gas phase as a result of trinitrotoluene detonation;
2) C-atoms recombination results in the formation of nucleus, with the unique chemical state of carbon atoms on their surfaces being responsible for diamond nucleation and growth;
3) The growth of NDP goes through incorporation of C-atoms from gas phase into the nucleolus where sp^3-bonds formation occurs.