X-ray Diffraction Analysis of Nano-diamonds: Spatial Structure Computer Models

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The scheme of a diffractometer that employs high-intensity synchrotron radiation (SR) with monochromatization ($\Delta\lambda/\lambda = 4\cdot10^{-4}$) and practically without radiation polarization has been shown as well as experimental diffraction patterns of detonation nano-diamonds (DND) that were registered with the application of SR of the VEPP-3 storage accelerator, the Joint Usage Center at BINP SB RAS, Novosibirsk.

Experimental and theoretically-computed diffraction patterns of spherical nano-diamonds (ND) and graphite&diamond have been given. Theoretically-computed diffraction patterns are given. They point out a diffraction change when an interface arises, in the reflection area of diamond (111), (220), and (311): fullerene&diamond, nano-tube&diamond, icosahedral diamond (of 20 diamond tetrahedrons), fullerene&graphite&diamond, glycine&diamond (spherical and cylindrical models [111]), spherical nano-diamond with defects (replacement of alternating coordination spheres (CS) in nano-diamonds with compressed and extended CS. We used the models of spherical nano-diamonds to demonstrate the surface looseness to be up to 3 CS, density of the surface heterogeneity, possible existence of nano-diamonds with an equal number of atoms in their core and shell etc. A method has been given to find out parameters of the crystal lattice of detonation nano-diamonds (DND) along with their size basing on comparison of an experimental diffraction pattern and a diffraction pattern theoretically computed according to the spatial structure model. This method is an alternative to another one based on the diffraction equation $n\lambda = 2d_{hkl}\sin\theta_{hkl}$. We have demonstrated computer models of nano-diamonds (ND), including hybrid spherical two-phase nano-diamonds of the shell&core type: spherical nano-diamonds, graphite&diamond, fullerene& graphite&diamond, glycine&diamond etc.