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Diffraction Studies of Nanocrystalline Diamond and SiC in Real and Reciprocal Spaces. Bogdan Palosz, Inst. of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland.

Nanocrystals have a non-uniform structure, where the arrangement of atoms in the grain interior (the core) is different than that at the surface (the surface shell). This difference may be very small and missed in a conventional diffraction experiment. We show that the key in a quantitative characterization of the atomic structure of nanocrystals is acquiring a diffraction data in a very large range of the reciprocal space ($Q = 20\text{-}30 \text{ \AA}^{-1}$), what requires high energy X-rays or hot neutrons. Only such data can provide the accuracy needed for a meaningful description of the atomic structure of nano-grains. It concerns the analysis in real (Bragg) as well as in reciprocal spaces (PDF). With application of very large- Q neutron diffraction at LANSCE (HIPPO and NPDF stations, Q up to 50 \AA^{-1}) we were able to examine distribution of strains in nano-diamond and SiC as a function of the grain size, and trace their evolution in nano-ceramics sintered under high pressures. Also, using the Wilson method, different atomic thermal vibrations of the inner and surface atoms were evaluated.

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