

High Pressure Diffraction Studies of Nanocrystalline Materials

B. Palosz, S. Stel'makh, E. Grzanka, S. Gierlotka, & W. Palosz*

High Pressure Research Center UNIPRESS, ul.

Sokolowska 29/37, 01 142 Warsaw, Poland

** BAE Systems/NASA, Huntsville, Alabama 35812, USA*

Key words: **nanocrystals, high pressure, surface structure, diffraction.**

Experimental evidence obtained for a variety of nanocrystalline materials suggest that the crystallographic structure of a very small size particle deviates from that in the bulk crystals. In this paper we show the effect of the surface of nanocrystals on their structure by the analysis of generation and distribution of *macro*- and *micro*-strains at high pressures and their dependence on the grain size in nanocrystalline powders of SiC. We studied the structure of SiC nanocrystals by in-situ high-pressure powder diffraction technique using synchrotron and neutron sources and hydrostatic or isostatic pressure conditions. The diffraction measurements were done in HASYLAB at DESY using a Diamond Anvil Cell (DAC) in the energy dispersive geometry in the diffraction vector range up to $3.5 - 4 \text{ \AA}^{-1}$ and under pressures up to 50 GPa at room temperature. In-situ high pressure neutron diffraction measurements were done at LANSCE in Los Alamos National Laboratory using the HIPD and HIPPO diffractometers with the Paris-Edinburgh and TAP-98 cells, respectively, in the diffraction vector range up to $26 \text{ \AA}^{-1}$ and under pressures up to 8 GPa.

Examination of the response of the material to external stresses requires non-standard methodology of the materials characterization and description. Although every diffraction pattern contains a complete information on *macro*- and *micro*-strains, a high pressure experiment can reveal only those factors which contribute to the characteristic diffraction patterns of the crystalline phases present in the sample. The elastic properties of powders with the grain size from several nm to micrometers were examined using three methodologies: (1), the analysis of positions and widths of individual Bragg reflections (used for calculating *macro*- and *micro*-strains generated during densification) [1], (2), the analysis of the dependence of the experimental apparent lattice parameter, *alp*, on the diffraction vector *Q* [2], and (3), the atomic Pair Distribution Function (PDF) technique [3]. The results of our studies show, that SiC nanocrystals have the features of two phases, each with its distinct elastic properties.

[1] B.Palosz, et al; J. Phys.: Condens. Matter **16** S353-S377 (2004).

[2] B.Palosz et al., Phase Transitions, **76**, 171-185 (2003).

[3] B. Palosz et al., Mat. Res.Soc. Proc. **778**, U1.11.1-6 (2003).