

NANOCRYSTALS UNDER HIGH PRESSURE

B. Palosz, E. Grzanka, S. Gierlotka, and S. Stelmakh

Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokolowska 29/37, 01 142 Warszawa, Poland

Keywords: high pressure, nanocrystal, strain distribution, bulk modulus, Bragg reflection

e-mail: palosz@unipress.waw.pl

This work concerns application of high-pressure X-ray diffraction to examination of the structure of nanocrystalline materials. In general, high pressure is a unique tool for investigation of interatomic interactions: high pressure suppresses the interatomic distances and, thus, "forces the material" to show the nature of interactions between its components like atoms/ions or lattice defects [1]. A tentative model of a nanocrystal assumes that it has a non-homogeneous structure [2]. High-pressure diffraction technique can serve for determination of different elastic properties of inner and surface parts of the nanocrystalline grains, which relate directly to different lengths of the atomic bonds in the interior and at the surface of the grains. Here, application of *in situ* high pressure powder diffraction technique for examination of specific structural properties of nanocrystals is demonstrated for nanocrystalline powders of diamond and SiC having the average grains dimension from several to several tens of nm in diameter. Limitations and capabilities of the experimental techniques themselves and methods of diffraction data elaboration applied to nanocrystals with very small dimensions (< 30 nm) are discussed.

High-pressure *in situ* diffraction experiments were performed in DAC at Station F3 under the pressure of up to 40 GPa. The high pressure, high temperature experiments were performed in the six-anvil cubic press MAX80 at Station F2.1, HASYLAB at DESY, Hamburg. The measurements of *micro*- and *macro*-strains were performed for dry powders and in different pressure media.

Examination of polycrystals under pressure using diffraction methods is a well established technique. For polycrystalline materials high pressure studies are dedicated to studies on phase transformation, measurements of physical parameters like compressibility, characterization of microstructural behaviour like deviatoric stresses, *micro*-strains, yield strength, etc. In this work, dedicated to nanocrystalline powders of diamond, SiC and GaN, we attempt to find out if there are any specific properties of these materials which are dependent on, and correlated with, (1) the grain dimensions and, (2) the surface of the crystallites. For "ordinary polycrystals" both such effects can be ignored, but may be significant in nanocrystalline materials. In the analysis of the lattice compression one finds, that the lattice parameters determined from the positions of Bragg reflections do not have the usual meaning of a constant. What one calculates for individual reflections are "apparent lattice parameters", alp , the value of which

depends on the reflection [2]. This is due to a complex structure of a nanocrystal constituting a two-phase, core/surface shell system, for which a unique value of the lattice parameter loses its meaning. In consequence, no unique compressibility coefficient can satisfactorily describe the behaviour of nanocrystals under pressure. We offer a tentative interpretation of the distribution of *macro*- and *micro*-strains in nanoparticles of different grain size.

Because a nanocrystalline specie constitutes a two-phase (core-shell) system, Fig. 1, there is an obvious uncertainty as to the real meaning of the measured values of the apparent lattice parameters as determined from the Bragg reflections. This causes that evaluation of the elastic properties of nanocrystals requires a new approach. In this work we attempt to determine the type of the real structure of nanocrystals in comparison with conventional polycrystalline samples. We conclude that nanocrystalline samples should be characterized by two moduli (that of the core and that of the shell). Similar dilemma concerns the yield strength of nanocrystals.

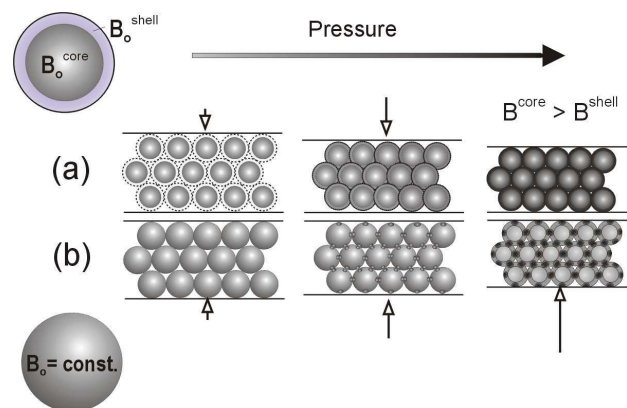


Figure 1. Compression of (a) core-shell structure of a nanocrystal and (b) a perfect small single crystal

Acknowledgements: The authors are indebted to staff of F3 and F2.1 Stations at HASYLAB by DESY for continuous support during numerous experiments there performed.

References

- [1] B. Palosz, S. Stelmakh, E. Grzanka, S. Gierlotka, R. Pielaszek, U. Bismayer, S. Werner, and W. Palosz, *J. Phys.: Condens. Matter* **16** (2004) S353-S377.
- [2] B. Palosz, S. Stelmakh, E. Grzanka, S. Gierlotka, W. Palosz, "Nanocrystallography", in: *Z. Kristallography*. **222** (2007) 580-594.