

Surface relaxation in nano-diamonds examined with application of real and reciprocal space methods

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Structure of commercial UD96 powder from Microdiamant AG and the same powder purified by different chemical treatment procedures using ozone and a mixture of sulfuric acid/chromic anhydrite mixture were examined using large-Q neutron diffraction (NPDF at LANSCE). Both real (PDF) and reciprocal (Bragg) space analysis was employed to examine a tentative core-shell model of nanodiamond powders. Elaboration of diffraction data was based on the concept of the "apparent lattice parameters" (alp), i.e. on determination of the values of lattice parameters calculated for individual Bragg reflections and supplemented by PDF analysis. Nanodiamond grains show a nonuniform structure where the outmost surface shell of about 3 Å thick shows a diamond type structure which is expanded by 3-5% compared to the diamond lattice in the grain interior - in the core. Analysis of the diffraction data was performed assuming that a single grain has, (i), a simple core shell structure or, (ii), a complex multi-shell structure where the tensile strain present in the outmost surface layer is relaxed through a modulation of compressive and tensile strains present in radial direction. There is a non-diamond envelope surrounding individual nano-grains, which behaves as a "gas-like" carbon stable up to 1000°C, and which transforms into a graphite-type phase at about 1200°C. Depending on chemical and thermal treatment of nanodiamond the lattice parameter of the crystalline nanograin core changes by about 0.1%.