s8.m28.p8 **The Analysis of the Diffuse Background on C60 Fullerite X-Ray Pattern.** Liubov Lugovskaya, Liudmila Aleshina, Anatoly Fofanov, Roman Osaulenko. *Petrozavodsk State University, Petrozavodsk, pr. Lenina, 33, 185640, Russia. E-mail: LiubovL@psu.karelia.ru*

Keywords: C60 fullerite; X-Ray; Amorphous component

X-ray researches of a powder sample of fullerite C60 were carried out on Cu K_{α} radiation. The X-ray pattern is indexed in cubic syngony with the unit cell period is equal (14.19±0.01) Å, space group is Fm $\overline{3}$ m. Interesting feature of the x-ray pattern is availability a diffuse background that testifies to presence at a sample of an amorphous component. The purpose of the given work was determination of the short-range order type in amorphous component in a cubic fullerite sample. Scattering intensities normalized by Warren method were compared to the experimental intensity distributions for amorphous carbon and schungite. Intensity distributions for amorphous components of a fullerite, amorphous carbon and schungite are sharply various. Distributions curves of s - weighed interferential functions H(s) and pair functions D(r) were calculated from the fullerite normalized intensity. Position of the first maximum on D(r) curve makes 1.53 Å, the first coordination number is equal 4, the average electronic density is equal 1.05 $Å^{-3}$. The specified values correspond to the similar data for two crystal carbon modifications: diamond and lonsdalite which is called hexagonal diamond. The shortest interatomic distance for C60 fullerene is equal 1.41 Å, and the coordination number is equal 3. Values of radiuses of the coordination spheres and the coordination numbers estimated for the fullerite amorphous component, sufficiently enough correspond to calculations for lonsdalite. Dispersions of coordination spheres are great, that is the configuration is strongly deformed. Also the calculations of diffraction patterns were carried out by Debye formula for a) single C60 molecule; b) the atom configuration corresponding to 25 unit cells of lonsdalite with the size (1a·5b·5c) and c) atom configurations in one unit cell of diamond. Positions of diffuse background maxima of an experimental curve correspond to results of model calculation for lonsdalite. The model curves of intensity distribution for fragments of C60 fullerene did not give concurrence to experiment in the field of first two maxima. Moreover, the following two maxima on fullerene C60 model curves are displaced and decrease on intensity. Thus, the short-range order in amorphous component of cubic C60 fullerite is formed on lonsdalite type.

s8.m28.p9 **Real Structure Analysis of Nanocrystalline and Submicrocrystalline Materials Using X-Ray Diffraction.** Zdenek Matej, Viktoria Cherkaska and Radomír Kuzel, *Department of Electronic Structures, Faculty of Mathematics and Physics, Charles University in Prague, Ke Karlovu 5, 121 16 Praha 2, Czech Republic. E-mail: matej@karlov.mff.cuni.cz*

Keywords: Profile analysis; Nanocrystalline materials; Deconvolution

Physical properties of nano- and submicro-crystalline materials are attractive object of study for research and industry development. Small size of coherently scattering domains and presence of lattice defects is the well-known reason of diffraction line broadening. Conventional way of X-ray line broadening analysis is based on integral breadths β or FWHMs (Williamson-Hall plot) or on Fourier coefficients (Warren-Averbach method). Description of line broadening can be phenomenological or it can be connected to a model of material microstructure. Single line Fourier coefficients as well as whole powder diffraction pattern can be calculated from such phenomenological or microstructure models. The anisotropic broadening, asymmetry and shift of diffraction lines can be accounted by a microstructure model. Simple shape (sphere, cube) of grains and lognormal distribution of their size is assumed in most cases. The Wilkens model of restrictedly random dislocations can describe deformation component of line broadening. Parameters of this model (dislocation density ρ and a R_e parameter describing dislocation correlation) and usually also two parameters of the size effect model can be determined and refined by the analysis of measured diffraction patterns. An interesting way of diffraction pattern analysis is represented by new methods based on the whole power pattern fitting [1], [2] (WPPM - introduced by the group of P. Scardi) and the multiple whole profile and Fourier coefficients fitting [3], [4] (MWP-fit - by team of T. Ungár). These methods are still in progress and authors of these methods are developing applicable software (PM2000 [1], [2], MWP-fit [3], [4]). New methods and relevant programs (MWP-fit and PM2000) are applied to nano- and submicro-crystalline samples of copper, iron and germanium obtained by high-pressure torsion deformation. Results of new and traditional methods are compared and potential of the X-ray analysis in the study of microstructure of nanocrystalline materials is demonstrated. It is shown that new methods of line profile analysis can reliably separate the size and strain broadening. The main problem is a correlation of two size parameters and especially the dislocation density ρ and the cut-off radius parameter R_e. Improvement of microstructural model for description of nanocrystalline materials obtained by severe plastic deformation is desirable. All measurements were realized on common laboratory diffractometers and hence for some methods (program MWP-fit, Warren-Averbach method) diffraction data deconvolution [5] was necessary.

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