The analysis of the diffuse background on C60 fullerite x-ray pattern.

Liubov Lugovskaya, Liudmila Aleshina,
Anatoly Fofanov, Roman Osaulenko.
Petrozavodsk State University, 185640, Russia,
Petrozavodsk, pr. Lenina, 33

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 $Fm\bar{3}m$. 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.

The research described in this publication was made possible in part by Award No. PZ-013-02 of the U.S. Civilian Research & Development Foundation for the Independent States of the Former Soviet Union (CRDF) and of Ministry of Education of Russian Federation