Nanocomposites and nanomaterials

Study of the structure of ball-milled fullerenes C_{60}

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The structural changes that occur in fullerenes C_{60} at mechanical activation processing are studied. Based on model atomic configurations obtained by reverse Monte Carlo method, the quantitative characteristics describing the structure of fullerite C_{60} in the initial state and after ball-milling are established.

The bond angles distributions for the reconstructed atomic configurations in fullerenes C_{60} in the initial state and ball-milled ones were calculated. It was shown that it is characterized for the pristine fullerenes C_{60} by a broad maximum, which decomposes into two components with the positions of ~ 110 and ~ 117°. It stays in place after ball-milling treatment for 1 hour, but a low intensive broad asymmetric maximum with position of ~60° appears, what indicates displacements of carbon atoms from equilibrium positions in the structure of molecules C_{60}. Further increase of milling time results in disappearance of maxima characteristic of structure of the molecule. The distribution takes the form typical for carbon materials in the amorphous state [1,2].

Statistical analysis of atomic rings in the structure of ball-milled fullerenes was performed using S. King criterion. The pristine molecule of C_{60} is characterized by 5- and 6-fold rings. At the initial stage of ball-milling treatment (1-3 hours) the molecules partially decomposes into individual atoms, what results in appear of essential amount of 3-fold rings with simultaneous decrease of the percentage of 5- and 6-fold ones. After 14 hours of the processing, 3-fold rings are dominated in the carbon material produced, what indicates full amorphization of fullerenes C_{60}.

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1. *Rud A. D., Kiryan I. M.* Quantitative analysis of the local atomic structure in disordered carbon // J Non-Cryst. Solids. – 2014. – **386**. – P. 1-7.
2. *Rud A.D. , Kirian I.M. Lakhnik A.M.* Topological characteristics of local atomic arrangements at crystalline-amorphous structural transition in graphite // http://arxiv.org/pdf/1412.1982v1.pdf