UNIDIMENSIONALLY DISORDERED STRUCTURES IN CRYSTALLINE FULLERITE FILMS

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Fullerite, the condensed crystalline phase of fullerene molecules bounded with Van der Waals forces, is a new and extremely interesting object for physics of carbon materials.

According to current notion C_{60} fullerene crystal (fullerite) at the room temperature and normal pressure possesses f.c.c. lattice (Fm3m spatial group), with each node corresponding to one C_{60} molecule performing almost free rotation. In spite of distinction of the molecules shape from spherical (actually they are truncated icosahedrons), the rotation enables centrosymmetric nature of dispersion interaction between neighbor molecules and their close packing [1].

High interest to thin fullerite-based films is caused by their physical and physico-chemical properties. It was found that they have non-linear optical characteristics, are promising materials for solar energy converters, exhibit high tribological characteristics, may be used to production of superhard coatings, etc. That stimulated appearance of a lot of works, devoted to investigations of crystal structure, growth mechanisms, and search of fields of applications for such films.

C_{60} fullerite thin films are characterized by close packed f.c.c. structure with the lattice parameter of 1.416 nm. According to observations of various authors, C_{60} films have different structure states, phase transformations. However it turned out, that only a few works devoted to detailed investigations of crystalline defects of C_{60} fullerite thin films.

Real close packed crystals of h.c.p. and f.c.c. structures in many cases contain stacking faults, which mutual arrangement may be not chaotic, but ordered, what results in formation of superlattices of stacking faults. An interest in study of such structural states is determined by the fact that these states may occur in the materials possessing unique physical properties [2]. C_{60} fullerite films are good object for study of such structures.

In our previous investigations [3] it have been shown that at the most TEM micrographs of C_{60} films, taken at moderate resolution mode, the characteristic banded contrast is observed, indicating presence in the structure a lot of bidimensional defects (fig.1). A detailed analysis of electron diffraction pattern confirmed that such contrast is caused by defects like stacking faults, twin boundaries, or partially disordered polytype phases.

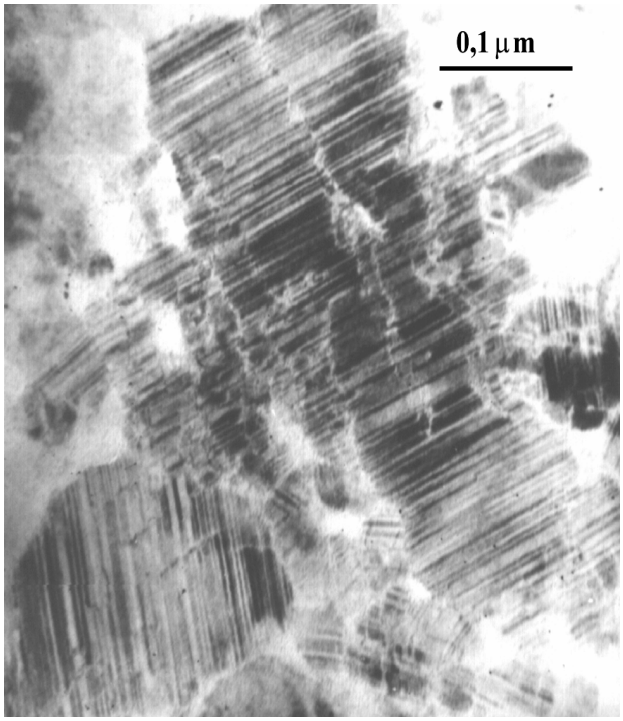
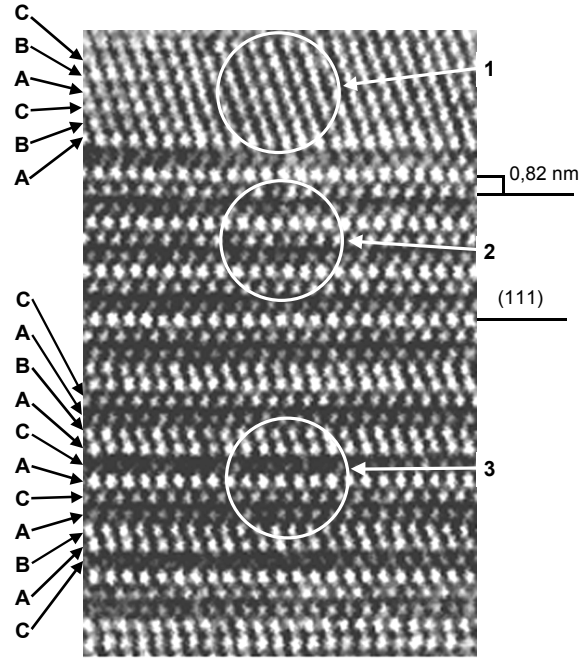


Figure 1. Banded contrast on TEM micrographs approving that C_{60} fullerite films contain a lot of planar defects.

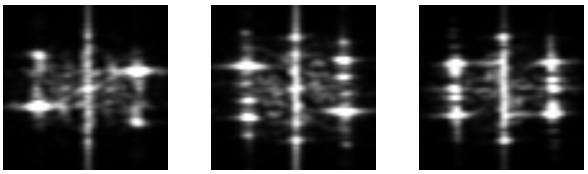
In the structure of C_{60} fullerite films the areas exist where beside the twins and individual stacking faults a polytypic structure is observed with ordered positioning of stacking faults on the planes of (111) type. For the purpose of detailed analysis a fragment of the structure with the polytype is shown at the fig.2.

For the designation of layers alternation the certain sequence of letters ABCABC, etc., is used, each of the three letters corresponding to the one of the three possible positions of the (111) plane in close packed structure. At the top area of the image the sequence of ABCABCABC… is realized, that corresponds to f.c.c. structure. At the bottom area of the image the order of layers alteration of CABACACABAC… is characteristic, that corresponds to ten-layered polytype structure. Analyzing the image we can see that

between the areas of f.c.c. structure and polytype structure an area of h.c.p. structure exist.



a



b

Figure 2. The structure of C_{60} film with polytype: **a** – high resolution electron micrograph showing fragments of f.c.c. structure (1), h.c.p. structure (2), and the polytype CABCACABAC (3); **b** – simulated by Fourier transform diffraction patterns from areas 1-3.

Conclusions

For the fullerite crystals the co-existance of different close packed structures is typical. It results from weak Van der Waals binding forces between the fullerene molecules in a solid phase. It is known that at a room temperature as well as at higher temperatures spherical molecules of fullerene, while keeping their position in certain nodes of crystal lattice, at the same time freely rotating around their centers. For such molecular crystals extremely low stacking fault energy should be characteristic. One may expect that such crystals will easily twin, will contain significant number of stacking faults, twin boundaries, and other planar defects. The possibility of formation of different polytype structures in such crystals is very high. They are such polytype states that we observe at the images, obtained by high resolution TEM.

References

1. Natsik V.D., Lubenets S.V., Fomenko L.S. // Fizika Nizkih Temperatur. – 1996. vol.22. №3. – P. 337. (In Russian)
2. Olikhovskaya L.A., Rud A.D., Ustinov A.I., Chuistov K.V. // Metallofiz. Noveishie Tekhnol. – 1986. vol.10. №3. – P. 32-37. (In Russian)
3. Solonin Yu.M., Grayvoronskaya E.A., Galiy O.Z. // Poroshk. metal. – 2001. vol.91. № 11/12. – P. 91-99. (In Russian)