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Measuring of fullerene molecular form factor in condensed C_{60} films

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Dependence of the fullerene molecule form factor on the (*hhh*) reflection order has been measured in experiment for epitaxial C_{60} films prepared by condensation in quasi close volume. The experimental dependence has been found to be close to theoretical one calculated using the rotation model. It is shown that the molecular diameter can be determined accurately by measuring the argument of $\sin(\pi nD/d_{hhh})$ using the integral intensity ratio of 6^{th} and 7^{th} order (*hhh*) reflections and determining independently the interplanar spacing d_{hhh}.

Экспериментально измерена зависимость модуля формфактора молекулы фуллерена от номера порядка отражения (*hhh*) для эпитаксиальных пленок C_{60}, полученных конденсацией в квазизамкнутом объеме. Установлено, что экспериментальная зависимость близка к теоретической, вычисленной по модели вращения. Показана возможность прецизионного определения диаметра молекулы *путем измерения величины аргумента функции* $\sin(\pi nD/d_{hhh})$ по соотношению интегральной зависимости шестого и седьмого порядков отражения (*hhh*) и независимого измерения межплоскостного расстояния d_{hhh}.

Recently, several works have been published aimed at fullerene matrix doping with semimetals, elemental semiconductors and semiconductor compounds [1–3]. The interaction of intercalated semiconductor atoms and molecules with C_{60} ones must result in a dramatic changes in the material electron properties. A wide application variety has been forecast for those materials in optoelectronics, solar energetics, and formation of functional layers in organic semiconductor devices [2, 4, 5]. The doping changes substantially the fullerene matrix properties due mainly to changes in the C_{60} molecule electron shell. These changes must manifest themselves as changes in the molecule X-ray form factor that can be revealed using the integral intensity dependence on the reflection order [7].

The fullerene molecule form factor, F_m, can be calculated in the frame of rotation model [7, 8]. According to that model, centers of 60 carbon atoms are statistically distributed over the surface of a sphere:

$$F_m = 60 f_C \cdot \frac{\sin(\pi SD)}{\pi SD}, \qquad (1)$$

where f_C is the carbon form factor; $S = 2\sin\theta/\lambda$, D being the fullerene molecular sphere diameter. For the Bragg (*hkl*) reflections, $S = 1/d_{hkl}$, where $1/d_{hkl}$ is the reciprocal lattice vector module. Therefore, the argument of $\sin(\pi SD) = (\pi D/d_{hkl})$. Measuring d_{hkl} from the Bragg reflection positions, the fullerene molecule diameter D and its changes under various factors can be determined using the form factor dependence on the reflection order.

The purpose of this work is to determine experimentally the form factor dependence on the (*hhh*) reflection order for C_{60} films and to elaborate a procedure for calculation