A dense new version of crystalline carbon C_8

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By condensation of carbon plasma flow in a vacuum, a new cubic form of carbon was synthesized and identified for the first time by the electron-diffraction method. It has a crystal structure *Im* 3 (No. 204) with 16 atoms in a cell. The calculated density is equal to 4.1 g/cm^3, which exceeds by 15% the density of cubic diamond.

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Condensation of high-speed flow of carbon plasma on cooled substrates makes it possible to synthesize and conserve different modifications of carbon under normal conditions.[1,2]

In this paper we report a new, diamond-like modification of carbon obtained by us, whose density is close to that of the metallic form of diamond, and we analyze the structure of this modification.

The experimental setup and the technique of depositing the diamond-like layers are described in Ref. 3. The crystal structure of the carbon films was investigated with

TABLE I. Electron-diffraction pattern of the carbon phase.

$h^2+k^2+l^2$	hkl	d_{exp}	$d_{calc.}$ [1]	$I_{calc.}$ [2]
2	011	3,02	3,025	100
4	002	2,13	2,139	87
6	112	1,74	1,746	11
8	022	1,52	1,513	14
10	013	1,352	1,353	69
12	222	1,234	1,235	1
14	123	—	1,144	17
16	004	—	1,070	8

the ÉMV-100 L electron microscope. We used thin carbon films 200–1000 Å in thickness, which were deposited on a freshly cleaved KCl single crystal.

The carbon films were largely a homogeneous condensate. The micro electron-diffraction pattern of this material has diffuse rings with the interplanar spacing 2.09 (2), 1.15 (4), 0.74, and 0.59 Å, indicating that the "quasi amorphous" phase has a high dispersion (10–20 Å). In addition we observe individual formations measuring 100 to 3000 Å. We obtained from these formations single-crystal (with axes of the [001] and [011] bands) and polycrystal electron-diffraction patterns (Table I), which are indexed in the cubic system with a body-centered lattice period of 4.28 Å.

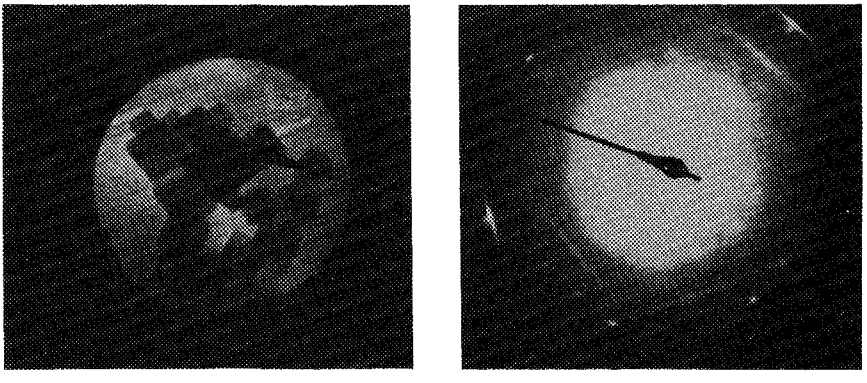

FIG. 1. Electron-microscope pictures of highly dispersed carbon film with morphologically formed crystals: a—Single crystals of the cubic system up to 2.8×10^{-5} cm in size (×42000); b—electron-diffraction pattern of the phase with a perfect structure.

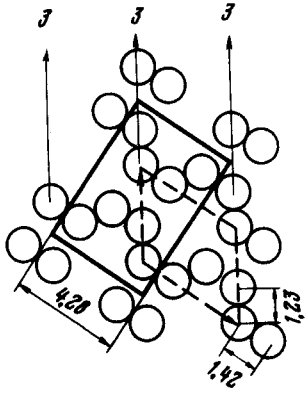

FIG. 2. Atomic plane (011) in the $Im\,3$ structure (No. 204, 16*c* in $16f\,(x, x, x)$ at $x = 1/6$.

The electron-diffraction patterns of the deposits of faceted microcrystals up to 3000 Å in dimension were examined (Fig. 1a). The morphology of the crystals indicates that they belong to the cubic system. The micro electron-diffraction pattern with Kikuchi lines (Fig. 1b) obtained from them shows that they are essentially perfect crystals. The interplanar spacing, which is also indexed in the body-centered cube with a period of 4.34 Å, was determined from the pairs of Kikuchi lines. This indicates that the crystal structure of the faceted crystals is identical to the polycrystal formations observed in the film.

On the basis of extinction of the body-centered cube (Table I) and the structural-type Le and Si,[4] to which the synthesized carbon phase can be related because of the proportionality of the period, we determined the space group No. 204 with 16 carbon atoms in the cell in the $16f$ position (x, x, x) at $x = 1/6$. The intensity of the diffraction maxima for the polycrystal, which was calculated from the proposed model, is in agreement with the visual estimate of the intensity of the diffraction rings in the electron-diffraction pattern.

The arrangement of the carbon atoms in the structure is shown schematically in Fig. 2. The synthesized phase consists of coordination tetrahedrons, which are identical to cubic and hexagonal diamonds but with a closer packing. The coordination number in the structure, as in diamond, is 4, but its coordination tetrahedron is slightly deformed. The density of the material, $\rho = 4.1$ g/cm^3, was determined from the number of atoms (16) in the unit cell and from its volume. This value, which exceeds the density of cubic and hexagonal diamonds by 15%, is close to the density of metallic carbon, whose existence at a static pressure of 1 Mbar has been proved by Vereshchagin *et al.*[5]

The high density of the new phase, which crystallizes in a finely divided carbon film, should evidently lead to high mechanical properties for the condensate. In fact, the microhardness of the 10–20 μm thick diamond-like carbon films exceeds that of the more densely packed (111) faces of natural diamond single crystals.[6]

[1]Calculated value for the lattice constant $\alpha = 4.279$ (4) Å.

[2]Values computed from the formula $p|F_{hkl}|^2 d_{hkl}$, where p is the recurrence factor, $F_{hkl} = f \times 48 \cos 2\pi hx \times \cos 2\pi kx \times \cos 2\pi lx$, f is the atomic scattering function for electrons, and $x = 1/6$.

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