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FORMATION OF A FILM-SUBSTRATE INTERFACE IN THE SILICON-DIAMOND SYSTEM

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The paper presents results of research on the forces of interaction of a pair of isolated carbon atoms and of a carbon atom in the gas phase with diamond and silicon substrates in relation to the distance between them. Based on the results obtained, the conclusion is drawn that the transition of atoms to an ordered array in formation of a single-crystal film is caused by the forces of interaction between atoms of the precipitate whose electronic structure can change with a change in the energy of interaction.

In recent years, in connection with the demands of practice, intense efforts have been made to find a method for obtaining homogeneous epitaxial films of diamond. Available predictions indicate that such films possess the best and reproducible properties and a long working life. It is known that devices produced on the basis of silicon, germanium, gallium arsenide, and other semiconducting materials with admixtures introduced to obtain the necessary type of conductivity age rapidly; this is not typical of devices manufactured on the basis of diamonds. Application of homogeneous epitaxial films of diamond in engineering will make it possible to employ its unique features and produce long-life different-purpose devices of extremely high quality. However, the manufacture of such films that comply with the requirements of modern production is associated with certain difficulties that up to now cannot be overcome within the limits of the existing concepts.

Up to now there is a widely held view [1] that atoms condensed on the face of a crystal experience the influence of the force field of the crystal lattice, which strives to continue the "bricklaying" that at one time led to formation of the substrate. In other words, the substrate forces new atoms to be arranged in a certain order. It is meant here that an atom or a molecule is regarded as a structural unit that can be an invariant part of a lattice. In our opinion, these ideas are wrong and are the main reason for futile attempts at obtaining homogeneous epitaxial films of diamond.

The aim of the present work is the determination of the structure of the force field of diamond and silicon substrates, the creation of a model of the boundary layer between adjoining phases, and the laying of a foundation for the new approach suggested by us to solve the problem of the building up of homogeneous epitaxial diamond films.

On the basis of the Mie equation [2]

$$U = Ar^{-n} - Br^{-m} \tag{1}$$

(where U is the potential energy between molecules at the distance r from one another; A, n, B, and m are constants) we determined the forces of interaction of carbon atoms that are not valence-bound in relation to the distance between them for an isolated pair of particles and of interaction of an atom of the gas phase with a crystal substrate. For the relative force of interaction F/F_{max} of an isolated pair of particles as a function of the distance between them the following expression is obtained:

$$\frac{F}{F_{max}} = \frac{\left(\left(\frac{m+1}{n+1}\right) r_{min}^{n-m} r^{-n-1} - r^{-m-1}\right)}{\left(\frac{m-n}{n+1}\right) r_{min}^{-m-1}}, \tag{2}$$

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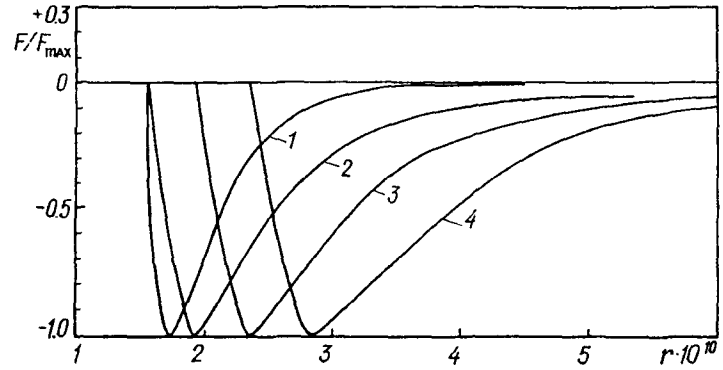

Fig. 1. Dependence of the relative force of interaction between atoms as a function of the distance r between them: 1) of an isolated pair of carbon atoms, 2) of a carbon atom of the gas phase with a diamond substrate, 3) the same, with a silicon substrate, 4) of a silicon atom of the gas phase with a silicon substrate. r, m.

where F_{max} and F_{min} are the force and the interatomic distance that correspond to the minimum of the curve $F(r)$.

The relative force of interaction of a substrate with gas-phase atoms that are located an arbitrary distance r from the plane of the surface can be represented in the form

$$\frac{F}{F_{max}} = \left[\frac{r_{min}^{n-m} r^{-n+2}}{(n-2)} - \frac{r^{-m+2}}{(m-2)}\right] \Big/ r_{min}^{-m+2} \left[\frac{m-n}{(m-2)(n-2)}\right]. \quad (3)$$

Curves of the relative force of interaction between atoms as a function of the distance between them, calculated by us from formulas (2) and (3), are presented in Fig. 1. From this figure it is seen that the dependences of the relative force of interaction between both isolated atoms and gas-phase atoms and the substrate on the distance between them are depicted by similar curves each of which is characterized by the horizontal asymptote $F = 0$ at $r = \infty$ and the vertical asymptote $F = \infty$ at $r = 0$. Although the curves are somewhat displaced with respect to one another, they all confirm the same fact that at large distances r the atoms virtually do not interact either with one another or with the substrate. As the distance r decreases, attractive forces appear that in absolute value increase up to a certain distance r_{min} but then decrease and at $r = r_0$ become equal to zero. With a further decrease in r repulsive forces that increase prevail, tending to infinity as $r \to 0$. The state in which $r = r_0$ and the forces of interaction are equal to zero and the potential energy is at a minimum corresponds to the position of equilibrium.

The foregoing data (Fig. 1) show that the force field of the substrate has a considerable value only in the interval $(r_0, 3r_0)$, whereas at large distances it is negligibly small and cannot exert a substantial influence on the formation of the atomic structure of the precipitate. Therefore the long-standing idea that the structure of an epitaxial film is formed by the force field of the substrate is incorrect. In actual fact *the reason for the transition of atoms to an ordered arrangement in formation of an epitaxial film is the presence of forces of interaction between atoms of the precipitate whose electronic structure can change with the interaction energy* [3]. Guided by this idea, we constructed a two-dimensional model (Fig. 2) of a film-substrate interface in the silicon-diamond system. This model takes account of the relative dimensions of the atoms of adjoining phases and the equilibrium distances between them. It is assumed that at the initial stage the surface of the silicon substrate has a perfect lattice. Since the carbon atoms that are sorbed on it possess a certain freedom of motion, they occupy positions that are energetically most favorable. Thus, for example, carbon atom 1, while interacting with the substrate, is located at the distance Si–C = $1.88 \cdot 10^{-10}$ m from silicon atom 2, rather than at the distance Si–Si = $2.34 \cdot 10^{-10}$ m as claimed by the old widely held theory. Carbon atom 3, interacting mainly with one carbon atom 1 and two silicon atoms 2 and 4, is located to the right of atom 1 and somewhat below it. A pore of somewhat increased dimensions is formed in this case between atoms 1, 2, 3, and 4. Atom 5 will be located higher than atom 3 on the same principle of energetic encouragement. The entire first layer is built in a similar way. Since atom 3 turned out to be lower than

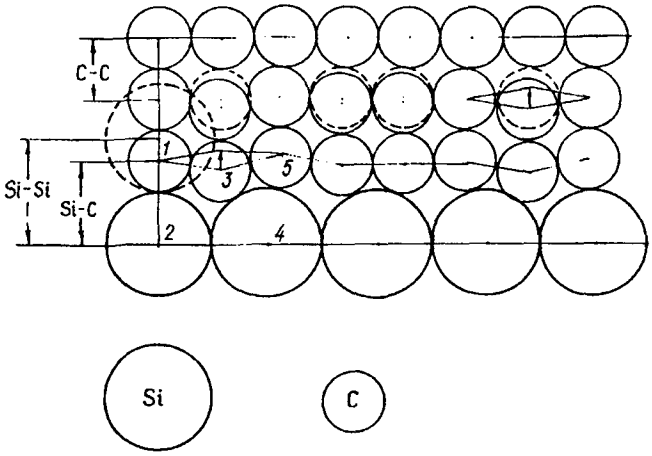

Fig. 2. Two-dimensional model of a film-substrate interface in the silicon-diamond system.

1 and 5, the latter atoms developed forces whose resultant (shown by an arrow in Fig. 2) tends to shift atom 3 and level them out in a horizontal plane.

Thus, the structure of the first layer consisting of carbon atoms of the precipitate is formed under the influence of the force field of both the silicon substrate and the carbon atoms (of the precipitate). The construction of the second and subsequent layers follows the same principle, but only under the action of the forces of interaction between the atoms of the precipitate, since the force field of the substrate is negligibly small at these distances. Under these conditions, a mono-, poly-, or amorphous structure of the building-up layer can be formed depending on the parameters of the synthesis in conformity with the phase diagram of the structures of the given substance.

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