ANISOTROPY OF THE SURFACE OF CARBON MATERIALS

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In this work, a model of the surface layer of perfect single crystals is used and the role of surface energy in physical processes occurring in the region of nanosized carbon materials is clarified. Of these, diamond, graphite, carbyne and fullerenes have been investigated. The thickness of the surface layer of diamond with cubic symmetry is 8.2 nm and is a nanostructure. The average size of the synthesized nanodiamond is of the order of ~ 8 nm. The value of the surface energy σhkl calculated by us along the diamond planes (100), (110), and (111) is in good agreement with experiment and other calculations. The thickness of the surface layer of graphite along the a axis is equal to $R(I)_a = 8.0$ nm and also represents a nanostructure. But along the c axis we have a layer thickness of about 1.5 nm and the number of monolayers is only 2. On this c axis, graphite can be created a monolayer by turning it into graphene. The σ_{hkl} value calculated by us along the a and c planes of graphite is 25957 and 5515 mJ/m², respectively. Carbines represent a polymeric polyyne or cumulene chain composed of sp-hybridized carbon atoms. If we imagine that the thickness of the surface layer of carbyne is stretched into a one-dimensional chain along the c axis, then the length of this chain is up to 200 nm for α-carbyne. The thickness of the surface layer of fullerenes significantly exceeds the thickness of the surface layer of pure metals. The surface energy of fullerenes σ_{hkl} increases with an increase in the number of carbon atoms $C_{36} \rightarrow C_{96}$. It also changes in the series $(111) \rightarrow (100) \rightarrow (110)$.

Keywords: *diamond, graphite, carbyne, fullerenes, nanostructures, surface layer thickness, surface energy, anisotropy.*

Introduction

This work is a continuation of works [1-3], where for the first time a model of the surface layer of perfect single crystals was constructed and the role of surface energy in physical processes occurring in the nanoscale region was clarified. Calculations of the surface energy will be carried out according to the formula derived under the assumption that there are no first-order phase transitions in these substances up to their melting point, which for crystals with a body-centered (bcc) and face-centered (fcc) cubic structure is given by the relations [4], where Z is the number of formula units of the unit cell, l_{hkl} is the thickness of the first coordination sphere in the [hkl] direction, and is the lattice constant:

$$\text{Im}\,3\text{m},\ Z = 2;\ l_{100} = a;\ l_{110} = a\sqrt{2};\ l_{111} = a/\sqrt{3},$$
$$\text{Fd}3\text{m},\ Z = 4;\ l_{100} = a;\ l_{110} - a/\sqrt{2};\ l_{111} = 2a/\sqrt{3}. \tag{1}$$

In works [5, 6] for the thickness of the surface layer R and surface energy σ, we obtained the following relations:

$$R(I) = \left[\text{kg}/\text{mol}\cdot\text{m}^3/\text{kg}\cdot\text{m}^{-2}\right]\cdot 0{,}24\cdot 10^{-9}\cdot M/\rho,\ \text{nm}$$
$$R(I)_{x=a} = \left[\text{m}^3\cdot\text{m}^{-2}\right]\cdot 0{,}54\cdot 10^{-11}\cdot x(a)^3,\ \text{nm}$$
$$R(I)_{y=b} = \left[\text{m}^3\cdot\text{m}^{-2}\right]\cdot 0{,}54\cdot 10^{-11}\cdot y(b)^3,\ \text{nm}$$
$$R(I)_{z=c} = \left[\text{m}^3\cdot\text{m}^{-2}\right]\cdot 0{,}54\cdot 10^{-11}\cdot z(c)^3,\ \text{nm} \tag{2}$$
$$\sigma_a = \left[\text{mJ}/\text{m}^2\cdot\hat{E}/\hat{E}\right]\cdot 10^{-3}\cdot T_m\cdot R_a(I)/R(I),\ \text{mJ}/\text{m}^2$$
$$\sigma_b = \left[\text{mJ}/\text{m}^2\cdot\hat{E}/\hat{E}\right]\cdot 10^{-3}\cdot T_m\cdot R_b(I)/R(I),\ \text{mJ}/\text{m}^2$$
$$\sigma_c = \left[\text{mJ}/\text{m}^2\cdot\hat{E}/\hat{E}\right]\cdot 10^{-3}\cdot T_m\cdot R_c(I)/R(I),\ \text{mJ}/\text{m}^2$$

Here M is the molar mass of the crystal, ρ is its density, a, b, c are the unit cell parameters of the crystal, and Tm is its melting point. In this work, we investigate the thickness of the surface layer and the surface energy of carbon materials.

3. Diamond

In general, 11 varieties have been identified among crystals and polycrystalline formations of diamond [7]. We will consider only the single crystals shown in Figure 1.
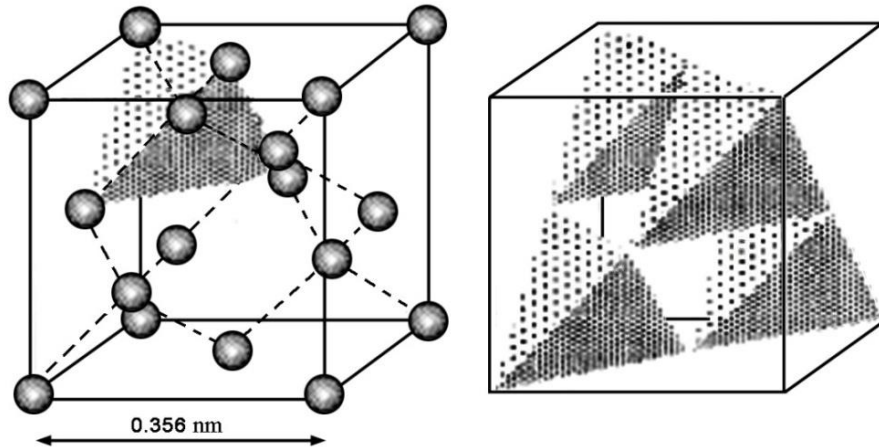

Fig.1. The structure of diamond (allotropic form of carbon C): "ball" model (left) and polyhedral model (right) [8].

Of all the proposed structural modifications of diamond, the structure (allotropic form of carbon C), which belongs to the holohedral class Oh, having the symmetry of the Fedorov space group Oh7-Fd3m, is most confirmed theoretically and experimentally. Lattice parameter at a temperature of 25 ºC and p = 1 atm. is equal to a = 3.57 Å [9], and the melting point T_m = 3973-4273 K, density ρ = 3.47-3.55 (g/cm^3), molar mass M = 12.01 (g/mol).

The structural cell of a diamond crystal is two cubes with a period of 0.356 nm, shifted relative to each other along the diagonal of the cube [9], then instead of (1) one should write:

$$\sigma \approx 2 \cdot 10^{-3} T_m,$$
$$\text{Fd3m}, Z = 4; l_{100} = \sigma; l_{110} - \sigma/\sqrt{2}; l_{111} = \sigma/\sqrt{3}. \tag{3}$$

Using (2) and (3), we calculate the surface energy anisotropy (table 1).

Table 1. Anisotropy of the surface energy of diamond

Diamond	(hkl)	Structure	T_m, K	R(I), nm	σ_{hkl} by (1), mJ/m^2	σ_{hkl} by [10], mJ/m^2	σ_{hkl} by [11], mJ/m^2
C	100	Fd3m	4273	8,2 (23)	8546	9100	-
	110				6104	6274	-
	111				5027	5270	4999±355

Let us now analyze Table 1. The thickness of the surface layer of diamond R(I) = 8.2 nm, that is, this layer is a nanostructure, which contains 23 monolayers of diamond. In this layer with atoms of pure metals and non-metals, there is a reconstruction and relaxation associated with the rearrangement of the surface [1-3]. The size effects in the R(I) layer are determined by the entire collective of atoms in the system (collective processes). Almost classic dimensional effects are observed only in nanoparticles and nanostructures [1-3]. Experimentally, they can be observed in very pure single crystals with grazing incidence of X-ray radiation, when the angle of incidence is equal to or less than the critical angle of total internal reflection.

The value of σ_{hkl} calculated by us for the planes (100), (110) and (111) is compared with the results of [10] and [11]. The calculations are based on the work of Harkins [10], published back in 1942. It is performed theoretically on the basis of Gibbs thermodynamics. Assuming the C-C bond energy in diamond equal to 90 kcal/mol, and the cohesion energy of diamond equal to twice the surface energy, he obtained the σ_{hkl} values presented in Table 1. The results of the experimental measurement of the surface energy of diamond by the Griffiths method were carried out in 2017 in [11] along the (111) plane and are also presented in Table 1. This experimental value of the surface energy of diamond is very close to the value of σ_{hkl} obtained by us (Table 1). Theoretical estimates of the surface energy of diamond for the (100) plane were carried out in many works (mJ/m^2): 9400 [12], 6513 [13], 6118 [14].

4. Graphite

Graphite is a unique native mineral, an allotropic modification of the element carbon, which is the most stable in the earth's crust. Graphite has that unique set of qualities that make it indispensable for problems in nuclear physics and power engineering [15]. The hexagonal lattice of graphite belongs to the space group C6/mmc-D^4_{6h} with four atoms per unit cell. The parameter a of the hexagonal cell is 2.46 Å, the parameter c = 6.74 Å, the theoretical density of such a crystal is 2.267 g/cm^3. In each plane, carbon atoms form a network of regular hexagons with an atom spacing of 1.42 Å. The bonds within the layers, which have a covalent nature, represent trigonal hybrids (2s, 2px, 2py) (Figure 2) [8]. Melting temperature range T_m = 4218-4163 K.
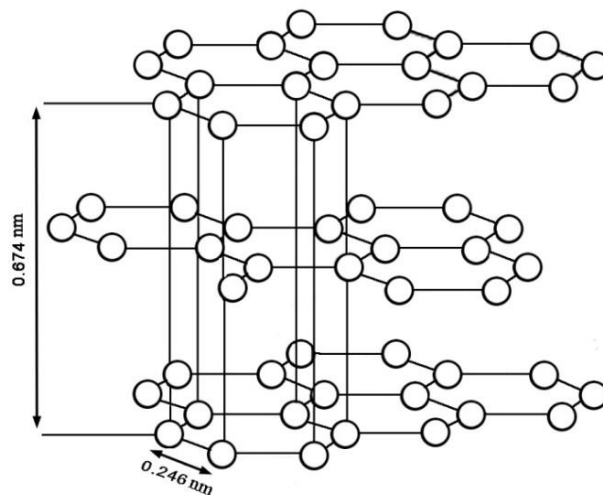

Fig. 2. Hexagonal graphite C [8].

Let us determine the thickness of the surface layer of hexagonal graphite and the anisotropy of its energy. The thickness of the surface layer of diamond R(I) = 8.2 nm, which almost coincides with R(I)$_a$ = 8.0 nm and also represents a nanostructure. But along the c axis we have a layer thickness of about 1.5 nm and the number of monolayers is only 2. On this *c* axis, graphite can be created a monolayer by turning it into graphene.

To determine the free surface energy of pyrographite by the Gilman method in a vacuum, a special installation was constructed. The experiments were carried out with pyrographite grade P2100V with the maximum sample thickness. The free surface energy of pyrographite of the indicated grade was found to be σ_c = 5000 mJ/m^2 [11], which is close to that obtained by us in Table 2.

Table 2. Thickness of the surface layer and anisotropy of the surface energy of graphite

Graphite	Structure	R(I)$_a$, nm	R(I)$_c$, nm	σ_a, mJ/m^2	σ_c, mJ/m^2
C	C6/mmc- D^4_{6h}	8,0 (33)	1,7 (2)	25957	5515

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5. Carbyne

Carbines represent a polymeric polyyne ($–C\equiv C–)_m$ or cumulene ($=C=C=)_n$ chain, consisting of carbon atoms in sp-hybridization (Fig. 3a, b). Polymer chains in carbyne crystals are packed in the form of hexagons along the (001) face. The presence of bends in the chains causes displacement of the layers (Fig. 3c).
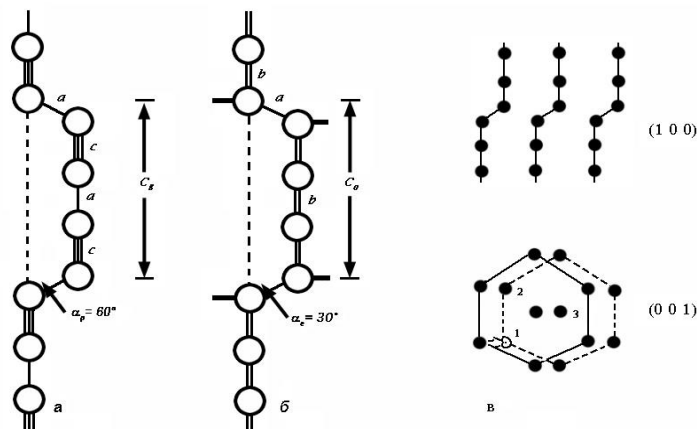

Fig. 3. Heimann's model of α-carbyne (a) and β-carbyne (b); c - two-layer model [16].

The hexagonal cell of the α-carbyne crystal has the following crystal lattice parameters: $a = b = 0.894$ nm and $c = 1.536$ nm; for β-carbyne - $a = b = 0.824$ nm and $c = 0.768$ nm [17]. The density of carbyne crystals is 1.9-2.0 g/cm^3. The melting point is about 3970 K. Using these data, we estimate the thickness of the surface layer and the anisotropy of the surface energy of the carbine (formula 2). Here R(I) = 36, since the molar mass of carbon in the unit cell is M = 12x6 = 72, where 6 is a six-atomic chain [18], and $\rho \approx 2.0$ g/cm^3.

Table 3. Surface layer thickness and surface energy anisotropy of carbyne

Carbin	Structure	R(I)$_a$, nm	R(I)$_c$, nm	σ_a, mJ/m^2	σ_c, mJ/m^2
C	α-carbin	38,6 (43)	196,7 (128)	4257	21692
C	β-carbin	30,2 (37)	40,0 (52)	3330	4411

The thickness of the surface layer of carbyne differs significantly from those for diamond and graphite, but closer to carbon materials like fullerenes, which we will discuss below. The anisotropy of the surface energy of carbines, which also have a hexagonal crystal cell, does not differ much from the surface energy of grphites.

6. Fullerene

Fullerene was discovered in 1985 by G. Kroto (Great Britain), R. Curl, R. Smelli (USA), for which they were awarded the Nobel Prize in 1996. A review of fullerenes for 15 years from 1991 to 2006 was carried out in [19]. The most recent monograph on the structure and stability of higher fullerenes is described in [20]. It discusses a completely new - molecular - form of carbon existence; these closed carbon clusters were able to capture and enclose within themselves individual atoms, several atoms, and even small molecules. All this is new and unusual from the point of view of theoretical chemistry and fundamental science in general.

Fullerenes are carbon clusters with an even, more than 20, number of carbon atoms forming three bonds with each other; atoms in fullerene molecules are located on the surface of a spheroid at the vertices of hexagons and pentagons. Examples of fullerenes are shown in Fig. 4 [21]. In [22], a relationship was found between the mass of the C_{cn} fullerene molecule and the properties of fcc fullerites, such as: the sublimation

energy, the distance between the centers of the nearest molecules, the Grüneisen parameter. compression modulus at zero pressure and temperature.

Based on the data of the correlation dependences, the parameters of the Mee-Lennard-Jones pair potential for the inter-fullerene interaction in fcc fullerites were reconstructed. On the basis of the obtained parameters of the potential, the properties of fullerites are calculated and good agreement with the data known from the literature is obtained. It is shown that at nc <15-20 crystals of fullerites C_{cn} are unstable. At the same time, fullerites where nc> 100 will have anomalously low surface energies, which should lead to fragmentation of nanoclusters from such large Cnc molecules. The parameters of the triple and critical points of fullerenes are estimated.
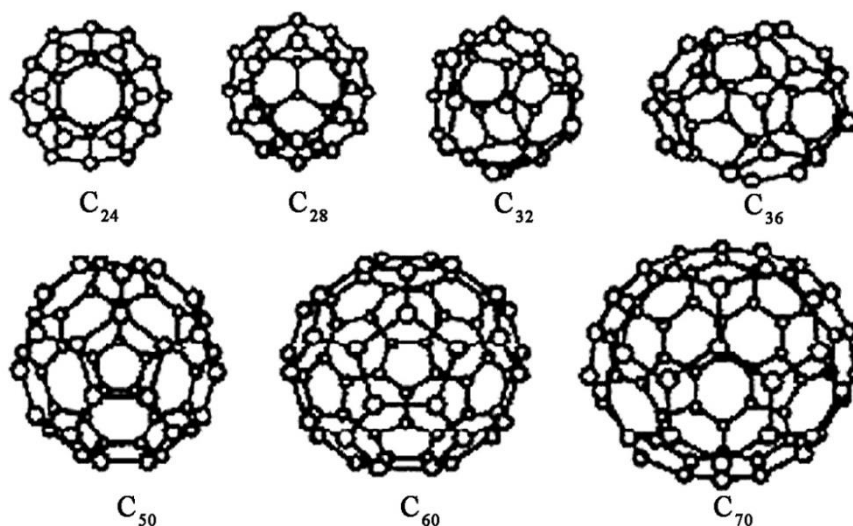

Fig. 4. Schemes of the structure of fullerenes [21]

The evolution of the parameters of the potential and the indicated properties with a change in the molecular weight of the fullerene has been studied. The parameters T_m, M, ρ for calculating R(I) and σ_{hkl} were taken by us from [22]. In addition, knowing the thickness of the surface layer R(I) and the crystal lattice parameter a, one can estimate the number of monolayers that form the R(I) layer (n = R(I)/a). Thus, for gold and silicon, we showed [23] that the R(I) layer contains 3 monolayers of gold and 4 monolayers of silicon. The same order of magnitude in the R(I) layer contains the number of monolayers of pure metals. Table 4 shows that the thickness of the surface layer of fullerenes R(I) significantly exceeds the thickness of the surface layer of metals.

It follows from Table 4 that the thickness of the surface layer of fullerenes R(I) in C_{84} and C_{96} exceeds 100 nm according to Glater [24], which is characteristic of nanostructures. At h ≈ 10 R(I), a phase transition occurs in the surface layer of fullerenes. For example, in fullerene C_{60}, the phase transition is due to the action of the forces of pair van der Waals interaction, which have a significant noncentral component due to the anisotropy of the electron density on the surface of molecules [25]. So at 2600 K the fcc lattice transforms into a simple cubic (PC) lattice. In the PS structure, there is the possibility of hindered rotations of molecules around ordered axes between two energetically nonequivalent orientational configurations: pentagons and hexagons. The surface energy of fullerenes σ_{hkl} increases with an increase in the number of carbon atoms $C_{36} \rightarrow C_{96}$. It also changes in the series (111) $\rightarrow$ (100) $\rightarrow$ (110) (table 4).

7. Carbon materials

Carbon materials can be viewed as spatially cross-linked polymeric substances. In these compounds, carbon is tetravalent and is in one of three ground states corresponding to sp^3 -, sp^2 - and sp-hybridization of electrons. In a number of substances, carbon atoms are in different, including intermediate (sp^m-), electronic states. To describe them, the most convenient classification (Figure 5) by the type of chemical bonds, based on the hybridization of electron orbitals of carbon atoms [26]. Let us now compare the results obtained by us, presented in tables 1-4. Table 1 shows that the thickness of the surface layer of diamond is 8.2 nm and is a nanostructure. That is, nanodiamonds are of interest. Detonation nanodiamonds were first synthesized in 1963 by the explosive decomposition of powerful mixtures of explosives with a negative oxygen balance in a

non-oxidizing environment. Such diamonds are characterized by nanoscale particles, chemical resistance of the diamond core, and activity of the peripheral shell [27]. Moreover, as a result of detonation of a charge weighing 140 kg in an aqueous shell, particles of an average size of ~ 8 nm were obtained (compare with Table 1)

Table 4. Thickness of the surface layer and anisotropy of the surface energy of fullerene

Fullerene	(hkl)	Structure	T_m, K	M, g/mol	ρ, g/sm^3	R(I), nm	σ_{hkl} mJ/m^2
C_{36}	100	Fd3m	1404	432.40	1.810	40.61 (36) a=11.725 Å	1404
	110						1003
	111						1652
C_{60}	100	Fd3m	2031	720.66	1.484	85.56 (60) a=14.17 Å	2031
	110						1451
	111						2321
C_{70}	100	Fd3m	2260	840.23	1.547	93.39 (64) a=14.96 Å	2260
	110						1614
	111						2659
C_{76}	100	Fd3m	2387	912.84	1.582	98.09	2367
	110						1705
	111						2808
C_{84}	100	Fd3m	2547	1008.92	1.589	107.93	2547
	110						1819
	111						2997
C_{96}	100	Fd3m	2763	1153.06	1.452	135.00	2763
	110						1974
	111						3251

Nanodiamonds are complex objects, usually with a three-layer structure, including:
- a diamond core with a size of 4-6 nm, which contains from 70 to 90% of carbon atoms;
- a transitional carbon shell (intermediate layer) around the core of X-ray amorphous carbon structures with a thickness of 0.4 - 1.0 nm, which can contain from 10 to 30% of carbon atoms;
- the surface layer, in which, in addition to carbon atoms, other heteroatoms (N, O, H) can be located, forming a number of functional groups (all this is at a level of ~ 8 nm (compare with Table 1).

Nanodiamonds began to be produced by industry on a large scale and their use is increasing all the time (Figure 6). From Table 2, the thickness of the surface layer of graphite along the c axis is about 1.5 nm and the number of monolayers is only 2. Along this axis, a monolayer can be created from graphite, turning it into graphene, which can be called "nanographite". The unique electrical properties of graphene (due to its two-dimensional nanostructure), confirmed by numerous studies, are extremely interesting (usually two-layer structures, as in Table 2), both in fundamental and applied terms [28, 29].
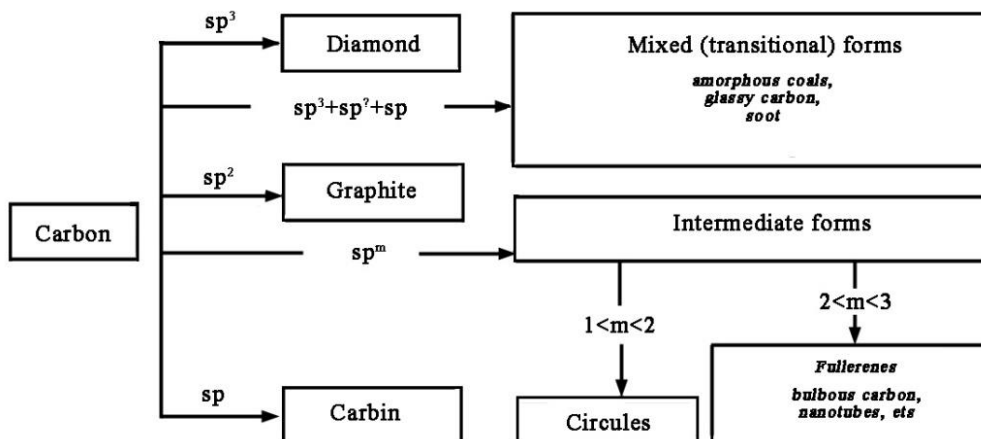

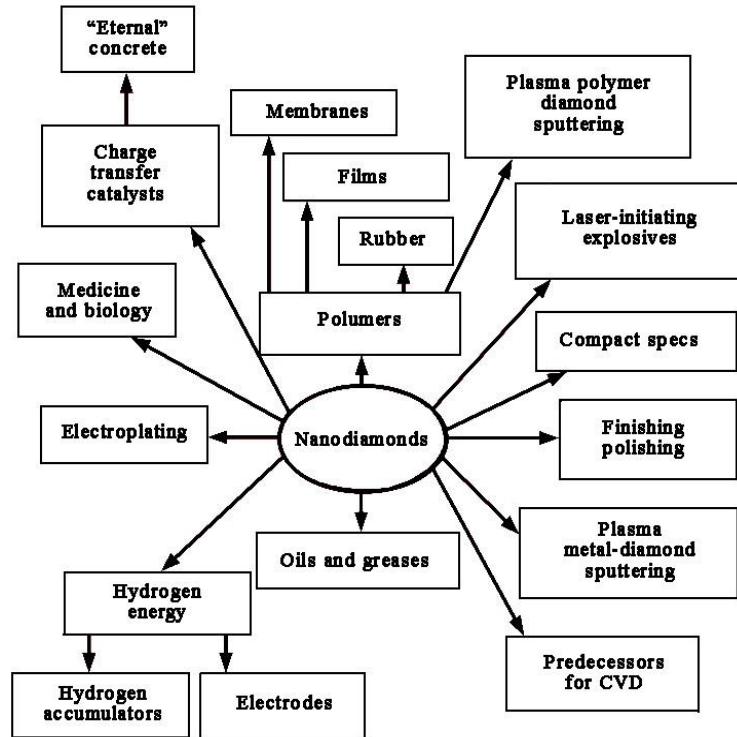**Fig. 5.** Classification scheme of allotropic forms of carbon [26].

Fig.6. Spheres of application of nanodiamonds [27].
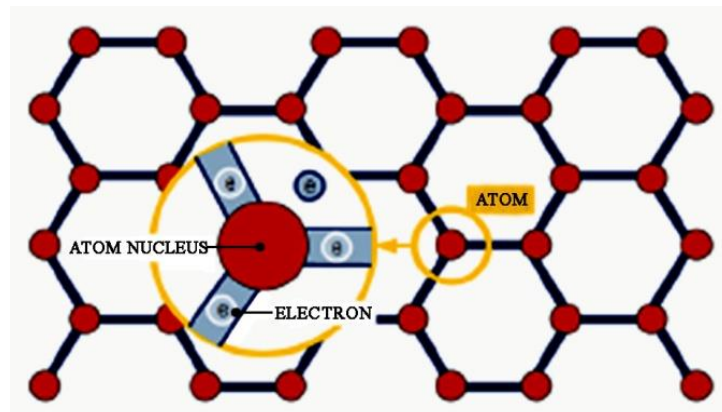

Fig.7. Schematic representation of grapheme.

    The amazing properties of graphene are due to the unique nature of its charge carriers - they behave like relativistic particles (Figure 7) [28]. Graphene has a unique structure and exceptional physical and chemical properties, which lead to many possibilities for its application (Fig. 8).

    As shown above, the structure of carbyne is formed by carbon atoms assembled into chains by double bonds (α-carbyne) or alternating single and triple bonds (β-carbyne). If we imagine that the thickness of the surface layer of carbyne is stretched into a one-dimensional chain along the *c* axis, then the length of this chain is up to 200 nm for α-carbyne (Table 3). This result was obtained in [30] and is shown in Figure 9.

    It turned out that carbyne is the most durable of all known materials. The specific strength of carbine is $6.0 \cdot 10^7$ - $7.5 \cdot 10^7$ N m/kg, while the specific strength of diamond is $2.5 \cdot 10^7$ - $6.5 \cdot 10^7$ N m/kg, graphene is $4.7 \cdot 10^7$ - $5.5 \cdot 10^7$ N m/kg, carbon nanotubes - $4.3 \cdot 10^7$ - $5.0 \cdot 10^7$ N m / kg. Carbyne is the toughest material known. The specific stiffness of carbyne is about 10^9 N m/kg, which is two times higher than the specific stiffness of graphene - $0.45 \cdot 10^9$ N m/kg. The use of carbine is shown in Figure 10. Fullerenes with a large thickness of the surface layer (Table 4), like rare minerals in nature, are quite rare. Their application in practice is also still limited (Figure 11).
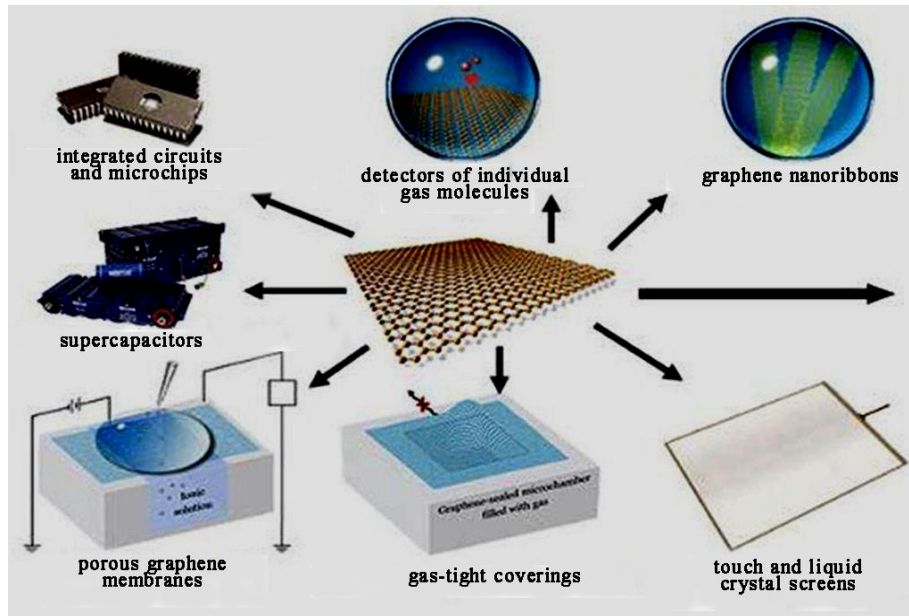
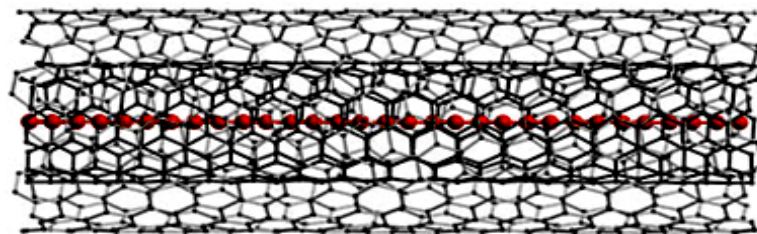**Fig.8.** Application of 2D structures of graphite - graphene

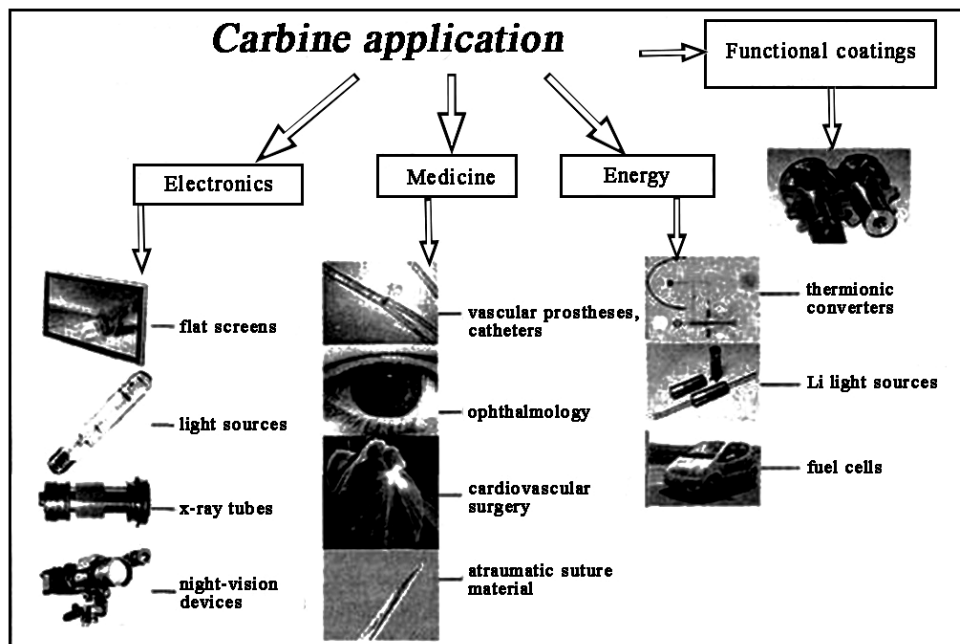**Fig.9.** Linear 1D structure of a carbyne molecule (red atoms) inside double-walled carbon nanotubes [30].

Fig.10. Application of Carbyne nanostructures

Fig.11. Application of fullerene nanostructures

Conclusion

Thus, our model of the surface layer showed that the surface of carbon materials is a nanostructure, the properties of which differ significantly from the bulk properties of the material. Currently, in various fields of science, industry and construction, materials are used that are united by dimensional features, namely, nanocrystals, nanoporous materials, nanostructures, and nanocomposites. The range of nanoobjects is extremely wide and continuously increasing, which makes it possible to obtain new catalytic systems in chemistry, engineering materials with unique material science characteristics, structures with nanometer geometry for recording information, converters of various types of energy, superconducting materials in physics, new drugs and their carriers in medicine.

Today, various kinds of materials, the structural elements of which are on the order of millionths of a millimeter, are beginning to be widely used all over the world to provide improved electrical, magnetic, optical and other consumer qualities. Analysis of the state and development trends of the nanoindustry at the present time allows us to conclude that the following types of carbon nanomaterials are the most promising: nanodiamonds, graphene, nanocarbines, fullerenes, which we have considered in detail, as well as soot, amorphous coals, glassy carbons and many other carbon nanomaterials, analysis and calculation of properties of which can be carried out according to the model we have outlined and tested.

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