Investigation of the unit cell parameter and dislocation structure of polycrystalline diamond films

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Abstract

The values of the unit cell (UC) parameter were measured and elements of the internal structure were determined in polycrystalline diamond films (PDFs) using x-ray diffraction. It was established that the values of the UC parameter were connected with the dislocation densities in mosaic PDF crystallites. The dislocation density was calculated from measured microdistortions and dispersion in the blocks based on the surface stretch forces that arise on the boundaries between blocks. This allowed more precise computing of the dislocation density. A similar connection between the UC parameter and dislocation density also exists in epitaxial diamond films and in plastic deformed natural type IIb and Ic diamonds. A regular relationship between physical values of the UC parameter and dislocation density in mosaic diamond materials was determined using mathematical modelling. An increase in the dislocation density results in a decrease in the UC parameter from 0.356 689 nm in more pure and perfect type IIa diamonds to a limiting value of 0.356 42 nm in PDF samples.

1. Introduction

Diamond is an insulator with wide bandgap. But in 1952 mosaic natural diamonds with a low specific resistance and with semiconducting characteristics were found. It is known that structure, admixture and structural imperfections determine electronic properties of crystalline solids. It was assumed that the semiconducting properties of these diamonds are explained by disturbance of their ideal structure. Scientists consider that the diamond with its unique properties is a prospective material for modern electronics, and have studied the nature and conditions of forming the semiconducting properties. For this reason, any deviations from ideal structure and atomic composition of diamond materials are important.

In [1] it was determined that the average value of the unit cell (UC) parameter ($a = 0.356\,683 \pm 1 \times 10^{-6}$ nm) of the semiconducting type IIb diamond group differs from the UC parameter of the more perfect and 'pure' type IIa diamonds, which is $0.356\,689 \pm 1 \times 10^{-6}$ nm [2]. In [1] it was assumed that the decrease in the diamond UC parameter could be explained by vacancies, imperfections of vacancy type or impurity atoms with a smaller atomic weight than carbon. Later during investigation of diamond film synthesis processes it was noticed that their UC parameter values are less ($0.356\,64$ nm [3] and $0.356\,42$–$0.356\,59$ nm this work) than for type IIa diamonds.

Using the suppositions of [1] we have estimated an influence of thermodynamic equilibrium vacancies on a modification of the non-doped diamond film UC parameter. It was established that such vacancies can reduce the UC parameter by only $\sim 1 \times 10^{-5}$ % or 4×10^{-8} nm. This estimated decrease lies outside the measurement accuracy of the UC parameter. Thus, vacancies cannot reduce the UC parameter to the values which occur in type IIb diamonds and in synthetic diamond films. In [4] the influence of impurity atoms of nitrogen, phosphorus and boron on the UC parameter in synthetic diamonds was investigated. These diamonds were prepared from hydrocarbons at high pressures and temperatures. It was established that all the above mentioned elements do not decrease the UC parameter, but increase it instead from $0.356\,60$ to $0.356\,70$ nm if their concentration increases from 0.002 to 0.12 at.%. The results obtained in [4] confirm an increase in the UC parameter with an increase in the impurity nitrogen concentration in natural type I diamonds. Thus, it is possible to conclude that the point imperfections formed by impurity atoms and vacancies are not the principal reasons behind the UC parameter reduction in natural type IIb diamonds and in synthetic diamond films.

In a series of papers and, in particular, papers [5, 6] it was shown that the semiconducting type IIb diamonds have a mosaic internal structure. It is known that in such crystals dislocation density can reach 10^{11}–10^{12} m^{-2} and more, and these dislocations form complicated dislocation systems, which are called dislocation inter-block (DIB) boundaries.

It is also known that the number of atoms which form these DIB boundaries is equal to about 1% of the total number of atoms.

Therefore, a study of the connection between the DIB boundaries and the UC parameter in mosaic diamond crystals is essential for understanding of electronic properties of diamond.

2. Diamond samples

In the present paper we have considered the three groups of diamond samples: the first group is polycrystalline diamond film (PDF) samples; the second group is single-crystal epitaxial diamond film (EDF) samples; and the third group is natural mosaic crystals such as IIb.

Samples of the first group were synthesized in our laboratory from a gas environment on Si substrates without introduction of admixtures by a high-gradient chemical transport reaction method [3]. Synthesis took place at substrate temperatures from 1073 up to 1273 K and gas mixture pressures from 5.33 up to 31.99 kPa. The gas mixture consisted of 2–4 vol% methane and 98–96 vol% of hydrogen. A graphite heater heated the gas mixture to a temperature of ~ 2273 K. All PDF samples had a thickness of 3–11 μm. We have chosen the samples with thickness nearly 5 μm.

To define the substructure of the synthesized PDF samples we used data obtained from a scanning electron microscope (SEM) and a transmission electron microscope (TEM). The SEM image of the PDF sample surface shows that they consist of crystallites with a size of 1–2 μm. On the other hand, TEM data and micro-electron diffraction investigations have shown that weakly disorientated diamond particles with a size from 0.03 to 0.1 μm are the basic elements
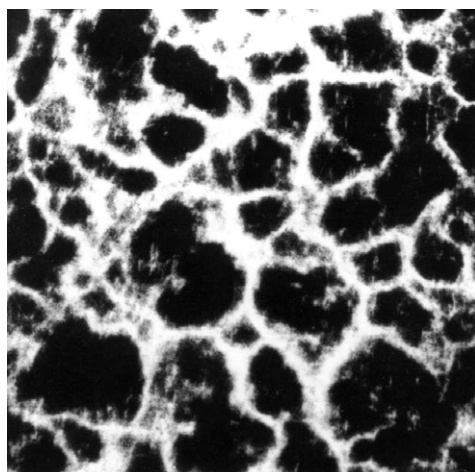
Figure 1. Cross section of a semiconductor mosaic type IIb diamond with luminous dislocations at the boundaries between blocks under the action of an electron beam (polished surface, area 300 μm square) [5, 6].

of the crystal grains. Thus, crystallites of the PDF samples consist of shallow diamond blocks and they have a mosaic structure.

Samples of the second group were deposited on substrates which were made from natural diamond single crystals. They were prepared in the Institute of Physical Chemistry of the Russian Academy of Sciences. All samples were synthesized from a gas mixture without doping. It was established that EDF samples with a thickness of 0.05–0.1 μm are single crystals. Their UC parameter is equal to $0.3567 \pm 8 \times 10^{-4}$ nm. Professor B V Spitsyn, the pioneer of the method for synthesizing diamond films from methane–hydrogen mixture [3], provided us with several EDF samples for examination. Study of these EDF sample structures by SEM has shown that they have a mosaic structure. For example, the EDF-3 sample consists of weakly disorientated blocks with sizes of about 1 μm.

Samples of the third group were not produced for this work. Instead we conducted the analysis of type IIb diamond structure using literature data. The real structure of type IIb diamonds has been described in many papers ([5, 6] and others). It has been established that type IIb diamonds are very non-homogeneous; some of them have a stratified structure. The authors of [5, 6] have detected on a cut of type IIb diamond a bright-blue glow of the dislocation boundaries between mosaic blocks under the action of an electron beam (figure 1). From this figure the average value of the block magnitude was estimated to be approximately ($\sim$10 μm). The authors of [7, 8] have also detected a bright-blue glow of the dislocation boundaries between mosaic blocks under the action of an electron beam in highly oriented diamond films.

Similar to the results of papers [5, 6], we also detected and studied a bright-light-blue glow under the action of an electron beam on surface areas with agglomerations of dislocations of a cleaved diamond (see figure 2): dark shadows running away from a crater are indicators of large dislocation densities. Such a bright-light-blue glow is typical for semiconducting diamonds of type IIb. These dislocations were created in natural non-conducting diamonds of type I and type IIa and in artificial diamonds by a laser impulse radiation. The presence of dislocations was confirmed by x-ray topography; their density was measured by a selective etching method and by x-ray diffractometry. We identified that the diamond areas with large dislocation density
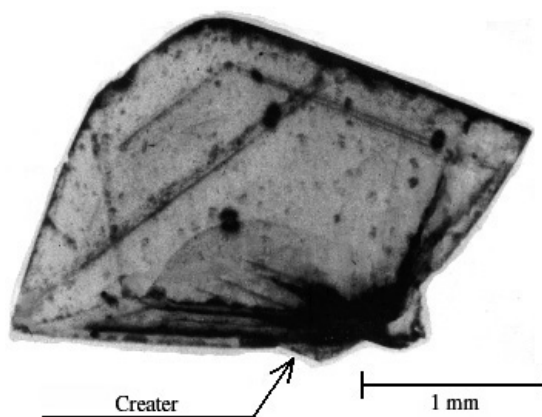
Figure 2. X-ray topogram of the diamond plate with dislocations on the edge of a split. These dislocations have bright-light-blue luminescence under the action of an electron beam.

also have large semiconducting conductivity, which is indicative for semiconducting diamonds of type IIb. Further details on this subject will be published elsewhere.

Based on the discussion presented above, we decided to investigate the connection between UC parameters of mosaic diamonds and dislocation densities, which are related to diamond's conductivity.

3. Measuring the diamond unit cell parameter

In this work the UC parameter was measured using a standard DRON-2 x-ray diffractometer at a grazing angle of the x-ray beam of $3°$. The measurements were made by radiation of the copper anode using the Bragg–Brentano Θ–2Θ scheme.

This device has high engineering parameters. The stabilization of anode voltage and anode current was maintained within an accuracy of 0.1% at fluctuations of a network tension of $\pm 7\%$ compared to the nominal tension. The overall error of measurement intensity over 10 h operation is no more than 0.5%. The diffractometer has a precise system of tube and goniometer alignment, ensuring the reliable fixing of an alignment position. This diffractometer is fitted with β-filters made from nickel (Ni). The measurement accuracy of angles in this type of device is $0.02°$.

To measure the UC parameter we used the reflection from (331) planes. The diffraction angle for these planes was $2\Theta \approx 140°$.

The selection component reflection $K_{\alpha 1}$ of the copper anode was based on a standard method proposed by Reschinger. The positions of diffraction peaks were determined by a mode of medians [9]. We have also conducted an analysis of possible factors which affect the accuracy of the UC parameter definition.

(1) For an estimate of total stresses (residual) $\sigma_{total} = \sigma_{thermal} + \sigma_{intrinsic}$ we carried out a strain-measuring examination of PDF samples using the well known '$\sin^2 \psi$' method. It was established that diamond films deposited on Si substrates do not show a noticeable presence of σ_{total}. Therefore, intrinsic stresses from structural mismatches $\sigma_{intrinsic}$ are small. The thermal stresses $\sigma_{thermal}$ also are small, as their thermal expansion coefficients are close, $\alpha_D = 3.56 \times 10^{-6} \text{ K}^{-1}$ and $\alpha_{Si} = 3.59 \times 10^{-6}$ [10].

(2) The effect of displacement of diffracted beams for light atoms, such as carbon, is very small, so it is possible to ignore this effect.

(3) The error caused by x-ray refraction is approximately 0.003%; it needs to be taken into account only at $\Delta a \leqslant 0.000\,02$ nm.

(4) The correction for divergence of the primary ray was not taken into account because of its insignificance.

(5) Temperature fluctuations yield a correction of an order below the measurement accuracy of the UC parameter, which we took into account.

(6) The influence of the PDF texture was reduced to a minimum using the Soller diaphragms with an angular divergence $\alpha = 1.5°$ on primary and diffracted bunches in the vertical plane. Therefore, this influence was not taken for the definition of the measurement accuracy of the UC parameter in PDF samples.

The analysis carried out by us has shown that the greatest error in the given method is an instrument error associated with measuring the angles (0.02°). It is a systematic error $\Delta\alpha_{SYS}$ in the definition of the UC parameter: $\Delta a_{SYS} \approx \Delta a_\Theta \approx 4 \times 10^{-5}$ nm.

The calculated significance of the mean-square deviation of measurement of the UC parameter in each PDF sample is $\sigma \leqslant 2 \times 10^{-5}$ nm. When calculating the full error, if the condition $\sigma \leqslant 0.5\Delta a_{SYS}$ is satisfied, it is possible to conclude that the full error of the UC parameter measurement is equal to the systematic error. Hence, $\Delta a \approx \Delta a_\Theta \approx 4 \times 10^{-5}$ nm.

From measurement diffraction angles 2Θ in samples of the first group we established that their value depends on synthesis conditions: temperature of substrates, pressure of the gas mixture in the reaction chamber and composition of the gas mixture. From the values of diffraction angles the interplanar spacing was calculated and the UC parameter derived for each sample. We have selected certain PDF samples and arranged them in table 1 in order of magnitude of their diffraction angles and UC parameter values. From table 1 it can be seen that sample 18 has the maximum UC parameter values of $0.356\,59 \pm 4 \times 10^{-5}$ nm. The minimum value is $0.356\,42 \pm 4 \times 10^{-5}$ nm. This was established in three series of PDF synthesis experiments. In the upper part of the table containing literature data we have included UC parameter values for samples from the most perfect and 'pure' type IIa diamond [2] to a PDF(SP) from the papers [3].

4. Study of the PDF substructure

The second part of the present investigation involved measuring the diffraction peak broadening and ascertaining their connection with the parameters of the PDF substructure. Broadening of the diffraction peaks provides information on the PDF substructure.

Measurements of the diffraction peak broadening were carried out for reflections from (111) and (331) atom planes. To reference the physical broadening β we used a standard sample, which was made from annealed nickel powder with a particle size L of ≈ 2000 Å. The standard sample has reflections near to PDF sample reflections. Reflection parameters of the standard sample were found to be $b_{111} = 2.0 \times 10^{-3}$ rad and $b_{331} = 4.15 \times 10^{-3}$ rad. These data were used by us to evaluate the physical broadening of maximum β from measured diffraction reflections from (111) and (331) planes of PDF atom samples. After this the Gaussian function approximation method was applied to determine the block size D and micro-distortions ξ from the b values [9]. The results are summarized in table 2. The sizes of blocks in samples IIb (L) [5, 6] and EDF-3 are displayed in the upper part of this table.

We have calculated the dislocation density in the PDF samples using data from table 2.

In order to improve the calculated dislocation densities we utilized another method. The method is based on Hooke's law and the energy of the surface stretch that arises on the block

Table 1. Unit cell parameter and internal structure of diamond samples.

Sample	$2\Theta_{(331)} \pm 0.02°$	a (nm)	Internal structure of the samples	Reference
IIa	—	$0.356\,689 \pm 1 \times 10^{-6}$	Nearly perfect and 'clean' diamonds	[2]
IIb (L)[b]	—	$0.356\,688^a$	Mosaic diamond	[5, 6]
EDF-3	—	$0.356\,687^a$	Mosaic diamond film	[3]
IIb (ave.)	—	$0.356\,683 \pm 1 \times 10^{-6}$	Mosaic diamonds	[1]
PDF(SP)[c]	—	$0.356\,64 \pm 1 \times 10^{-5}$	Nearly perfect PDF	[3]
18	140.63	$0.356\,59 \pm 4 \times 10^{-5}$	PDF	This work
12	140.65	$0.356\,56 \pm 4 \times 10^{-5}$	PDF	This work
11	140.72	$0.356\,48 \pm 4 \times 10^{-5}$	PDF	This work
13	140.73	$0.356\,47 \pm 4 \times 10^{-5}$	PDF	This work
24	140.74	$0.356\,46 \pm 4 \times 10^{-5}$	PDF	This work
17	140.76	$0.356\,44 \pm 4 \times 10^{-5}$	PDF	This work
23	140.78	$0.356\,42 \pm 4 \times 10^{-5}$	PDF	This work

[a] The significance of the UC parameter a is determined by a method involving interpolation of data of size Γ (a local dislocation density, see below) according to equation (5).
[b] The Lang's sample.
[c] The Spitsyn's samples.

Table 2. The substructure parameters of the diamond samples.

Sample	The reflective planes (hkl)	$B_{int} \times 10^3$ (rad)	$\beta \times 10^3$ (rad)	$\xi \times 10^3$	D (nm)	Reference
IIb (L)	—	—	—	—	10^4	[5, 6]
EDF-3	—	—	—	—	10^3	This work
18	(331)	17.6	17.1	1.2	46	This work
	(111)	4.7	4.2			
12	(331)	18.1	17.6	1.3	53	This work
	(111)	4.4	3.9			
11	(331)	20.9	20.5	1.6	57	This work
	(111)	4.5	4.0			
13	(331)	25.8	25.4	1.8	34	This work
	(111)	6.2	5.9			
24	(331)	26.7	26.4	2.1	53	This work
	(111)	5.3	4.9			
23	(331)	29.3	28.9	1.7	22	This work
	(111)	8.4	8.2			
17	(331)	32.2	31.9	2.7	49	This work
	(111)	5.3	4.9			

surface. The application of this method assumes the following approximations. The blocks have the shape of a cube with an average edge value D. Dislocations, which form DIB boundaries, are concentrated in thin layers on the boundaries and create a local dislocation density Γ. The local dislocation density Γ is similar to the dislocation density of the two crystals division, if their parameters are slightly different. As the average surface of blocks is much greater than the crystallite average surface, the surface of the blocks only was used in calculations.

The dislocations, which form boundary layers between blocks, strongly distort the diamond lattice. Hence, the energy of the carbon atoms which form DIB boundaries differs

Table 3. The UC parameter reduction and dislocation density in diamond samples.

Sample	Δa (nm)	$\Delta a/a_0$	Γ (m^{-2})	Reference
IIa	0	0	$\leqslant 10^8$	This work
IIb (L)	-1×10^{-5}	-2.8×10^{-6}	2.5×10^{13}[a]	[5, 6]
EDF-3	-2×10^{-5}	-5.6×10^{-6}	2.5×10^{14}[a]	This work
IIb (aver.)	-6×10^{-5}	-1.68×10^{-5}	3.04×10^{15}[b]	[1]
PDF-SP	-4.9×10^{-4}	-1.37×10^{-4}	1.06×10^{16}[b]	[3]
18	-9.9×10^{-4}	-2.78×10^{-4}	1.91×10^{16}	This work
12	-1.29×10^{-3}	-3.62×10^{-4}	1.98×10^{16}	This work
11	-2.09×10^{-3}	-5.86×10^{-4}	2.65×10^{16}	This work
24	-2.29×10^{-3}	-6.42×10^{-4}	2.86×10^{16}	This work
17	-2.49×10^{-3}	-6.98×10^{-4}	3.11×10^{16}	This work
13	-2.19×10^{-3}	-6.14×10^{-4}	3.2×10^{16}	This work
23	-2.69×10^{-3}	-7.54×10^{-4}	4.3×10^{16}	This work

[a] The Γ values, calculated from the measured sizes of blocks D.
[b] The Γ values, determined by interpolation of known significances a.

from the energy of carbon atoms located within the blocks. From the meaning of surface tension, there is energy on the boundaries between blocks, which results in surface tension forces. Under the action of these surface tension forces in blocks, pressures arise due to elastic stresses, which cause a relative change in the volume of the blocks:

$$\frac{\Delta V}{V_0} = 3\frac{\Delta D}{D_0}, \tag{1}$$

where $\Delta V = V - V_0$; V—the average volume of the blocks in investigated samples; V_0—the volume of the same blocks in an unstrained diamond; $\Delta D = D - D_0$; D—the average size of block edges in investigated samples; D_0—the size of an unstrained diamond block edge. As the pressure inside the block will be identical over the entire volume, the relative modification of a block edge will correspond to a relative modification of the UC parameter: $\Delta D/D_0 \approx \Delta a/a_0$, where $\Delta a = a - a_0$; a is the UC parameter of investigated samples and a_0 is the UC parameter of an unstrained diamond. Unstrained diamond values were taken from natural type IIa diamond [2]. All measured UC parameter values of semiconducting type IIb diamonds, EDF samples and PDF samples are less than a_0, that is $a < a_0$. Hence, $\Delta a < 0$ and, accordingly, $\Delta D < 0$. According to this $\Delta a/a_0$ and $\Delta D/D_0 < 0$. The data in table 3 and the coefficient of diamond volume compression $K = 5.85 \times 10^{11}$ N m^{-2} allows the determination of average values of the pressure in sample blocks:

$$p = 3K\left(-\frac{\Delta D}{D_0}\right) = 3K\left(-\frac{\Delta a}{a_0}\right) = -3K\frac{\Delta a}{a_0}. \tag{2}$$

As $\Delta a/a_0 < 0$ and $\Delta D/D_0 < 0$ then, accordingly, $p < 0$. Hence, the surface tension creates compressive efforts.

It is known that the UC parameter in silver, bismuth islets [11, 12] and nanodiamonds [13] diminishes under an action of the surface tension forces. In nanodiamonds the UC parameter decreases to as low as 0.352 33 nm.

Taking into account that a pressure which arises in cubic-shaped blocks is related to the surface energy as follows:

$$p = \frac{4 \cdot E_r}{D}, \tag{3}$$

one can find the energy of the block boundaries.

It is known that surface energy for small-angle boundaries is equal to [14]

$$E_r = E_0 \varphi (A - \ln \varphi), \tag{4}$$

where $E_0 = Gb/4\pi(1 - \nu) = 21.19$ is the constant for diamond; A is the magnitude, which takes into account the approximate energy of the dislocation core; $\varphi = b\Gamma D$ is the angle of the block disorientation; Γ is the dislocation density; $G = 6.58 \times 10^{11}$ N m^{-2} is the modulus of the displacement; and ν is the Poisson's coefficient. Equation (4) is valid not only for small block disorientation angles, but also for greater angles, $\varphi \geqslant 30°$.

From equation (4) we have calculated angles φ of block disorientation and have determined local dislocation densities Γ, where boundaries form between mosaic blocks (table 3).

Based on an analysis of the obtained outcomes and a comparison of tables 1–3 it is possible to conclude that the diamond UC parameter is related to the dislocation density within dislocation boundaries between blocks. The upper limit of the UC parameter values is defined on the equilibrium distances between carbon atoms in a crystal lattice of 'pure' type IIa diamond, which we accepted as $a_0 = 0.356\,689 \pm 1 \times 10^{-6}$ nm. This value is set by the nature of the carbon chemical bond in a diamond crystal lattice. The lowest value of the UC parameter ($\sim$0.356 42 nm in PDF samples) is limited by the compressibility of diamond and the decrease in surface energy between blocks resulting from interaction of dislocations due to their high density. The connection between the unit cell parameter and the dislocation density was modelled by the Boltzmann mathematical model, which has the following form:

$$a = a_{\mathrm{LIM}} + \frac{a_0 - a_{\mathrm{LIM}}}{1 + \exp\left(\frac{\Gamma - \Gamma_0}{d_\Gamma}\right)}, \tag{5}$$

where a_{LIM} is the limiting minimum value of the UC parameter at large dislocation densities ($\Gamma \to \infty$); a_0 is the UC parameter of an ideal unstrained 'pure' type IIa diamond (corresponds to $\Gamma \to 0$); Γ is the current local dislocation density; $d_\Gamma = 1.11 \times 10^{16}$ m^{-2} is the constant of proportionality, that is a permanent value for the given crystalline substance. At $\Gamma = \Gamma_0$, the value of the UC parameter is equal to $(a_{\mathrm{LIM}} + a_0)/2$.

The graph of the UCP experimental relationship to dislocation density (5) is shown in figure 3.

This graph displays the connection between of the UC parameter and dislocation density within the DIB boundaries in natural semiconducting type IIb diamonds, in mosaic EDF samples and in PDF samples consisting of crystal grains with a mosaic structure.

From figure 3 and table 3 one can see that the dislocation systems forming DIB boundaries in mosaic diamonds decrease the UC parameter and, accordingly, should increase the average x-ray density of the blocks. However, experimental examination of the weight density of mosaic diamonds indicates a decrease. In [1] the values of the weight density in the 14 semiconducting type IIb diamonds obtained ranged from 3.514 77 to 3.512 29 g cm^{-3}. The average weight density value was 3.515 06 g cm^{-3}. This is lower than the density of the perfect type IIa diamonds, which is $\rho = 3.515\,25$ g cm^{-3}. In the synthetic EDF samples and PDF samples with large dislocation densities the measured values of the weight density are even less than type IIb diamonds (table 4).

Thus, the reduction in the weight density of mosaic diamonds can occur only by an increase in their volume. However, x-ray density measurements indicate a reduction in the total volume of mosaic blocks. Hence, the increase in volume of mosaic diamonds can only result from expansion of the diamond lattice within the volume of the DIB boundaries.

The formation of an expanded diamond lattice within the DIB boundaries of mosaic diamonds can result in fundamental changes in the electronic properties of such diamonds. Natural semiconducting type IIb diamonds are an example of these effects. They have low
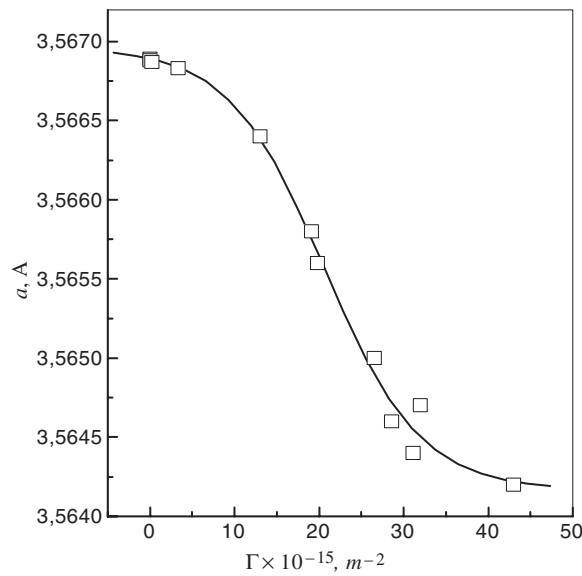
Figure 3. Relationship of the diamond UC parameter to dislocation density in diamond materials having a mosaic structure.

Table 4. The connection between the dislocation density, UC parameter and weight density in diamond materials.

Groups of diamonds	Dislocation density (m^{-2})	a (nm)	ρ (g cm^{-3})	Reference
Type IIa diamond (perfect)	$\leqslant 10^8$	$0.356689 \pm 1 \times 10^{-6}$	$3.51523 \pm 1.3 \times 10^{-5}$	[2]
Type IIb diamonds (average, mosaic)	3.04×10^{15}	$0.356683 \pm 1 \times 10^{-6}$	$3.51506 \pm 1.3 \times 10^{-5}$	[1]
PDF samples with the mosaic crystallites	1.9×10^{16}–4.3×10^{16}	$(0.35664$–$0.35642) \pm 4 \times 10^{-5}$	$(3.42$–$3.48) \pm 0.02$	[3]

specific resistance and hole electrical conductivity. This is in agreement with Shockley's representations [15] that dislocations with edge components in semiconductors with the structure of diamond form dislocation acceptor centres (DACs). The effect of the dislocation influence on the formation of electronic properties in diamond has been confirmed by our work on the creation of semiconducting properties in natural insulating diamond by the introduction of dislocation systems [16–19] under laboratory and natural conditions.

One more aspect of the functional dependence (5) can be noted. Such functional dependence can be used to interpolate between the UC parameter and dislocation densities in mosaic type IIb diamonds, EDF and PDF samples. From this dependence the UC parameter for the semiconductor diamond sample IIb (L) from [5, 6] was estimated, $a = 0.356688$ nm. The opposite calculation was also performed: on knowing the UC parameter for a sample from [3] the density of the dislocations within the DIB boundaries was estimated, $\Gamma = 1.06 \times 10^{16}$ m^{-2}. The results of these calculations are added to table 3.

5. Conclusions

In this work the relationship between the dislocation density and the UC parameter in diamonds, ranging from perfect type IIa natural crystals to synthetic PDF samples with mosaic crystallites, was investigated.

A method based on the surface tension forces that exist on dislocation boundaries between blocks of crystallites was applied to achieve a more accurate determination of the dislocation density in PDF samples.

The formula describing the dependence of the UC parameter on the density of the dislocations within the DIB boundaries was established.

An explanation is provided for the weight density reduction of mosaic diamonds, despite an increase in their x-ray density, on the basis of diamond lattice expansion within the DIB boundaries.

The basis for the formation of diamond electron properties is explained by the presence of dislocation systems within the diamond materials [17].

Acknowledgments

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