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THE EFFECT OF THE LASER-RADIATION POWER ON THE CHARACTERISTICS OF THE RAMAN LINE FOR DIAMOND SINGLE CRYSTALS

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The paper presents the results of the study of the effect exerted by exciting laser radiation on the Raman spectra of synthetic diamond single crystals plates (linear dimensions from 3 × 3 to 5 × 5 mm) having different impurity compositions. It has been found that an increase in laser radiation power from 70 to 480 mW (90–600 kW/cm^2) leads to heating of the samples by a few tens of degrees, which results in shifting of the Raman line maxima by ~0.5 cm^{-1} and in increased Raman line half-width up to ~0.15 cm^{-1}. As demonstrated by the spectral data, the heating temperature correlates with the optical density and geometry of the samples and also with the conditions of heat extraction from their surface. Based on the independent measurements of the crystal temperature at a certain distance from the excitation beam axis, it is shown that the variations of the characteristics of the principal Raman line are not determined by the local heating of the crystal studied under the effect of laser radiation. An analysis of the characteristics of the Stokes and anti-Stokes spectral components makes it possible to separate the temperature and impurity effects in the variations of the principal Raman line. Using diamond monocrystalline samples as an example, it has been revealed that the increased content of nitrogen as an impurity in the lattice from 3 up to 200 ppm leads to shifting of the Raman line maximum towards lower wave numbers by 0.08 cm^{-1} and to its broadening by 0.23 cm^{-1}.

Keywords: *synthetic diamond single crystals, Raman scattering, power of laser radiation, sample temperature, impurities.*

Introduction. Raman spectroscopy (Raman scattering) is one of the most informative methods for diagnosing the structure and phase composition of carbon materials, since each allotrope of carbon corresponds to a set of well-defined lines in Raman spectra. For a structurally perfect single crystal of diamond, the first-order Raman spectrum is a narrow single line with a peak maximum at 1332.5 cm^{-1} and a peak width at half-maximum (half-width) of 1.7 cm^{-1} at room temperature [1]. A detailed review of the effect of various factors on the main characteristics of Raman spectra of single crystals of natural and synthetic diamond, as well as CVD-diamond films, is given in [1, 2]. The position and half-width of the main peak in the Raman spectrum of diamond depend on external pressure, the presence of internal stresses, isotopic and impurity composition of the sample, etc. Therefore, the parameters of this line can serve as a measure of the degree of structural perfection of the sample. At the same time, in a number of cases (for example, when the impurity composition of the sample is varied), the characteristic changes in the position and half-width of the main RS line, caused by the presence of impurity atoms in the diamond lattice, are insignificant. Thus, according to the data reported in [3–5], the presence of nitrogen, which is the main impurity in single crystals of both natural and synthetic diamond, leads to a shift of the maximum of the main RS line to the low-frequency region by a value from tenths of a wavenumber to several cm^{-1} units. In this case, the half-width of the diamond RS-line increases with increasing concentration of nitrogen impurity [1, 5–7] and depends on the type of nitrogen defects [5]. Line broadening can reach 1.5 cm^{-1} for greater (1000 ppm) nitrogen concentrations. The study of such small effects using Raman spectroscopy is a complex task, since the parameters of the Raman line, in addition to the presence of impurity atoms in the diamond lattice, can be influenced by other factors whose effect exceeds the impurity effect. The significance of the temperature of the sample on the position of the maximum of the main diamond RS line should be noted. According to [8], an increase in the temperature of a diamond crystal from 300 to 350 K results in a 0.7 cm^{-1} shift of

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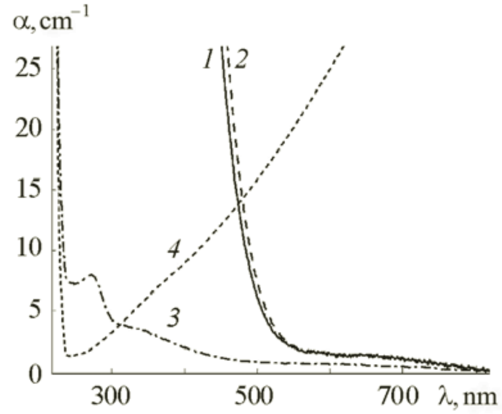

Fig. 1. Absorption spectra of samples Y1 (1), Y16 (2), W1 (3), and B6 (4) in the UV and visible ranges.

TABLE 1. Optical Characteristics of Samples

Sample	Impurity type	*n*, ppm	*l*, mm	*S*, mm^2	$\alpha_{\lambda = 481.5\text{ nm}}$, cm^{-1}	$\alpha_{\lambda = 514.5\text{ nm}}$, cm^{-1}	$\alpha_{\lambda = 552.4\text{ nm}}$, cm^{-1}
W1	Nitrogen	3	1.1	33	0.87	0.75	0.7
Y1	Nitrogen	161	1.05	70	10.5	4.0	2.1
Y16	Nitrogen	200	0.4	17	12.9	4.8	2.1
B6	Boron	19	1.5	45	14.5	17.0	20.4

Note: *n* is impurity concentration, *l* is sample thickness, *S* is the surface area of the sample, and α is the absorption coefficient.

the Raman line maximum towards low frequencies. Nonetheless, the temperature of the sample is usually not controlled in analysis of the structure of diamond single crystals by Raman scattering.

The purpose of this work is to analyze the effect of sample heating by the laser beam on the characteristics of a diamond RS line and to develop a methodology for taking this effect into account when determining impurities in samples.

Research Samples and Methods. Four single crystals of synthetic diamond with different impurity composition were studied. Monocrystals of diamond were grown by the temperature gradient method using non-press high-pressure high-temperature "cutting sphere" type devices (BARS-technology, V. S. Sobolev Institute of Geology and Mineralogy, Siberian Branch of RAS) [9]. Synthesis of crystals was carried out at the facilities of RUP "Adamas BSU" (Belarus). The impurity composition of the samples was varied by deliberate changes in the crystallization conditions.

The test samples were plane-parallel plates cut in the (111) plane with a thickness of 0.4–1.5 mm and linear dimensions from 3 × 3 to 5 × 5 mm. The level of internal stresses was controlled by analyzing the birefringence using a P-113 polarization microscope (LOMO). In crossed polarizers, all the samples have a relatively uniform gray color, which indicates that they have no noticeable internal stresses. Absorption spectra in the range of 0.2–0.9 μm were recorded using a Cary300 (Varian) spectrophotometer, IR absorption spectra were recorded using a Vertex 70 FTIR spectrometer (Bruker). The impurity composition of the samples was determined from the intensity of the absorption bands corresponding to impurity defects in the diamond lattice by using the proportionality coefficients provided in [1]. The impurity concentration is expressed in ppm, showing the number of impurity atoms per million lattice atoms.

The characteristics of the investigated samples are shown in Fig. 1 and Table 1. Samples W1, Y1, and Y16 contain nitrogen impurities in the form of single atoms in the substitution position (C-defect). The impurity concentration in the samples is 3–200 ppm. The sample W1 with a small amount of impurities is completely transparent in the visible range of the spectrum. For samples Y1 and Y16 with a high C-defect content, an edge of impurity absorption near 450 nm is observed in the visible range, and as a result the samples are yellow in color. Sample B6, doped with boron at the lattice nodes of diamond, is characterized by strong absorption of light in the red and near infrared regions of the spectrum, the intensity of which decreases in the short-wave region. Table 1 shows that the absorption coefficient of selected samples at the Raman excitation wavelength (λ = 514.5 nm) varies in the range of 0.75–17 cm^{-1}.

Raman spectra were recorded at room temperature using a 1403 Raman spectrometer from Spex, equipped with a double monochromator and cooled to T = 243 K of the photomultiplier R928. In the region of ~500 nm, the resolution of the spectrometer was 0.15 cm^{-1}. The spectra were recorded in backscattering geometry. An Ar$^+$-laser (λ = 514.5 nm) was used for excitation. The exciting beam was focused on the surface of the sample into a spot with a diameter of 10 μm. Laser radiation power was measured by an LM-2 power meter and was varied by installing neutral light filters NL in the range of 480–70 mW, the average power density in the laser spot varied from 89 to 611 kW/cm^2. The spectral half-width of the spectrometer slits was set to 0.25 cm^{-1}. To exclude the effect of the polarization state of the recorded radiation, a depolarizer (scrambler) was installed before the entrance slit of the spectrometer. Calibration of the spectral sensitivity of the system from the measuring monochromator and photomultiplier was carried out according to the standard procedure [10] with reference lamps: a 200-W tungsten-halogen lamp of the Q6.6A/T4QIICL type (220A model) and a tungsten lamp SI6-40 (at brightness temperatures 2000 and 2400 K). Parameters of the measured diamond RS lines were determined through approximation of the experimental data by the Lorentz function using Origin7 software. The measurements were carried out under normal atmospheric conditions and at a temperature of 293–296 K. In most experiments, diamond plates lay on the surface of a duralumin table of the spectrometer. For improved heat dissipation, some samples were clamped between two massive aluminum plates with an opening 1.5 mm in diameter to transmit light.

As indicated above, the characteristic change in the position of the main RS line, caused by the presence of impurities in the diamond lattice, amounts to several tenths of a cm^{-1}. To determine the exact position of the diamond RS line, an approach based on consistent recording of the Stokes and anti-Stokes components of the Raman spectrum was used. The energy of the phonon at which scattering occurs can be determined by the expression

$$\hbar\omega_0 = (E_{\mathrm{AS}} - E_{\mathrm{S}})/2\,, \tag{1}$$

where E_{AS} and E_{S} are the energies corresponding to the maxima of the anti-Stokes and Stokes components of the spectrum. Due to the symmetry of the Stokes and anti-Stokes components of the Raman spectrum with respect to the exciting laser line, the use of expression (1) makes it possible to loosen the requirements for the climatic conditions of the experiment and substantially improve the accuracy of determining the position of the Raman peak. Thus, according to [11], the use of this approach makes it possible to determine the position of the RS peak maximum for diamond within 0.05 cm^{-1}.

In the present work, reproducibility of the spectrometer parameters has been verified by a series of successive measurements (no less than 15) performed for the same sample. Samples Y1 and W1 were investigated. For both samples, the position of the line maximum determined by (1) remained constant despite significant changes in E_{AS} and E_{S}, most likely associated with a change in room temperature due to the heat released by the equipment placed in the laboratory. The standard deviation in determining the position of the RS line maximum is 0.04 cm^{-1}.

Results and Discussion. Figure 2 shows the dependence of the position of the maximum and half-width of the main Raman line on the laser radiation power. It can be seen that the line maximum shifted towards low frequencies with increasing laser radiation power (Fig. 2a). This effect is especially pronounced for samples B6 and Y16, having high absorption coefficients at λ = 514.5 nm. The maximum line shift for them reaches 0.5 cm^{-1} at a laser radiation power of 480 mW. The data obtained indicate a noticeable heating of the samples by exciting radiation. The experimental results shown in Fig. 2a are insufficient for drawing unambiguous conclusions about the influence of impurity atoms in the diamond lattice on the position of the maximum of the main RS line, since the presence of impurities in the diamond lattice apparently leads to an increase in the absorption of the laser radiation by the crystal and, as a consequence, its heating. At the same time, the influence of sample heating by the laser beam on the position of the main RS line maximum substantially exceeds the impurity effect.

From Fig. 2b it follows that the half-width of the main RS line of a diamond increases with increasing power of the exciting laser radiation. The above experimental dependences can be divided into two groups: the first — for samples Y1 and Y16, the second — for W1 and B6. For the selected groups, the dependencies have similar shapes, but are offset from each other in half-widths. Apparently, the shift is due to the different content of impurity atoms in the samples. It follows from the obtained data that an increase in the content of nitrogen impurity from 3 (sample W1) to 200 ppm (Y16) leads to a broadening of the main RS line by 0.2 cm^{-1}. The broadening of the line due to sample heating by the laser amounts to 0.1–0.15 cm^{-1} when laser radiation power is increased from 70 to 480 mW. Thus, at sufficiently high powers of the exciting radiation, the influence of sample heating by the laser beam on the half-width of the main RS line of diamond is comparable with the influence of impurities.

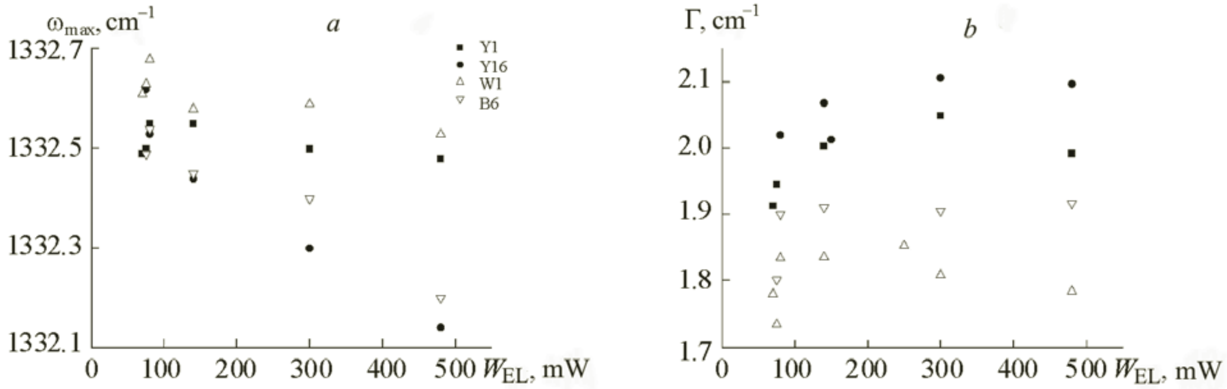

Fig. 2. Dependence of the position of the maximum (a) and half-width (b) of the main RS line of synthetic diamond single crystal samples on the power of the exciting laser radiation with λ = 514.5 nm.

It follows from the data presented that when studying the structure of diamond by means of Raman spectroscopy, it is necessary to monitor sample heating by the laser beam and take it into account when analyzing the results of the experiment. To monitor sample heating, it may be convenient to use a method based on comparing the intensities of the Stokes and anti-Stokes components of the Raman spectrum [2, 8, 12]. The temperature of the sample is determined from the expression:

$$I_S/I_{AS} = [(\omega_i - \omega_0)/(\omega_i + \omega_0)]^4 f(\omega) \exp(\hbar\omega_0/kT)\,, \tag{2}$$

where I_S and I_{AS} are the intensities of the Stokes and anti-Stokes lines, respectively; $f(\omega)$ is a coefficient that takes into account the differences in spectral sensitivity of the instrument at the frequencies of the Stokes and anti-Stokes lines; ω_i is the frequency of the exciting laser radiation; ω_0 is the frequency of the corresponding phonon. According to the data reported in [8, 12], the use of expression (2) makes it possible to determine sample temperature within 10 K in in the range of 273–750 K [12] or even up to 1300 K [8]. At $T < 273$ K, due to low intensity of the anti-Stokes component, accurate determination of the I_S/I_{AS} ratio is difficult. At high temperatures, expression (2) gives low values. The described method has obvious advantages, permitting temperature monitoring directly in the investigated region of the sample.

To verify the validity of the method and the use of expression (2), a series of successive measurements were performed for the same sample. Samples W1 and Y1 were investigated. At least 15 measurements were made for each of the samples. The power of the exciting laser radiation was 70 mW (90 kW/cm^2). After processing the measurement results using expression (2), for sample Y1 the average temperature was determined to be $T = 287.5 \pm 3.1$ K, and for the sample W1 $T = 296.5 \pm 2.7$ K. Note that the room temperature varied in the rage of 293–295 K when the sample Y1 was analyzed, and for sample W1 room temperature was 295–296 K. Clearly, the temperature of the sample Y1 determined from the spectral data is too low. One should take into account the significant differences in the absorption coefficients for these samples at the emission frequency of the Stokes and anti-Stokes components (Table 1). When Raman spectra are collected in backscattering geometry, radiation collected and analyzed by the spectrometer is scattered from the entire thickness of the sample. Therefore, the intensity of the Raman signal from absorbing crystals can be described by the expression [13]:

$$I = [1 - \exp(-(S + \alpha_1 + \alpha_2)L)] I_0 S/(S + \alpha_1 + \alpha_2)\,, \tag{3}$$

where S is Raman efficiency; α_1 and α_2 are absorption coefficients of the sample at the given wavelengths of the incident and scattered radiation; I_0 is the intensity of the incident radiation; L is sample thickness. Taking into account the fact that the efficiency of Raman scattering under ordinary conditions is small (substantially less than ($\alpha_1 + \alpha_2$)), expression (3) can be transformed into

$$I = [1 - \exp(-(\alpha_1 + \alpha_2)L)] I_0 S/(\alpha_1 + \alpha_2)\,. \tag{4}$$

According to [14], Raman efficiency for the Stokes component is:

$$S = \frac{3\hbar N^2 \omega_S{}^4}{2\pi c^4 \rho \omega_0} |\alpha_{z,y,x}|^2 (n_0 + 1)\,. \tag{5}$$

Here, ω_S is the frequency of the scattered radiation; ω_0 is the frequency of the scattering phonon; N is the number of unit cells per unit volume of the crystal; ρ is crystal density; $\alpha_{zy,x}$ is the polarizability tensor of the crystal; n_0 is the Bose–Einstein distribution:

$$n_0 = [\exp(\hbar\omega_0/kT) - 1]^{-1} . \tag{6}$$

Expression for the efficiency of the anti-Stokes component of the spectrum is similar to (4), but the term $(n_0 + 1)$ is replaced by n_0.

Considering that the frequencies of the Stokes and anti-Stokes components of the spectrum can be written as $(\omega_i - \omega_0)$ and $(\omega_i + \omega_0)$, expressions (4) – (6) can be used to express the intensity ratio of these components:

$$I_S/I_{AS} = K[(\omega_i - \omega_0)/(\omega_i + \omega_0)]^4 f(\omega) \exp(\hbar\omega_0/kT) ,$$

$$K = \left(\frac{\alpha_i + \alpha_{AS}}{\alpha_i + \alpha_S}\right)\left(\frac{1 - \exp\{-(\alpha_i + \alpha_S)L\}}{1 - \exp\{-(\alpha_i + \alpha_{AS})L\}}\right) , \tag{7}$$

where α_i, α_S, and α_{AS} are the absorption coefficients at the wavelength of the exciting laser radiation and at frequencies corresponding to the Stokes and anti-Stokes components of the spectrum. In a number of cases (for example, for structurally perfect type IIa or Ia diamond crystals), when the absorption coefficients at the frequencies of the Stokes and anti-Stokes components of the spectrum are equal, expression (7) is reduced to expression (2). Such cases are considered in [8, 12]. In the experiment described in the present work, for sample Y1, the values of α_S and α_{AS} differ by more than a factor of five (Table 1), therefore, Eq. (2) is not applicable in this case. The coefficients K for samples W1 and Y1, recalculated using expression (7), are 1.01 and 1.26, respectively. Taking into account the above considerations, the determined mean temperature value for sample W1 is 296.9 ± 2.7 K, and for sample Y1 it is 298.4 ± 2.9 K. These results make sense. Sample heating by the laser beam ΔT under the experimental conditions was small at 1.5 K for sample W1 and 4.5 K for sample Y1. Small values of ΔT are due to high thermal conductivity of the samples and a relatively low power (70 mW) of the exciting laser radiation. A slightly more significant sample heating of the sample Y1 is due to its larger absorption coefficient at the wavelength of the laser radiation compared to W1. Thus, the widely used expression (2) cannot accurately determine the temperature for light absorbing samples. In these cases, it is necessary to use the more general expression (7), which takes into account the actual absorption spectrum of the sample. According to the estimates of the authors, one can determine the absolute values of sample temperature to within 3 K using expression (7) in the temperature range near 300 K.

In the experiment described above, the minimum laser radiation power was used, which under the given conditions made it possible to reliably detect the anti-Stokes component of the diamond RS spectrum. However, in most known experiments (see, for example, [5–7]) performed on similar equipment, radiation of much higher power (200–300 mW) was used for Raman spectrum excitation. Under such conditions, sample heating by the laser beam is more pronounced and can affect the position and half-width of the main RS line. To assess the effect of heating, the experimental data for the samples under study were analyzed at various exciting laser radiation powers. The results obtained using (7) are shown in Fig. 3a. It can be seen that for all samples the temperature increases with increasing laser radiation power. However, the efficiency of heating by a laser beam differs significantly for different samples. The maximum heating is observed for samples B6 and Y16 and reaches 40–45 K at a laser radiation power of 480 mW. For samples Y1 and W1, the heating is much lower and does not exceed 10 K at maximum power. The differences are due to the samples having different absorption coefficients at λ = 514.5 nm, as well as different thicknesses (Table 1), that is, the fraction of absorbed laser radiation that results in sample heating is not the same. Based on this, the dependences of sample heating on the absorbed laser radiation power were analyzed. The power absorbed by the sample can be calculated using the expression

$$P_{abs} = P_0(1 - R)[1 - \exp(-\alpha_i L)] , \tag{8}$$

where P_0 is the power of the incident laser beam; R is the reflection coefficient of diamond at the given incident laser radiation wavelength; α_i is the absorption coefficient of the sample at the given incident laser radiation wavelength; L is sample thickness. For λ = 514.5 nm, the reflection coefficient at the diamond–air interface is 0.174 [1]. The obtained dependences are shown in Fig. 3b. It can be seen that the differences in the dependence of the temperature change of the samples on the power of the absorbed laser radiation are conserved. Apparently, sample heating greatly depends on sample size. Since the efficiency of heat removal from a heated body is proportional to its surface area, under the given experimental conditions the

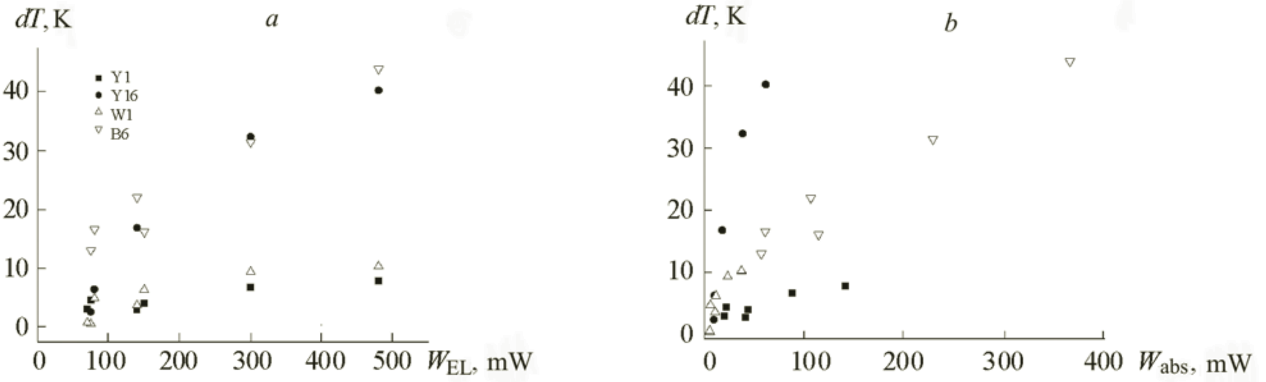

Fig. 3. Sample heating as a function of the total (a) and absorbed (b) power of the exciting laser radiation.

sample of a smaller surface area, other things being equal, should be heated more strongly. This effect manifests well when comparing the characteristics of samples Y1 and Y16. From Table 1 it follows that for samples Y1 and Y16 the surface area differs by a factor of 4 (70 and 17 mm^2). It can be seen in Fig. 3b that for the sample Y16, the slope of the function describing the dependence of temperature on the absorbed power is much greater than for sample Y1. At the same time, for samples W1 and B6 having similar surface areas, the experimental points are practically on the same curve.

The presence of such dependences on the size of the sample indicates that for diamond single crystals the heating of the sample by the laser beam has a bulk rather than a local character. To verify this assumption, the described experiment for testing the influence of laser radiation power on the heating of single crystals of synthetic diamond during the measurement of Raman spectra was repeated, but the samples were clamped between two massive aluminum plates with an aperture 1.5 mm in diameter to transmit light. The presence of this additional heat sink led to a decrease in the heating of samples determined by equation (7) by a factor of 3–4 in comparison with the previous experiment, where the crystals were lying freely on the spectrometer stage. In addition, independent temperature measurements were carried out for sample B6 away from the axis of the exciting laser beam using a thermocouple. The junction of the chromel-alumel thermocouple was mechanically pressed against the surface of the plate 1.5 mm away from the laser beam axis. A systematic increase in the thermoelectric power was observed with increasing laser radiation power. The temperature of the sample was established within 10–15 s, the spectrum collection time was 250 s. The temperatures determined with the thermocouple were 3–4 K below the values obtained by the method of comparing the intensities of the Stokes and anti-Stokes component of the spectrum using expression (7). Based on the above experimental data it can be concluded that, due to high thermal conductivity of diamond, heat is effectively transferred to the bulk of the crystal from the region where laser radiation acts on the sample, and the sample is heated relatively uniformly. Consequently, the changes in Raman spectrum parameters of diamond are caused by an increase in its temperature not only at the spot where laser radiation acts on the crystal, but in the entire volume of the sample.

The accuracy of the methods used to determine the position of the band maximum and sample temperature can be estimated by comparing the obtained temperature dependences of the half-width and the position of the maximum of the main diamond RS line with the known experimental and theoretical results. The influence of sample temperature on the parameters of the main RS line has been fairly well studied [1]. There are more than a dozen experimental studies (see, for example, [8, 15, 16]), where the position and half-width changes of the diamond line in the temperature range of 14–2300 K have been determined. In [17, 18] various theoretical models were proposed to describe the decay of an optical phonon from the center of the Brillouin zone. In most cases, the problem cannot be solved analytically. To describe the shape of the Raman band, a simplified Klemens model [19] has been most widely used. Decay of the optical phonon into two acoustic phonons belonging to the same branch but having opposite momenta is considered in this model. In this case, the dependence of the half-width of the RS line on the temperature $\Gamma(T)$ can be described by a simple expression

$$\Gamma(T) = \Gamma_0(1 + 2/[\exp(\hbar\omega_0/2kT) - 1]) , \qquad (9)$$

where Γ_0 and $\hbar\omega_0$ are the line half-width and the energy of the phonon from the center of the Brillouin zone at $T = 0$ K; k is the Boltzmann constant; T is the absolute temperature.

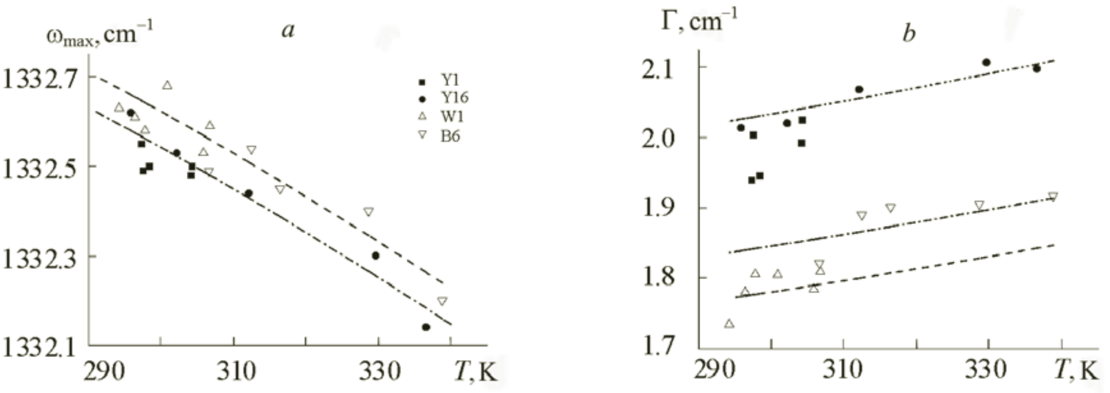

Fig. 4. Dependences of the peak position (*a*) and half-width (*b*) of the main RS line on the temperature for various samples of synthetic diamond; lines — theoretical predictions of the model [19]: a) Eq. (10) for $A = 9.5$ cm^{-1} and $\omega_0 = 1333.44$ and 1333.36 cm^{-1}; b) Eq. (9) for $\Gamma_0 = 1.64$, 1.70 and 1.87 cm^{-1}.

Since for the anharmonic approximation the real and imaginary parts of the intrinsic energy of the phonon are related by the Kramers–Kronig relation, the temperature shift of the RS line from the position corresponding to zero temperature $\Delta\omega(T)$ should be described by the same dependence, but with the opposite sign:

$$\Delta\omega(T) = -A(2/[\exp(\hbar\omega_0/2kT) - 1]) \,, \qquad (10)$$

where A is a constant, depending on the features of the dispersion curves of the sample. It was shown in [17] that the experimental results obtained both directly in [17] and in a number of earlier works (for example, [16, 20]) are well described by the expressions (9) and (10).

Figure 4 shows the temperature dependences of the half-width and the peak position of the main RS line for the investigated single crystals of synthetic diamond, both calculated from (9) and (10) and obtained from the experimental data. Fig. 4a shows that the experimentally detected shift of the main RS line of diamond observed with increasing sample temperature is well described by expression (10) for $A = 9.6$ cm^{-1}. The values of ω_0 depend on the impurity content in the samples. For crystals with a low content of impurities (type IIa) $\omega_0 = 1333.44$ cm^{-1}. An increase in the nitrogen impurity content from 3 (sample W1) to 200 ppm (Y16) causes ω_0 to decrease by 0.08 cm^{-1}.

A similar pattern is observed for the line half-width (Fig. 4b). Experimental dependences of the line half-width on temperature are in good agreement with the results of calculations using (9). The parameter Γ_0 increases with increasing impurity content in crystals. For type IIa crystals, $\Gamma_0 = 1.64$ cm^{-1}. An increase in the content of the nitrogen impurity from 3 to 200 ppm leads to a broadening of the main RS diamond line by 0.23 cm^{-1}, which correlates with the experimental data [5].

Good agreement of the obtained temperature dependences of the half-width and the peak position of the main diamond RS line with known experimental and theoretical data confirms validity of the methods used to determine these parameters. In addition, analysis of such temperature dependences for samples with different impurity composition in a diamond lattice makes it possible to separate the effects of temperature and impurity content on the parameters of the main RS line of a single crystal.

Conclusions. For the laser radiation power range of 70–480 mW (90–600 kW/cm^2), which is usually used to excite Raman scattering spectra of diamond, it is possible to heat the samples to several tens of degrees, which leads to a shift of the diamond Raman line maximum by ~0.5 cm^{-1} and an increase in the half-width of the Raman-scattering band of single crystals to ~0.15 cm^{-1}. Sample heating efficiency is determined by their optical density at the analyzing laser radiation wavelength and by their geometry, as well as by the conditions of heat removal from the surface of the samples during measurements. Due to high thermal conductivity of diamond, effective heat removal occurs to the bulk of the crystal from the region of action of laser radiation on it, and the sample is heated relatively uniformly.

For crystals with a high absorption coefficient at the laser radiation wavelength, the effect of sample heating by the laser beam on the parameters of the main Raman scattering line of diamond are comparable or even exceed the influence of impurities. It has been shown that in order to correctly determine the diamond temperature by the method of comparing the parameters of the Stokes and anti-Stokes components of the spectrum, it is necessary to take into account crystal absorption at the emission frequency of these components. According to the obtained experimental data, this technique makes it possible to monitor sample temperature during measurements to within 3 K, and the peak position of the Raman lines to within at least 0.05 cm^{-1}. It is shown that by analyzing the temperature dependences of the peak position and half-width of the Raman line of diamond samples with different impurity composition, the impurity effect and the temperature effect can be separated. Thus, for the investigated samples of single crystals of synthetic diamond, an increase in the content of nitrogen impurity in the lattice of diamond from 3 to 200 ppm results in a shift of the Raman line maximum to the low-frequency region by 0.08 cm^{-1} and its broadening by 0.23 cm^{-1}.

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