

Zoning of Diamonds from the Mir Kimberlite Pipe: Results of Fourier-Transformed Infrared Spectroscopy

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Abstract—Plates prepared of diamonds from the Mir kimberlite pipe were examined with FTIR spectroscopy. It is shown that B1 defects were formed by annealing during crystal growth, whereas B2 centers arose after growth cessation. The development of B2 centers in a natural diamond is the secondary process with respect to the aggregation of the nitrogen admixture. The kinetics of this process is related to the breakdown of an over-saturated solid solution. The results obtained make it possible to estimate the temperature and duration of natural diamond growth.

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INTRODUCTION

Most natural diamonds reveal zoning in the distribution of A, B1, and B2 defects of the crystalline structure (Beskrovanov, 2000), which exert an effect on many physical features (Vecherin et al., 1997) and are determined in quantitative terms by the systems of absorption in the IR range that bear the same names. According to the modern concept (Jones et al., 1992; Goss et al., 2003), an A defect consists of two replacing nitrogen atoms; the suggested model of B1 defect comprises four replacing nitrogen atoms and a vacancy. The annealing of diamonds results in the transformation of an A defect into a B1 (Allen and Evans, 1981; Evans and Qi, 1982), which is often termed the aggregation of nitrogen. The determination of nitrogen concentrations in the forms of A and B1 defects makes it possible to estimate the temperature and duration of annealing of natural diamonds, i.e., their residence time under conditions of the upper mantle (Taylor et al., 1990; Mendellsohn and Milledge, 1995) in line with the kinetic equation of the second order

$$C_{N(A)} = C_N/[1 + tC_N A_{Ar} \exp(-E_A/RT)],$$

where T is the temperature, t is the duration of diamond annealing, C_N is the total concentration of nitrogen, $C_{N(A)}$ is the concentration of nitrogen in the form of an A defect, at. ppm, A_{Ar} is the Arrhenius constant, $\ln A_{Ar} = 13.5$, and $E_A/R = 81\,626$ K (Taylor et al., 1990).

In terms of this model, the formation of B1 point defects results in the appearance of internode carbon atoms that further make up large B2 planar defects denoted as platelets. Their linear dimensions vary from a few nanometers (Allen and Evans, 1981) to a few micrometers (Sobolev et al., 1968; Woods, 1976) and

the thickness is measured by a few atomic layers (Humble, 1985; Barry, 1991). B2 defects are identified by an absorption band with a maximum in the range 1358 – 1378 cm^{-1} ; the exact position of this maximum is controlled by the defect dimension (Sobolev et al., 1968; Hanley et al., 1977; Clackson, 1990). B2 defects often contain nitrogen that is not a necessary structural constituent, because its content varies widely (Berger and Pennycook, 1982; Bruley, 1992; Fallon et al., 1995) and the isotopic nitrogen composition does not affect the position of the B2 band (Woods et al., 1993).

The theoretical study of the formation of B2 centers as an aggregation of internode carbon atoms showed that they originate in two ways (Goss et al., 2000, 2003). The first way consists in the diffusion of A defects that gives rise to the formation of B1 defect and a mobile internode carbon atom, which is captured by the B2 center. The dissociation of A defects into single nitrogen atoms with an equilibrium constant controlled by the temperature (Brozel et al., 1978) probably is an intermediate stage. The second way provides for the growth of B2 defects with the formation of a vacancy, which diffuses further toward an A defect, making up relatively mobile H3 centers; the diffusion of these centers to an A defect results in the formation of a B1 defect. Thus, the first mechanism implies that the formation of B1 defects is a cause of the growth of B2 defects, whereas, in the second mechanism, the formation of B1 defects is a consequence of the growth of B2 centers. While the second mechanism is realized, the ratio of the concentrations of B1 defects to the concentrations of atoms in the B2 centers is constant in all crystals or less than a certain limiting value if the B2 centers remain undestroyed. In some samples denoted as ordered (Woods, 1986), absorption coefficients in B1 and B2 systems are connected by a linear

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relationship. In disordered samples, such a correlation is absent. Woods (1986) explained this phenomenon by the destruction of B2 centers with the formation of dislocation loops and nitrogen-bearing microcavities (Hirsch et al., 1986; Evans et al., 1995). Another possible cause of the distorted proportionality related to the incomplete formation of B2 centers was not applied previously to the interpretation of zoning in natural diamonds described by many authors (Mendellsohn et al., 1991; Milledge et al., 1995; Beskrovnov, 2000; Bulanova et al., 2002; Appleyard et al., 2004). If the formation of B2 defects is not ended, then the characteristics of the B2 band may also be used to estimate the temperature and duration of diamond annealing and to supplement the data obtained from the determination of the degree of nitrogen aggregation. To elucidate a dominating mechanism of the formation of B2 defects in natural diamonds and to verify the hypothesis of the incomplete formation of B2 centers, it is necessary to investigate the distribution of nitrogen concentrations in the forms of A, B1, and B2 defects and to determine the position of the maximum of the B2 band through the volume of samples. The decreased ratio of the concentration of atoms in B2 defects to the concentration of B1 defects from the growth center outward will testify to the incomplete formation of centers and the growth following the first mechanism, whereas the increase in this ratio will indicate either the destruction of B2 centers or their formation by the second way.

EXPERIMENTAL AND SAMPLES

To ascertain the distribution of A, B1, and B2 centers through the volume, we examined five plates of diamonds $3 \times 4 \times 0.4$ mm in dimension sawed off from crystals along {100} and then polished. The diamonds from the Mir kimberlite pipe initially were plane-faced octahedrons of type I according to the classification proposed by Orlov (1984), which are typical of this deposit (Zinchuk et al., 2003). The photomicrographs of the studied samples with crossed polars are shown in Fig. 1. Samples 1–3 are quarters of the crystal sections; the growth centers are located in the lower-right corners. Sample 4 embraces the entire crystal, and, in sample 5, the growth center is located in the right-hand part of the photomicrograph. The nitrogen concentration in the forms of A and B1 defects, the integral absorption coefficient proportional to the amount of atoms in B2 defects, and the position of the maximum of the B2 band in the IR absorption spectra were determined for the prepared plates. The spectra were recorded with an FSM-1201 FTIR spectrometer equipped with a MIK-15 microscope. The records were obtained at room temperature with a resolution of 4 cm^{-1} and averaging of 256 measurements for the spectra of radiation intensity transmitted through the sample and of 512 measurements for background spectrum. The spectra were recorded from areas 0.3 mm in diameter with overlapping of analyzed areas. The nitrogen concentrations in

the forms of the A defects ($C_{N(A)}$, at. ppm) and B1 defects ($C_{N(B1)}$, at. ppm) were calculated from the absorption coefficients at frequencies of 1282 (α_{1282}) and 1175 cm^{-1} (α_{1175}) using calibrating coefficients (Bokii et al., 1986; Boyd et al., 1994, 1995): $C_{N(A)} = 16 \times 1.2(\alpha_{1282} - 0.41\alpha_{1175})$ and $C_{N(B1)} = 79 \times 0.4 \times 1.2(\alpha_{1175} - \alpha_{1282})$.

The position of the maximum absorption of the B2 band (ν_{B2}) was determined with interpolation of the spectra. The amount of excess carbon atoms ($C_{1(B2)}$, at. ppm) in the B2 defects was determined from the integral absorption coefficient of the B2 band (K_{B2}) that is proportional to the area of the B2 defects in a volume unit (Sumida and Lang, 1988): $C_{1(B2)} = 0.4 \times K_{B2}$ (Vasil'ev, 2005). The standard deviation of the nitrogen concentrations in the forms of the A and B1 defects was 6 and 13%, respectively, and 5% for the integral absorption coefficient for the B2 band. Section {100} is not optimal for the study of the heterogeneities in diamonds of an octahedral habit, because zones with different characteristics overlap due to the finite thickness of the plate. The width of such overlapping is 14% less than the plate thickness, and upon observation in the direction {100}, it is impossible to reveal distinct boundaries between consecutive zones in both the birefringence and distribution of the defects. Therefore, in the zones that correspond to the local maximum on the curve of the distribution of the measured concentration, the true concentration value is higher than the measured one, while in zones with a local minimum, the true concentration is lower than the measured value.

RESULTS

As can be seen from Fig. 1, all samples are zonal as commonly observed in natural diamonds (Varshavsky, 1968; Beskrovnov, 2000). Zones and sectors with normal growth mechanisms, dissolution boundaries, and other features, which would indicate significant variations in the conditions during the growth of these crystals, are not observed. Figure 1 also demonstrates the distribution of the total nitrogen concentrations in the A and B1 defects (C_N) in the volume of the studied samples and the degree of aggregation, i.e., the percentage of nitrogen in the form of the B1 defect [$C_{N(B1)}/C_N$ 100], (%), as well as the ratio of the nitrogen concentration in the B1 form to the concentration of excess carbon atoms B2 [$C_{N(B1)}/C_{1(B2)}$] and the position of the maximum on the B2 band (ν_{B2}). For the sake of clarity, the $C_{N(B1)}/C_{1(B2)}$ ratio and degree of nitrogen aggregation is enlarged ten times in one diagram.

Plate 1. In the central region, the nitrogen concentration is about 900 at. ppm; then, it abruptly falls to 400 at. ppm in the intermediate zone and remains at the level of 400–500 at. ppm in the marginal zone. The degree of nitrogen aggregation is 40% in the central zone, 23% in the intermediate zone, and 10% in the

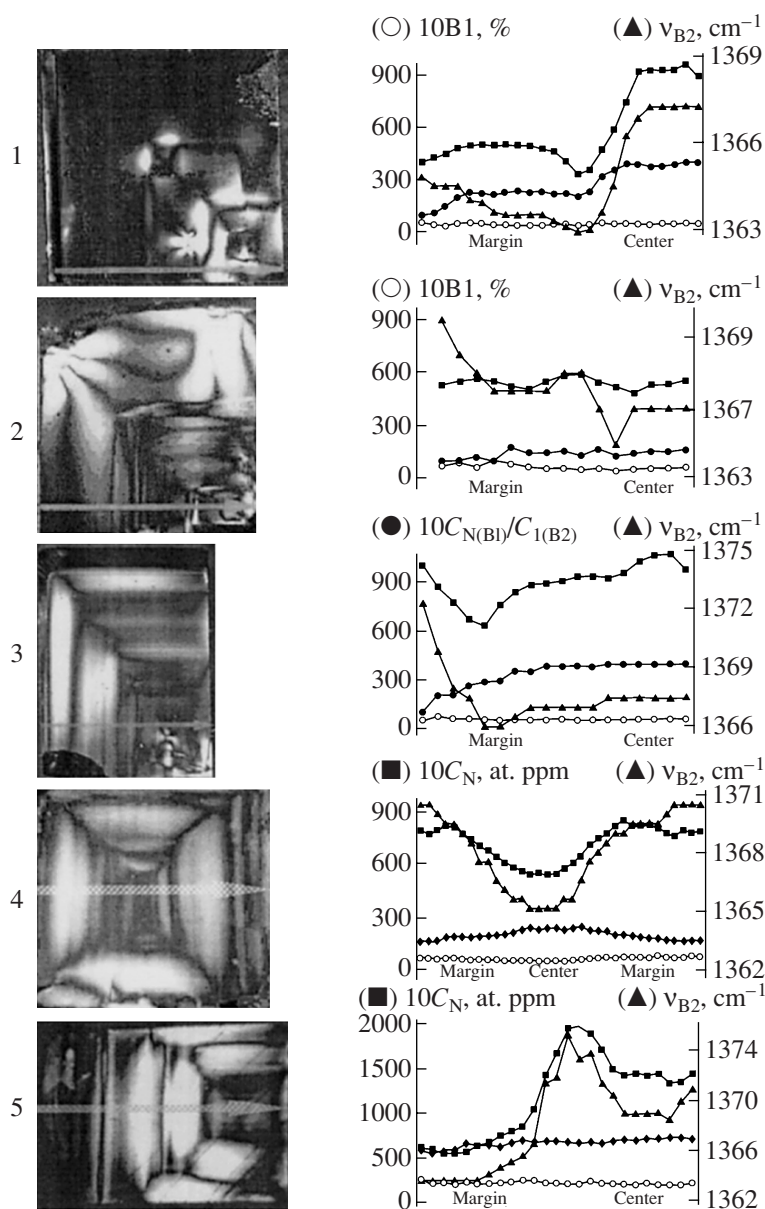


Fig. 1. Photomicrographs of plates 1–5 (crossed polars) E[100] and distribution of the total nitrogen concentration (filled box), percentage of nitrogen in the form of B1 defects (filled circle), position of the maximum of the B2 band (filled triangle), and ratio of nitrogen concentration in the form of B1 defects to the concentration of atoms in B2 centers (open circle). Arrows indicate measurement profiles.

marginal zone. The maximum of the B2 band shifts from 1367.3 cm^{-1} in the central part of the crystal to 1363.6 cm^{-1} and 1365.8 cm^{-1} in the intermediate and marginal zones, respectively. The $C_{N(B1)}/C_{1(B2)}$ ratio ~ 4 is virtually constant throughout the crystal and corresponds to the ordered diamond.

Plate 2. C_N slightly varies within the range 490–590 at. ppm. The relative nitrogen concentration in the form of B1 defects decreases from 16% in the center to 10% in the marginal zone. The $C_{N(B1)}/C_{1(B2)}$ ratio increases from 5–6 in the center to 8% at the periphery, i.e., is twice as high than in ordered diamonds. The posi-

tion of the maximum of the B2 band also changes: at the margin of the plate, the maximum falls on 1369.5 cm^{-1} , whereas, in the central part of the crystal, it falls on 1366.5 cm^{-1} ; the greatest wavelength (1366.1 cm^{-1}) was noted at one point in the intermediate zone with a minimum in the nitrogen concentration.

Plate 3. The sample reveals a distinct zoning along (111) across the entire volume. The nitrogen concentration at the center of crystal is 1070 at. ppm, decreases to 640 at. ppm in the intermediate zone, and increases to 1010 at. ppm in the marginal zone. The degree of nitrogen aggregation gradually decreases from 40% in

the center to 10% in the marginal zone. Despite the significant change in the concentrations of A and B1 defects, the $C_{N(B1)}/C_{1(B2)}$ ratio is almost constant throughout the crystal at a level of 5.8, increasing to 7.7 at the periphery, and falling to 5.1 at the outermost point. The maximum of the B2 band shifts from 1372.5 cm^{-1} in the marginal zone to 1366.1 cm^{-1} in the intermediate zone, and 1367.5 cm^{-1} in the central zone.

Plate 4. In contrast to the preceding plates, the nitrogen concentration increases from 550 at. ppm in the center of the crystal to 830 at. ppm in the peripheral zone and falls at the edge of the plate. The degree of nitrogen aggregation decreases from 25% in the center to 18% at the margin. The $C_{N(B1)}/C_{1(B2)}$ ratio rises from 5.7 in the center to 7.8 at the periphery. The shift of the maximum of the B2 band from 1365.2 cm^{-1} in the center to 1370.5 cm^{-1} at the margin indicates that, at the periphery, the B2 centers are much smaller than in the crystal center.

Plate 5. This sample is distinguished by a maximum concentration of nitrogen occasionally reaching 2000 at. ppm. In the growth center, the concentration is 1440 at. ppm and falls to 600 at. ppm at the margin. The degree of nitrogen aggregation gradually decreases from 72% in the center of the crystal to 58% at its periphery. The $C_{N(B1)}/C_{1(B2)}$ ratio remains constant at 5.8 ± 0.7 . The position of the maximum of the B2 band reflects the variation in the total nitrogen content and shifts from 1375.4 cm^{-1} to 1363.8 cm^{-1} .

DISCUSSION

The study of the distribution of the nitrogen defects A and B1, the integral absorption coefficient, and the position of the maximum absorption of the B2 band for the plates sawed off from natural diamonds led to the following conclusions.

(1) The degree of nitrogen aggregation in all of the studied crystals decreases from the center to the margin.

(2) The ratio of the nitrogen concentration in the form of B1 defects to the concentration of the atoms in the form of B2 defect varies insignificantly over the plates, but is distinct in different samples. The minimum $C_{N(B1)}/C_{1(B2)}$ ratio that equals 4 and fits ordered samples was noted only in plate 1.

(3) The maximum of the B2 band shifts toward the short-wave region at the periphery of the crystals. This trend is often disturbed through the crystal section. The short-wave position of the maximum of the B2 band corresponds to the regions enriched in nitrogen.

The results obtained indicate an irregular variation in the nitrogen concentration outward from the crystal center. Note that it is as yet impossible to establish whether a variation in the nitrogen concentration in the environment that affects the growth rate and crystal morphology (Stolk et al., 2003) or a shift of *PT* parameters is the cause of the zoning in natural diamonds and

to understand to what extent both factors are interrelated. The distribution of nitrogen and carbon isotopic compositions indicates that the composition of the environment changes during crystallization (Bulanova et al., 2002; Hauri et al., 2004).

The results of the measurements of the degree of nitrogen aggregation and calculated isotherms of diamond annealing at 1400 and 1450 K during 3 Ga are shown in Fig. 2. As can be seen, the different zones of one crystal do not fall on the same isotherm. Hence, the results of the study of zonal diamonds cannot be interpreted in terms of follow-up annealing of the crystal as a whole, because separate zones of one crystal cannot be annealed in different regimes over 3 Ga. It should be noted that the isotherm at $T = 1400\text{ K}$ corresponds to the isochron of 275 Ma at $T = 1460\text{ K}$ (Fig. 2).

As follows from Fig. 2, a higher temperature or greater duration of annealing corresponds to central parts of the crystals; deviations from this general trend are within the error limits of the determination of the degree of aggregation for most samples, except plate 4, which is distinguished by a high nitrogen content (2000 at. ppm) at a high degree of aggregation (up to 75%). It may be suggested that an appreciable percentage of nitrogen in this crystal occurs in the B2 defects that captured diffusing nitrogen atoms. Nitrogen that occurs in the B2 defects is not measured, and, thus, the recorded results underestimate the degree of aggregation. Another possible cause of the underestimation may be related to the change in the kinetics of the process with an increase in the nitrogen concentration owing to the interaction of the defects or variation in the volumetric characteristics of the diamond matrix. The diminishing degree of nitrogen aggregation from the crystal center to its periphery indicates that 15–75% of the B1 defects in the studied samples were formed during crystal growth, when the high temperature provided a sufficiently high rate of this process. Thus, one can judge the temperature and duration of postgrowth annealing only from the degree of nitrogen aggregation in the near-surface zone of the crystals.

The constant ratio of the nitrogen concentration in form of B1 defects to the concentration of atoms in the B2 defects admits two alternative explanations. (i) B2 centers were formed simultaneously throughout the crystal after the cessation of its growth. The rate of this process was lower than the rate of the formation of B1 defects. (ii) B1 and B2 defects were formed synchronously, and the time that elapsed from the onset of the growth of the diamond to its completion does not affect the completeness of their formation from internode carbon atoms.

In the latter case, the formation rate of the B2 centers is equal to or higher than the formation rate of B1 defects, and all samples must be ordered; but this assumption is denied by the unequal $C_{N(B1)}/K_{(B2)}$ ratios in different crystals. Hence, the B2 centers were formed largely after the cessation of crystal growth, whereas most B1 defects were formed from A defects at the

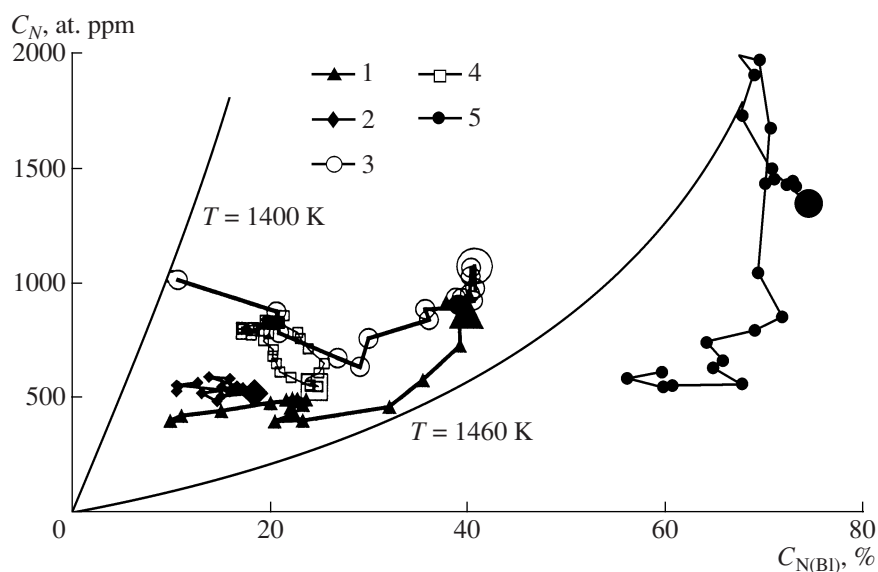


Fig. 2. Variation in the degree of nitrogen aggregation over the area of the studied plates 1–5. Large symbols correspond to central regions of crystals. Solid lines are calculated isotherms 1460 and 1400 K for annealing during 3 Ga equivalent to isochrons 0.275 and 3 Ga at a temperature of 1460 K, after Taylor et al. (1995).

thermodynamic parameters of crystal growth. In this case, the B2 centers are formed via intermediate stages with the formation of more simple defects (Vasil'ev et al., 2005), which serve as an efficient outlet or source of internode atoms depending on the external conditions.

It is known that the maximum of absorption band shifts toward the long-wave region with an increase in the dimensions of the B2 defects (Sobolev et al., 1968; Hanley et al., 1977; Clackson et al., 1990). The kinetics of the formation of the B2 centers as macrodefects has to be described in terms of the breakdown of an one-component oversaturated solid solution (Slezov and Sagalovich, 1987) that proceeds over three stages: (i) the origin of macrodefects at the initial stage, (ii) their growth without increasing in number and at an appreciable decrease in the degree of oversaturation, and (iii) their redistribution by dimensions at the final stage, while small defects are dissolved and large ones increase in size. In terms of this interpretation, the amount of B2 defects is determined by the initial degree of oversaturation with internode carbon atoms in the growing crystal, i.e., by the rate of their appearance in the beginning of aggregation, when a new diamond layer arises. Discrete internode carbon atoms are already mobile at room temperature and afterward are combined in more complicated multiatomic defects (Collins, 1999), whose possible structures were considered by Goss et al. (2003). The internode carbon atoms that appear during subsequent annealing induce further growth of the already existing B2 defects without the formation of new defects. The initial rate of aggregation depends not only on temperature, but also on the concentration of A defects. Therefore, in high-N crystals, the maximum of the B2 band is commonly located in

the short-wave region. This allowed Davies (1977) to derive a linear relationship between the position of the maximum of the B2 band and α_{1282} . Since B2 centers of different sizes occur in a crystal simultaneously, the shape of the B2 band reflects the distribution of the B2 centers by their dimensions. At the initial stage of aggregation, the contour of the B2 band is the most asymmetric with a shift toward the short-wave region, occasionally up to 1400 cm^{-1} . At the end of the process, B2 centers of minor dimensions dissociate, and the B2 band becomes less asymmetric with a shift in the maximum toward the long-wave region (Woods, 1986). In some samples, considerable postgrowth heating gives rise to the additional formation of B2 centers. In this case, the absorption band splits, indicating two stages of its generation. This approach is close to the interpretation of the growth of B2 defects as a coalescence of gas pores during long-term mantle annealing (Mal'kov and Askhabov, 1979); however, the possibility of the displacement of B2 defects themselves seems to be less probable.

If the nitrogen aggregation occurs after the cessation of crystal growth, i.e., is constant through the volume of the sample, then the $C_{N(BI)}/C_{B2}$ ratio must be constant, and, in this case, the position of the maximum of the B2 band is determined by the total nitrogen concentration, as was established in sample 5 with minimum variation in the degree of aggradation through the sample (Fig. 3). The positive correlation between the position of this maximum and the nitrogen concentration allows us to suggest a parabolic relationship between the position of the maximum and the dimensions of the B2 defects. Taking into account the data reported by Sumida and Lang (1988), Clackson (1990), and Kiflawi et al. (1998)

and accepting 3 nm as a minimal dimension of the B2 defects (Allen and Evans, 1981) at the short-wave limit of the maximum position at 1378 cm^{-1} (Vasil'ev et al., 2005), these points can be approximated by parabolic relationship $R_{B2}(v) = 0.089 \times (v_{B2} - 1380)^2 + 2$ (Fig. 4).

Assuming that the concentration of the atoms in the B2 defects is proportional to the square of their linear dimensions, accepting the concentration of the excess carbon atoms in the B2 defects as two atoms per unit cell, or 15.8 atoms/nm^2 (Humble, 1992), accounting a recalculation of at. ppm into cm^{-3} , and knowing the absorption spectrum $\alpha_{B2}(v)$, one can estimate the concentration of the defects properly as $B2(N_{B2}):N_{B2} = 0.4 \times 1.76 \times 10^{17}/15.8 \int \alpha_{B2}(v) R_{B2}^{-2}(v) dv$.

Integration was carried out within the limits $1350\text{--}1380 \text{ cm}^{-1}$. In the zones of plate 5 with the outermost position of the maximum of the B2 band, N_{B2} is 2.1×10^{15} and $1.3 \times 10^{17} \text{ cm}^{-3}$. These data indicate that the concentration of B2 centers in the volume of this crystal changes more than two times and is controlled by the total nitrogen concentration.

Let us make use of the simplest nucleation model for the estimation of the variable conditions at the formation of B2 defects in different zones of the crystal. Writing the relationship between the amount of nuclei of macrodefects of critical dimensions (further accepted as equal to N_{B2}), the concentration of the internode carbon atoms C_1 , and the temperature as $N_{B2} = C_1 \exp(-E_{B2}/RT)$, according to the classic equation of the equilibrium nuclei distribution by size (Vollmer, 1986). Here, E_{B2} is the energy of the formation of B2 centers of a critical size without taking into account the dependence of the critical size on oversaturation. Since the equilibrium concentration of the internode carbon atoms is negligibly low and their mobility is high, then their concentration in the crystal is proportional to the rate of formation, i.e., to the rate of nitrogen aggregation $C_1 \approx dC_1/dt = 1/4dC_{N(A)}/dt \approx C_N^2 \exp(-E_A/RT)$. After transformation, we obtain $RT/(E_{B2} + E_A) \approx 1/\ln(C_N^2/N_{B2})$.

This relationship allows us to estimate a change in the diamond growth temperature from the center to the margin of the crystal without determining the absolute value: $T/T_{\max} = \ln(C_N^2/N_{B2})_{\max}/\ln(C_N^2/N_{B2})$.

The curves of $T/T_{\max}$ variation through the volume of the studied samples are shown in Fig. 5. The minimum C_N^2/N_{B2} value corresponds to the high-N part of plate 5. Accepting that the maximum temperature of diamond growth is 1700 K (Bulanova, 1993), one can estimate a temperature range during crystal growth. In plate 5, the maximum temperature 1700 K corresponds to the growth center, while the minimum temperature is 1560 K . Diamonds from plates 2 and 3 grew at a tem-

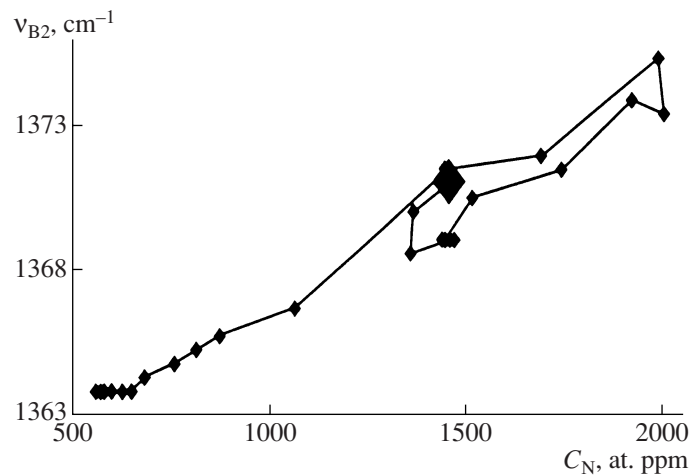


Fig. 3. Position of the maximum absorption of the B2 band versus the total nitrogen concentration in the forms of A and B1 defects in plate 5 with a constant degree of aggregation over the area. Large symbol is the outermost measurement point in the central region of the crystal.

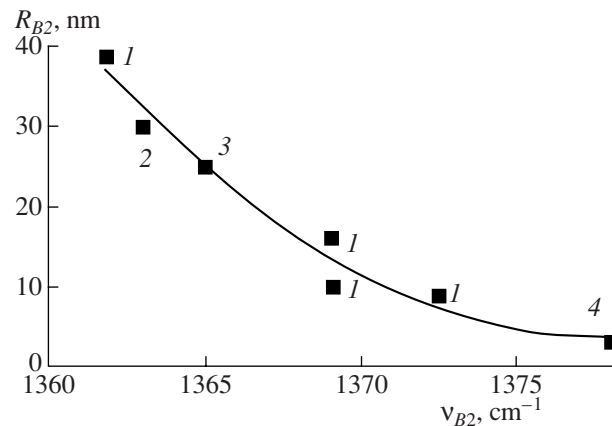


Fig. 4. Position of the maximum absorption of the B2 band versus the dimensions of the defects. (1) Clarkson et al. (1990), (2) Kiflawi et al (1998), (3) Sumida and Lang (1988), (4) limited recorded values (Allen and Evans, 1981; Vasil'ev et al., 2005).

perature of about 1630 K with deviations of $<20 \text{ K}$. In plate 1, the growth temperature gradually fell from 1660 to 1440 K . Crystal 4 grew at a temperature increasing from 1600 to 1630 K ; however, this range lies within the uncertainty limit. It is noteworthy that the variation in the nitrogen concentration in the studied plates does not accompany variation in the growth temperature, as exemplified in plate 5. As follows from Fig. 5, the falling temperature is not a crucial cause for the cessation of diamond growth, because the growth temperature of the marginal zones differs from one sample to another. This suggestion requires confirmation by further and a more detailed study of the surface layers of diamonds.

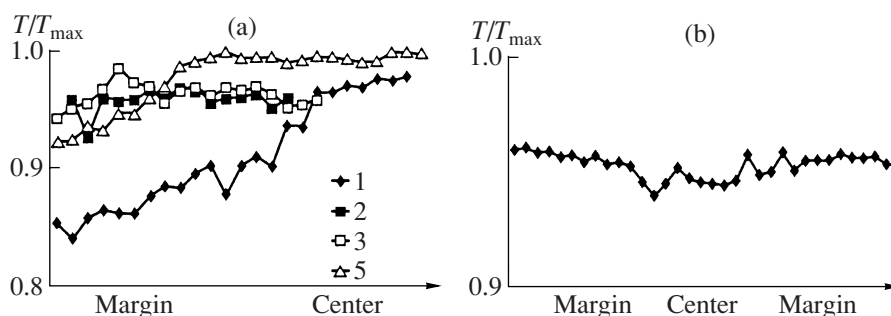


Fig. 5. Relative variation in the temperature during diamond growth: (a) plates (1–3, 5), (b) plate 4.

Thus, the shift of the maximum of the B2 band moving from the growth center toward the periphery is controlled by the evolution of the temperature of annealing, which can be estimated from the kinetic parameters of the formation of B1 and B2 defects, the distribution of B2 centers by their size, and the nitrogen concentration. While these data are available, one can determine not only the temperature of diamond growth, but also estimate the duration of this process from a variation in the degree of nitrogen aggregation. Another important aspect of this study pertains to the elucidation of relationships between temperature, rate of diamond growth, and concentration of nitrogen admixture. Unfortunately, the absence of experimental data on the formation of B2 centers under various conditions hampers the determination of the absolute temperature of diamond growth and the duration of this process. It should be noted that these estimates are impossible for nitrogen-free diamonds and for crystals with destroyed B2 defects as was established for the samples of ultradeep diamonds from Brazil (Kaminsky, 2001).

In summary, it may be concluded that the degree of nitrogen aggregation is determined not only by the regime of postgrowth annealing of the diamond, but to a greater extent, by the temperature and duration of annealing during the process of crystal growth. The amount of B2 centers bears information on the temperature at the first stage of annealing, determines their further dimensions, and remains almost unchanged under various postgrowth effects. The position of the maximum of the B2 band may be used in the description of diamonds as a characteristic that enhances the reliability of the comparison of crystals derived from different sources.

CONCLUSIONS

The study of the distribution of A, B1, and B2 defects within octahedral diamond crystals from the Mir kimberlite type has shown that B1 defects were formed from A defects through annealing during crystal growth. The formation of B1 and B2 centers should be regarded as consecutive processes; thereby, the amount of B2 centers is determined by the nitrogen

concentration in the diamond and the initial temperature of annealing. The distribution of B2 defects using their dimensions is a sensitive indicator of the variation in the temperature characterizing diamond formation. Therefore, a further study focused on the development of a mineralogical geothermometer based on B2 centers is of current importance.

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