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1999 J. Phys.: Condens. Matter 11 4925

(http://iopscience.iop.org/0953-8984/11/25/311)

Annealing behaviours of defects in electron-irradiated diamond probed by positron annihilation

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Received 19 February 1999, in final form 6 April 1999

Abstract. Annealing behaviours of defects in electron-irradiated diamond were studied using the positron annihilation technique. For a type IIa specimen after 3 MeV electron irradiation with a dose of 1×10^{18} cm^{-2}, the major species of vacancy-type defects was determined to be neutral monovacancies, V^0. The trapping rate of positrons by V^0 decreased above 600 °C annealing, but the annihilation mode of positrons trapped by vacancy-type defects was observed even after 900 °C annealing. For a type Ib specimen after the irradiation, the major species of vacancy-type defects was determined to be negative monovacancies, and the formation of nitrogen–monovacancy pairs, N–V, was observed after 650 °C annealing. The annihilation probability between positrons and electrons with a broad momentum distribution was found to be increased by the trapping of positrons by N–V.

1. Introduction

Diamond has been investigated for use in solid state devices for high power and high frequency applications that can operate in a radiation environment or at high temperature [1]. For high heat-load optical components used in synchrotron radiation system or the free electron laser, a diamond single crystal was reported to be superior to other monochromator materials [2, 3]. To develop reproducible doping techniques of electrically active impurities, knowledge of electric and annealing properties of point defects is crucial. Since radiation damage introduces colour centres [4], the study of defects in diamond is also important. The positron annihilation technique is regarded as a powerful means of studying defects in metals and semiconductors [5]. Using this technique, native defects and irradiation-induced defects in natural and synthesized diamond have been studied [6–11]. The results of these studies show that the positron annihilation technique can be a useful tool for studying point defects in diamond and diamond-like carbon. From measurements of optical absorption, luminescence and electron spin resonance (ESR), a great number of studies for point defects in diamond has been carried out [4, 12]. However, the relation between defects detected by the positron annihilation and their optical properties or defects detected by ESR is not fully established. Since positrons are a sensitive probe for vacancy-type defects, the results obtained by the positron annihilation technique could be used to identify optical centres or ESR active defects. In the present

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0953-8984/99/254925+10$19.50

work, we report a study of annealing properties of defects introduced by electron irradiation in synthesized diamond.

In condensed matter, a positron annihilates with an electron mainly into two γ rays. The annihilation line is broadened due to the momentum component of the electron, P_L, parallel to the direction of the annihilation line. The energy of the γ rays is given by the relation: $E_\gamma = 511 \pm \Delta E$ keV. The Doppler shift, ΔE, is obtained by the relation: $\Delta E = P_L c/2$, where c is the speed of light. When a positron is trapped by vacancy-type defects, the annihilation probability of positrons with core electrons decreases and hence that of positrons with valence electrons increases. Because the momentum distribution of core electrons is broader than that of valence electrons, the Doppler broadening spectrum is narrowed by the trapping of positrons by vacancy-type defects. The energy distribution of γ rays corresponding to the annihilation of positrons with valence electrons is also affected by the trapping of positrons by defects [13]. The change in the Doppler broadening spectrum is characterized by the S parameter or the W parameter; S and W mainly characterize the fraction of the annihilation of positron-electron pairs with the low and the high momentum distributions, respectively [14]. When positrons are trapped by vacancy-type defects, both the decrease in the fraction of positrons annihilating with core electrons and the change in the momentum distribution corresponding to the annihilation of positrons with valence electrons increase S (or decrease W). The lifetime of positrons trapped by vacancy-type defects increases because of a reduced electron density in such defects. Measurements of the lifetime spectra of positrons provide useful information for the identification of vacancy-type defects [15].

2. Experiment

The synthesized single crystals of diamond (type Ib and IIa) used in the present experiments were grown at Sumitomo Electric Industries. The classification system of diamond is based on macroscopic properties of diamonds; the origin of such properties is mainly nitrogen and boron impurities [4]. In type Ib diamond, nitrogen is present on isolated substitutional sites, and almost all commercial synthesized diamonds are type Ib, containing around 100 ppm of nitrogen. Nitrogen is also the major impurity in type IIa diamond, but, generally, its concentration is lower than the detection limit of infrared absorption. By the double-crystal x-ray diffraction method, the crystallographic quality of the specimens was found to be close to that of commercial Si single crystals [16]. The concentration of nitrogen atoms in the type Ib specimens was estimated to be 50–120 ppm. The specimens were irradiated with 3 MeV electrons up to a dose of 1×10^{18} cm^{-2}. During the irradiation, the temperature of the specimens was kept below 90 °C. After electron irradiation, furnace annealing was performed in the temperature range between 100 and 900 °C for 30 min in a vacuum of 1×10^{-3} Pa.

Doppler broadening spectra of the annihilation radiation and lifetime spectra of positrons were measured as a function of isochronal annealing temperature. Doppler broadening spectra were measured using the coincidence technique of two 511 keV γ rays [17]; an NaI scintillation detector was placed in collinear geometry with a Ge detector. With this setup, the peak-to-background ratio was obtained to be 2×10^4. At each annealing temperature, the spectrum contained 8×10^6 counts. The observed spectra were characterized by the S parameter (the central region of the spectrum was defined to be 511 ± 0.8 keV) and the W parameter (the wing region of the spectrum was defined to be from 511 ± 3.0 to 511 ± 6.1 keV).

Lifetime spectra were measured by a fast–fast system with BaF_2 scintillators attached to XP2020Q photomultiplier tubes. The full width at half maximum (FWHM) of the time resolution was about 230 ps. At each annealing temperature, the spectrum contained

8×10^6 counts. The lifetime spectrum of positrons, $I(t)$, is expressed by

$$I(t) = \sum \lambda_i I_i \exp(-\lambda_i t) \quad (1)$$

where λ_i and I_i are the annihilation rate of positrons of the ith component and its intensity, respectively. The ith lifetime of positrons, τ_i, is given by $1/\lambda_i$. In the present experiments, the observed lifetime spectra were analysed using the computer program RESOLUTION [18].

3. Results and discussion

3.1. Irradiation-induced defects in the type IIa specimen

Figure 1 shows the S parameter and the mean lifetime of positrons, τ_M, for the electron-irradiated type Ib and IIa specimens as a function of annealing temperature. The lifetime spectra of positrons for the type Ib specimen were analysed assuming one annihilation mode. For the type IIa specimen, the spectra were decomposed into two components, and τ_M was calculated by the relation $\tau_M = \tau_1 I_1 + \tau_2 I_2$. Uedono *et al* [19] reported the annihilation characteristics of positrons in the type Ib and IIa specimens before electron irradiation. Thus, before the discussion about irradiation-induced defects, their results are summarized as follows.

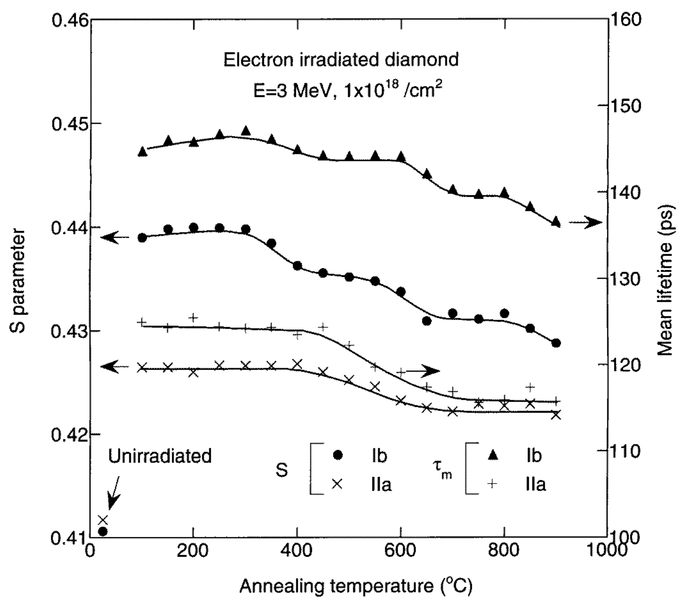

Figure 1. The S parameter and the mean lifetime of positrons for the electron-irradiated type Ib and IIa specimens as a function of annealing temperature. The values of S for the unirradiated specimens are also shown. The lifetimes of positrons before the irradiation are 106 and 98.7 ps for the type Ib and IIa specimens, respectively [19]. The lifetime spectra of positrons for the type Ib specimen were analyzed assuming one annihilation mode, and the spectra for the type IIa specimen were decomposed into two components. The solid lines are intended to serve as a guide to the eye.

For the specimens before electron irradiation, Doppler broadening spectra and the lifetime spectra were measured in the temperature range between 20 and 290 K. It was found that the lifetime of positrons was almost constant in the measured temperature range, and the average lifetimes were obtained to be 106 and 98.7 ps for the type Ib and IIa specimens, respectively. The obtained lifetime of positrons for the type IIa specimen is close to the calculated lifetime of positrons annihilated from the free state, τ_f, in diamond (93–96 ps) [20]. Thus, it was concluded that almost all positrons in the type IIa specimen annihilate from the free state. For the type Ib specimen, the observed increase in the lifetime of positrons is attributable to the trapping of positrons by vacancy-type defects. In general, such an annihilation mode increases the value of S, but for the type Ib specimen S is smaller than for the type IIa specimen. From several experiments performed by Uedono and co-workers [21–23], for Si, it was found that the characteristic value of S for vacancy–oxygen or vacancy–fluorine complexes is smaller than that for the positron annihilation from the free state. Since the major impurity is nitrogen for the type Ib specimen, the observed decrease of S is attributable to the annihilation of positrons with electrons of nitrogen atoms. Because the lifetime of positrons for the type Ib specimen is longer than τ_f, a candidate for the defects detected by the positron annihilation is open spaces adjacent to nitrogen atoms, such as nitrogen–vacancy complexes. It is known that the C–N bond on which the unpaired electron is situated is about 10–14% longer than the usual C–N bond length [12]. Thus, Uedono *et al* [19] also discussed the effects of the annihilation of positrons trapped by open spaces introduced by substitutional nitrogen atoms on the positron annihilation parameters.

In figure 1, for each specimen, the overall annealing behaviour of S agrees with that of τ_M. For the type IIa specimen, S and τ_M start to decrease above 500 °C annealing, but the decrease of these parameters seems to saturate above 700 °C annealing. The annealing behaviour of these positron annihilation parameters can be attributed to the annealing of the irradiation-induced defects. By using the two state trapping model of positrons [14], the trapping rate of the defects, κ, is given by

$$\kappa = (I_2/I_1)(\lambda_f - \lambda_2) \tag{2}$$

where $\lambda_f = 1/\tau_f$. κ is related to the concentration of defects, C_d, by

$$\kappa = \mu_d C_d = v_+ \sigma C_d \tag{3}$$

where μ_d is the specific positron trapping rate of the defect, v_+ is the thermal velocity of positrons and σ is the trapping cross section. Figure 2 shows τ_2 and κ calculated from equation (2) for the type IIa specimen as a function of annealing temperature. The lifetime of positrons annihilated from the free state, $\tau_{f(cal)}$, can be calculated by the relation $1/\tau_{f(cal)} = I_1/\tau_1 + I_2/\tau_2$. For the type IIa specimen, $\tau_{f(cal)}$ was calculated to be 108–117 ps. The derived value of $\tau_{f(cal)}$ is longer than the lifetime of positrons obtained for the type IIa specimen (98.7 ps) before electron irradiation, but, considering the uncertainty in the calculation of $\tau_{f(cal)}$, the difference between τ_f and $\tau_{f(cal)}$ is acceptable. For example, the uncertainty of $\tau_{f(cal)}$ could be caused by an incorporation of two or more annihilation modes into the first annihilation mode, and/or that of the time resolution of the system into the annihilation mode with the short lifetime.

In figure 2, before the annealing treatment, τ_2 is obtained to be 143 ps. Since this value is close to the lifetime of positrons trapped by monovacancies, V (146 ps, [15]), the second annihilation mode can be attributed to the annihilation of positrons trapped by V. One can estimate the charge state of defects from the temperature dependence of the trapping rate of the defects. The model which describes the trapping of positrons by charged vacancies in semiconductors was developed by Puska *et al* [24]. According to this model, μ_d for neutral vacancies is almost independent of temperature, but μ_d for negatively charged vacancies is larger than that for neutral ones, and the difference is enhanced at low temperature. The Doppler broadening spectra and the lifetime spectra for the type IIa specimen before the annealing treatment were measured in the temperature range between 20 and 290 K [19]. In these measurements, no increase of S or I_2 corresponding to negatively charged defects was observed at low temperature. This suggests that the defects detected by the second component

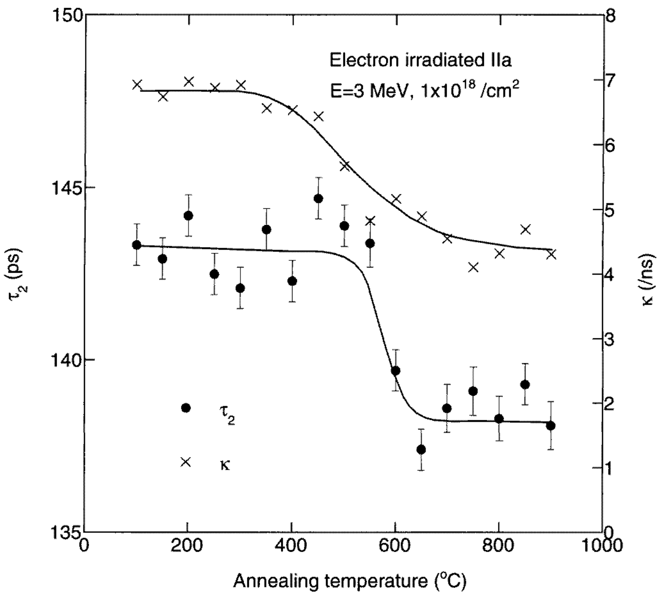

Figure 2. The second lifetime of positions, τ_2, and the trapping rate of positrons by the defects, κ, for the electron-irradiated type IIa specimen as a function of annealing temperature. For the as-irradiated specimen, the major species of vacancy-type defects was identified as V^0. The solid lines are intended to serve as a guide to the eye.

are neutral. Thus, the major species of the defects detected by the second annihilation mode can be identified as neutral monovacancy, V^0, and the change in the value of κ shown in figure 2 can be related to the annealing behaviour of V^0.

The irradiation-induced defects in diamond have been studied by optical measurements. The optical absorption band, GR1, has been associated with V^0 [4]. Clark *et al* [25] reported that the intensity of the GR1 band decreased in three annealing stages (275–350, 400–575 and 625–800 °C). From measurements of ESR spectra [12, 26], it was reported that self-interstitials, I, are mobile below 80 K, and trapped by impurities during irradiation. The annealing stages of the GR1 band, therefore, were reasonably attributed to not only the migration of V^0 into sinks but also the recombination between V^0 and I [12, 25, 26]; free interstitials are introduced by the dissociation of I–impurity complexes.

In figure 2, κ decreases with increasing annealing temperature, but it saturates above 700 °C annealing. This annealing behaviour is different from that of the GR1 band. As shown in figure 2, the decrease of τ_2 was observed above 600 °C annealing. The decrease in the lifetime of positrons trapped by vacancy-type defects suggests an increase in the density of electrons in such defects. The change in the electron density could be due to the change in the configuration of atoms near the defects. Thus, the observed decrease of κ cannot be simply attributed to the migration of V^0 or the recombination between V^0 and I. The presence of the defects at high annealing temperature (>800 °C) might be due to the formation of complexes between V^0 and impurities. The concentration of V^0 can be estimated from equation (3), but, at this stage, μ_d for V^0 is not known. For Si, μ_d for neutral divacancies was estimated to be 1×10^{15} s^{-1} [27, 28]. Thus, using $\mu_d = 5 \times 10^{14}$ s^{-1}, C_d was estimated to be 8×10^{-6} for the specimen after 900 °C annealing. Since the impurity concentration in the type IIa specimen is expected to be several ppm, the formation of V–impurity complexes is not negligible. The major impurity of diamond is known to be nitrogen. From the comparison between the results obtained for the type IIa and Ib specimens, however, it can be concluded that the formation of nitrogen–monovacancy complexes, N–V, is not an origin of the defects observed above 800 °C annealing. We shall return to a discussion of this point in the next section.

The decrease of τ_2 observed above 600 °C annealing could be due to the relaxation of atoms surrounding V^0. The GR1 band is a zero-phonon line corresponding to the electric transition of V^0, and its levels are regarded as an E ground state (with an A_1 just above (0.008 eV)) and a T_2 at 1.673 eV; the Mulliken system is used to show the spectroscopic levels [4]. The local softening of V^0 could change the ground and the excited states of such defects, and could decrease the intensity of the GR1 band. Thus, the relaxed V^0 is a candidate for the defects observed above 800 °C annealing. From the annealing behaviour of κ shown in figure 2, assuming that σ of the defects observed above 800 °C annealing is close to that of V^0, about 60% V^0 introduced by electron irradiation is converted into the relaxed monovacancy-type defects above 800 °C annealing.

3.2. Irradiation-induced defects in the type Ib specimen

In figure 1, for the electron-irradiated type Ib specimen before the annealing treatment, the lifetime of positrons was obtained to be 145 ps. Since this value is close to τ_2 obtained for the electron-irradiated type IIa specimen, almost all positrons are considered to annihilate from the trapped state by V in the type Ib specimen. For this specimen, S and the lifetime of positrons are larger than those for the type IIa specimen. This means that, for the type Ib specimen, the fraction of positrons trapped by defects, F_d, $(= \mu_d C_d/(\lambda_f + \mu_d C_d))$ is higher than that for the type IIa specimen. In the present experiments, since the temperature of the specimen during electron irradiation is lower than the migration temperature of V, the concentration of V for the type Ib specimen is the same as that for the type IIa specimen. For type Ib diamond, the ND1 band is known to be produced by electron irradiation [4]. This band is interpreted as arising from negatively charged monovacancies, V^-. While the GR1 band is a dominant signal for relatively pure diamond (type IIa), an intense signal of the ND1 band is observed when a sufficient concentration of nitrogen is present in the specimen (type Ia and Ib). The role of nitrogen atoms is to convert the monovacancies from V^0 to V^- by charge transfer from nitrogen 'donors'. Thus, in the present experiments, for the type Ib specimen, the observed high value of F_d can be attributed to the attractive long range Coulomb potential of V^- and the resultant increase of μ_d.

For electron-irradiated type Ib diamond, it is known that the intensity of the ND1 band decreases above 630 °C annealing, and the centre corresponding to N–V (1.945 eV) starts to be observed after such a annealing treatment [4, 29, 30]. After 800 °C annealing, the major monovacancy-type defect was reported to be N–V [30]. Thus, in this section, first, the effect of nitrogen atoms coupled with V on the positron annihilation parameters is discussed, then overall annealing behaviours of the positron annihilation parameters are reconsidered. For the positron annihilation in vacancy–impurity complexes, since the effect of impurities coupled with vacancies on the Doppler broadening spectrum tends to appear in the high momentum region [23, 31], the W parameter is sensitive to such defects. Figure 3 shows the W parameter for the electron-irradiated type Ib and IIa specimens as a function of annealing temperature. In this figure, the vertical axis was inverted, thus one can easily compare the annealing behaviour of W with that of S. For the type Ib specimen, below 600 °C annealing the annealing behaviour of W seems to be close to that of S, but above 650 °C annealing W started to increase rapidly. Since the onset temperature of the increase in W agrees with that of the formation of N–V, the observed decrease of W can be attributed to the increase in the fraction of positrons trapped by N–V.

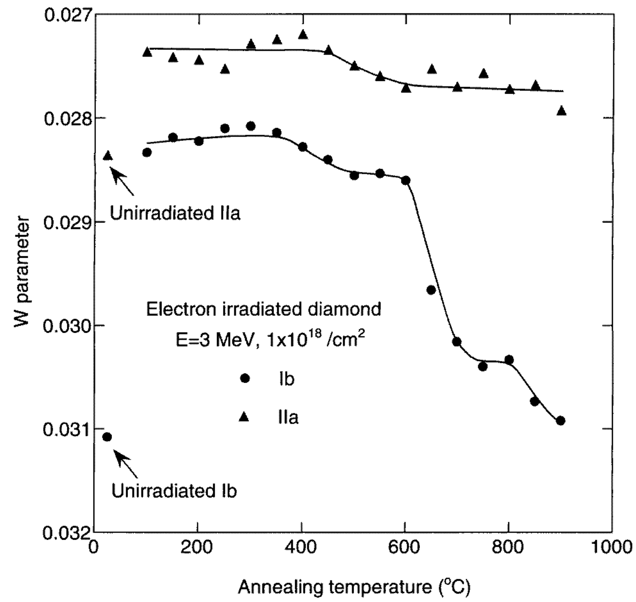

Figure 3. The W parameter for the electron-irradiated type Ib and IIa specimens as a function of annealing temperature. The values of W for the unirradiated specimens are also shown. The vertical axis was inverted in order to compare the annealing behaviour of W with that of S (figure 1). The solid lines are intended to serve as a guide to the eye.

For more detailed interpretation of the change in the Doppler broadening spectra, the difference between the spectra for the specimen before and after electron irradiation was calculated. The spectrum for the unirradiated specimen is shown in figure 4; the horizontal axis shows ΔE. The differences between the spectra are shown in the same figure; the spectrum for the unirradiated specimen was subtracted from the spectra for the electron irradiated specimen after 100, 600 and 900 °C annealing. In figure 4, it can be seen that the Doppler broadening spectrum mainly consists of the narrow and the broad components. The broad component clearly observed at $\Delta E > 4$ keV corresponds to the annihilation of positrons with core electrons [17]. The narrow component observed at $\Delta E < 4$ keV corresponds to the annihilation of positrons with valence electrons. For the electron-irradiated specimen, the positive values at $\Delta E < 1$ keV are attributed to the lowering of the crystal symmetry due to the trapping of positrons by vacancy-type defects [13]. Figure 5 is an expanded view of the subtracted spectra shown in figure 4. In figure 5, for the specimen after 100 and 600 °C annealing, the negative values at 4 keV$< \Delta E < 8$ keV are attributed to the decrease in the annihilation probability of positrons with core electrons by the trapping of positrons by vacancy-type defects.

For the specimen after 900 °C annealing, at $\Delta E = 2$–4 keV, the subtracted counts are larger than those for the specimen after 100 and 600 °C annealing (figure 5), and they are positive at $\Delta E = 3.5$–4.0 keV. The observed subtracted spectrum cannot be explained by the trapping of positrons by 'pure' vacancy-type defects. As mentioned above, since the major vacancy-type defects are N–V after 800 °C annealing, it can be concluded that the observed increase in the annihilation probability between positrons and electrons with the broad momentum distribution is due to the annihilation of positrons trapped by N–V.

From the above discussion, for the specimen above 650 °C annealing, the observed decrease of S cannot be attributed only to the decrease in the concentration of defects by the

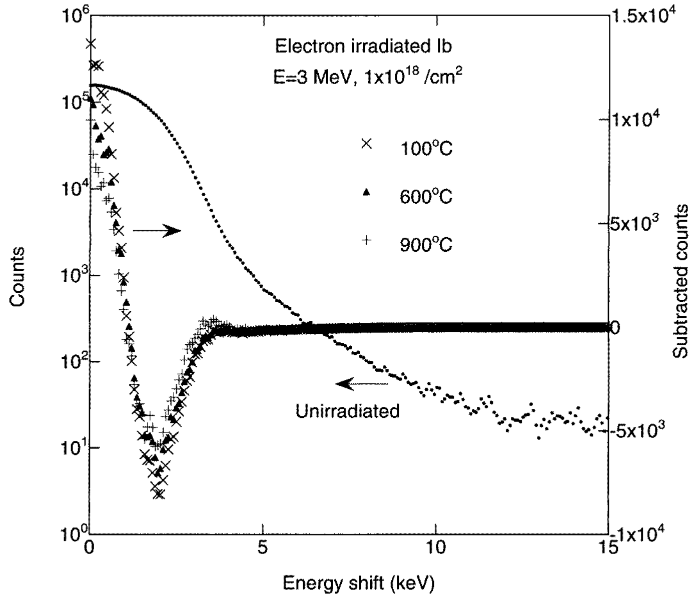

Figure 4. The Doppler broadening spectrum for the unirradiated type Ib specimen. The differences between the spectra for the unirradiated specimen and the irradiated specimen after 100, 600 and 900 °C annealing are also shown; the spectrum for the unirradiated specimen was subtracted from the spectrum for the irradiated specimen.

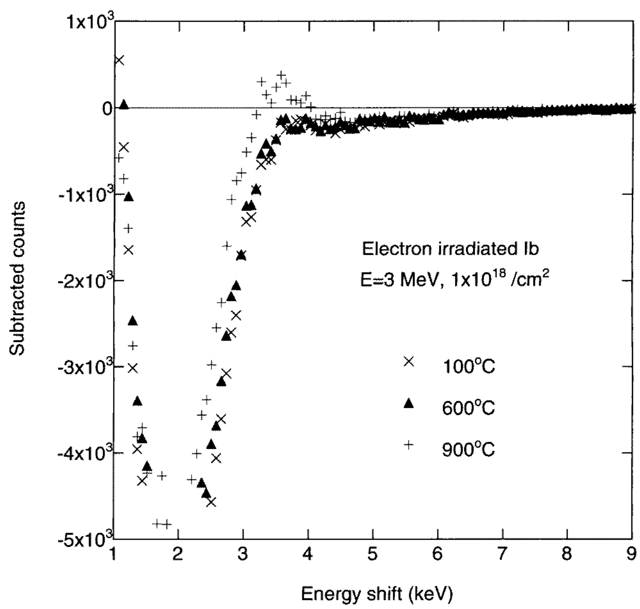

Figure 5. An expanded view of the subtracted spectra shown in figure 4.

annealing treatment (figure 1). For the specimen after 900 °C annealing, the lifetime spectrum of positrons cannot be analysed by two-component analysis, but it was well analysed by assuming one annihilation mode, and the derived lifetime (136 ps) is longer than τ_f. These facts suggest that almost all positrons annihilate from the trapped state even after 900 °C annealing. Thus, the difference ($\Delta\tau = 9$ ps) between the lifetimes for the as-irradiated specimen and the specimen after 900 °C annealing can be associated with the increase in the density of electrons due to the coupling of nitrogen atoms with V. From the comparison between the results for the type Ib and IIa specimens, the observed high trapping fraction of positrons by N–V is likely to be due to the negative charge state of N–V. Since the measurements of ESR and the hole-burning effect of N–V suggest that the ground state of N–V is a spin triplet [29, 32, 33], the number of electrons at N–V is considered to be even. Loubser and van Wyk [12], therefore, suggested that N–V captures an extra electron to form a six-electron centre. According to this model, N–V would consequently acquire a negative charge. However, from quantum-beat spectroscopy and *ab initio* calculation, Lenef and coworkers [34, 35] reported that the properties of N–V can be explained assuming that N–V is neutral. In the present experiments, if the charge state of N–V is neutral, the trapping fraction of positrons by vacancy-type defects for the type Ib specimen should be close to that for the type IIa specimen, but that is not the case. Thus, assuming that the charge state of N–V is neutral, in order to explain the observed high trapping rate of positrons into N–V, one needs other trapping processes of positrons.

From the above discussion, the effect of nitrogen atoms coupled with V on the positron annihilation parameters is now clear. For the type IIa specimen, since the overall annealing behaviour of W is close to that of S (figures 1 and 3), the effect of nitrogen atoms on the annealing behaviour of V^0 is likely to be negligible. The effect of other impurities such as Ni on the positron annihilation parameters is not established, but, if such impurities couple with V, the corresponding change in the electric structure is considered to appear in the annealing behaviours of S or W. Thus, the annealing behaviour of defects for the type IIa specimen is likely to be discussed neglecting the formation of impurity–V complexes.

In figure 3, after electron irradiation, W for the type Ib specimen is larger than that for the type IIa specimen. This means that, for the type Ib specimen, the nitrogen-related defects are already formed just after electron irradiation, and the annihilation mode of positrons trapped by such defects is incorporated into the derived positron annihilation parameters. In the temperature range between 100 and 600 °C, the annealing behaviour of W is close to that of S; W (or S) starts to increase (or decrease) above 400 °C annealing, and seems to saturate at 500–600 °C annealing (figures 1 and 3). Although the onset temperature of the change in the positron annihilation parameters for the type Ib specimen is about 100 °C lower than that for the type IIa specimen, the relaxation of V, which is observed for the type IIa specimen, is considered to occur in the type Ib specimen after 400–500 °C annealing.

4. Conclusions

We have presented a study of annealing behaviours of vacancy-type defects in electron-irradiated type Ib and IIa diamond. The Doppler broadening spectra of the annihilation radiation and the lifetime spectra of positrons were measured as a function of annealing temperature (100–900 °C). For the type IIa specimen, the species of the major vacancy-type defects detected by the positron annihilation was determined to be V^0. κ and τ_2 started to decrease above 500 °C annealing, but the trapping of positrons by vacancy-type defects was observed even after 900 °C annealing. Since the defects (V^0) corresponding to the GR1 band are known to be almost annealed out below 800 °C annealing, the relaxed V^0 is a candidate for the defects observed above 800 °C annealing.

For the type Ib specimen, the effect of nitrogen atoms coupled with V was clearly observed by the W parameter. From the detailed analysis of the Doppler broadening spectra, the increase in the annihilation probability between positrons and electrons with a broad momentum distribution ($\Delta E = 3.5$–4.0 keV) was observed for the specimen after 900 °C annealing. This fact was attributed to the trapping of positrons by N–V. The lifetime of positrons trapped by N–V was shorter than that of positrons trapped by V. This suggests that the electron density in N–V is higher than that in V. The annealing behaviours of the positron annihilation parameters were well explained assuming that the charge state of N–V is negative.

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