Jpn. J. Appl. Phys. Vol. 36 (1997) pp. 605–611
Part 1, No. 2, February 1997

# Anomalous Temperature Dependence of Positron Trapping due to Divacancies in Si

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(Received October 2, 1996; accepted for publication November 18, 1996)

The temperature dependence of positron lifetime and trapping rate due to electrically neutral divacancies in Si has been determined for temperatures from 5.5 K to 210 K. The charge state of divacancies was verified through the Hall effect, electron spin resonance and infrared absorption measurements. The positron lifetime at neutral divacancies was 280 ps at low temperatures and increased to 295 ps at around 30 K. This is explained in terms of the lattice relaxation effect accompanying the positron trapping. The positron trapping rate due to neutral divacancies was found to increase upon cooling, to decrease after reaching a maximum at around 30 K and to increase again below 10 K. The observed temperature dependences of the trapping rate could not be explained by existing models. The temperature dependence was found to be reproduced by the Breit-Wigner formula for resonance phenomena. Possible reasons were discussed.

KEYWORDS: positron trapping, positron lifetime, divacancies, Si, temperature dependence

## 1. Introduction

Positron annihilation spectroscopy (PAS) is a powerful method to study vacancy defects in crystalline solids. This method has been extensively applied to the study of defect in semiconductors in the last ten years.[1–3] Several important features have been reported so far on the subject of defects induced by irradiation, deformation and heat treatment. Recently, first-principles calculations have been used to determine the detailed positronic, electronic and atomic states at defects and provide information for defect identification.[4]

Positrons implanted from a radioactive source such as sodium-22 into target materials are thought to slow down to thermal energy within ~10 ps.[5] Positrons in solids diffuse to annihilate with electrons in the bulk or to be trapped by vacancy defects. Positron lifetime is proportional to the square of an overlap integral between positron and electron wavefunctions.[6] Hence, positron lifetime at vacancies has a tendency to increase with the open volume size of vacancies due to the reduction of electron density. Theoretical calculations indicate that positron lifetime is sensitive even to small (several %) lattice relaxation around vacancies.[7–10] This feature provides a reasonable explanation for the temperature-dependent positron lifetime due to vacancies in GaAs. Positron trapping rate into defects is proportional to the defect concentration and specific trapping rate. The specific trapping rate is the trapping rate per defect. Positron trapping by a defect occurs *via* two successive processes; diffusion to the defect and transition into the bound state. Positron trapping due to small vacancies such as monovacancies and divacancies is usually limited to transition since positrons approach them immediately.[11] The vacancy-positron binding energy is usually on the order of 1 eV.[12,13] The transition rate of a free positron into the bound state in a vacancy is enhanced when the wavefunction of the positron sufficiently overlaps the trapping potential and the binding energy is effectively dissipated through elemental excitations. In the case of metal vacancies, the binding energy is thought to be dissipated through electron-hole excitations.[14] The magnitude and temperature dependence of the positron trapping rate calculated using the second-order perturbation theory (Fermi's golden rule) agree with experimental results.[14]

Positron trapping characteristics in semiconductors may be different from those in metals due to (i) the variety of defect charge states depending on the Fermi level, (ii) the low free electron density and (iii) the existence of the band gap which is of an order comparable to that of positron-vacancy binding energy. The dissipation of binding energy through electron-hole excitations may be difficult when the binding energy is lower than the band gap energy. Hence, the phonon emission process and localized electron excitation should be taken into account. A long-range Coulomb interaction may occur between the positrons and charged defects due to the absence of screening by free electrons. Consequently, the specific trapping rates for vacancies depend on the charge state of vacancies. The positron trapping rate for negatively charged vacancies in Si is known to increase upon cooling and to saturate at low temperatures (negative temperature dependence).[15–18] It is expected that shallow levels are formed as a consequence of the Coulomb attraction from an analogy with shallow acceptors and donors.[19] These shallow levels may provide precursor states for the transition of positrons into deep bound states. In previous studies,[17,18] the phonon cascade mechanism was proposed to interpret the negative temperature dependence of the trapping rate for divacancies: positrons drop down to a deeper state as a result of successive transition between shallow levels accompanied by phonon emission. Puska *et al.* investigated the validity of the phonon cascade mechanism using a theoretical calculation based on the second-order perturbation theory.[19] Their results show that the transition rate between shallow levels associated with phonon emission is lower than the positron annihilation rate in the bulk while the transition rate from one of the shallow states to the deep ground state is higher than the annihilation rate in the bulk. The above results suggest that positron trapping occurs *via* two steps and not *via* phonon cascade; positrons are first trapped by one of the shallow

levels and then drop down to the deep ground state. The negative temperature dependence of the trapping rate is well explained considering the thermal detrapping from shallow levels to the free state in the two-step trapping kinetics.[19,20] Thus, the negative temperature dependence of the trapping rate for negatively charged vacancies may be dominated by the shallow levels but not by the transition to the deep ground state.

Neutral vacancies are thought to be simple deep traps for positrons due to the absence of the Coulomb potential. Thus, the trapping characteristics for neutral vacancies seem to be different from those for negative vacancies. In many previous works, it is tacitly assumed that the trapping rate due to neutral vacancies was independent of temperature.[21–23] Puska's theory shows that such an assumption may be justified when the binding energy is dissipated through electron excitations. However, no experimental evidence for a temperature-independent trapping rate for neutral vacancies has been obtained to date. In fact, neutral vacancies have been reported to show apparent temperature dependences.[24,25] Recently, first-principles calculations show that lattice relaxation is induced accompanied by positron trapping into vacancies.[9,10] This implies a strong interaction between positrons and vacancies. Positron diffusion experiments revealed that the positron effective mass in Si is $1.2m_0$, where $m_0$ is the static electron mass.[26,27] The increased effective mass also indicates the strong coupling between positrons and lattice vibration. It is therefore expected that the multiphonon emission process may be one of the channels for positron trapping by neutral vacancies.

Thus, it is important to investigate the temperature dependence of the positron trapping rate due to neutral vacancies. In this work, we carried out positron lifetime measurement for neutral divacancies in Si induced by electron irradiation. It is known that one donor level at $E_V + 0.27\,\mathrm{eV}$ and two acceptor levels at $E_C - 0.41\,\mathrm{eV}$ and $E_C - 0.23\,\mathrm{eV}$, where $E_V$ and $E_C$ denote the energy of the top of the valence band and the bottom of the conduction band, respectively, are associated with divacancies in Si.[28,29] Hence the charge state of the divacancies is controlled to be neutral by adjusting the Fermi level within the lower half of the band gap. In our previous work, we found a temperature-dependent trapping rate due to neutral divacancies induced by 15 MeV electron irradiation from 15 K to 300 K.[16] However, the measurement was a little bit rough and hence we could not find critical differences between neutral and negatively charged divacancies. In this work, we accurately determined the temperature dependence of the positron trapping rate due to neutral divacancies from 5.5 K to 210 K. We performed the Hall effect measurement to determine the Fermi level. It is known that the 3.3 $\mu$m (0.38 eV) infrared (IR) absorption band arises from an internal transition of single-negative divacancies. This absorption band is not observed when divacancies are neutral but observed after optical ionization by white light.[30–32] It is also known that electron spin resonance (ESR) spectra, designated Si:G6 and Si:G7, which can be distinguished by their $g$-values arises from single-positive and single-negative divacancies, respectively.[28] To verify the presence of divacancies and their charge state, we also employed ESR and IR measurements. Consequently, we found a unique temperature dependence of the trapping rate due to neutral divacancies at low temperatures which could not be explained by conventional models.

## 2. Experimental

Specimens used in this work were floating-zone grown Si crystals doped with boron ($4\times10^{14}\,\mathrm{cm^{-3}}$). The specimens were irradiated with 3 MeV electrons at a fluence of $7\times10^{17}\,\mathrm{e^-/cm^2}$ at around 60°C using a dynamitron accelerator in the Japan Atomic Energy Research Institute. The Fermi level of the specimens after the irradiation was determined to be $E_V + 0.40\,\mathrm{eV}$ at room temperature using the Hall effect measurement. The Hall effect measurement at low temperatures was very difficult to perform due to the reduction of free carrier density. This suggests that the Fermi level is pinned at almost the same point. Isochronal annealing was performed in the temperature range between 250 and 450°C for 20 min in a dry argon ambience.

The positron source was prepared by depositing $^{22}$NaCl ($\sim6\times10^5$ Bq) onto a titanium thin film with a thickness of 3 $\mu$m. The positron source was sandwiched by two specimens and positron lifetime measurement was carried out using a conventional spectrometer with a time resolution of about 200 ps from 5.5 K to 210 K. About $2\times10^6$ counts were accumulated in each spectrum. The source components were determined to be 130 ps and 520 ps with intensities of 9% and 0.5%, respectively, from the measurement for the unirradiated specimen. These source components seem to come from the positron annihilation in the titanium film and in the sodium itself. After subtracting the source and background components, a lifetime spectrum $L(t)$ was decomposed into two lifetime components using a computer program named PATFIT-88:[33]

$$L(t) = (I_1/\tau_1)\exp(-t/\tau_1) + (I_2/\tau_2)\exp(-t/\tau_2). \quad (1)$$

Here, $\tau_i$ are the lifetimes and $I_i$ are the intensities ($I_1 + I_2 = 1$). In the framework of the two-state trapping model in which positrons are assumed to annihilate in the bulk state or the trapped state at vacancy defects, the lifetimes $\tau_1$ and $\tau_2$ have the following values:[34]

$$\tau_1 = \frac{1}{\tau_B^{-1} + \kappa}, \quad (2)$$

$$\tau_2 = \tau_V. \quad (3)$$

Here, $\tau_B$ is the positron lifetime at the bulk which is determined to be $222\pm2$ ps from a measurement for unirradiated specimens, $\tau_V$ is the positron lifetime at vacancy-type defects and $\kappa$ is the net positron trapping rate due to the detects:

$$\kappa = \frac{I_2}{I_1}(\tau_B^{-1} - \tau_2^{-1}) \quad (4)$$

The validity of the analysis based on the two-state trapping model can be checked by the difference between $\tau_1$ determined by eq. (1) and that calculated by eq. (2). The

trapping rate is further expressed as $\kappa = \mu C = \sigma \nu_+ C$, where $\mu$ is the specific trapping rate, $\sigma$ is the trapping cross section, $\nu_+$ is the thermal velocity of positrons ($\sim 10^7 (T/300)^{1/2}$ cm/s) and $C$ is the defect concentration.

The presence of divacancies and their charge state were verified through IR and ESR measurements. The IR measurement was carried out at 7 K using a JEOL FT-IR JIR-100 spectrophotometer. To avoid the optical ionization of divacancies due to the light source, a band-pass filter which restricted the photon energy from 0.30 to 0.39 eV was installed in the spectrophotometer. The ESR measurement was carried out at 20 K with an X-band (9 GHz) microwave incident on a $TE_{100}$ cylindrical cavity using a JEOL JES-TE300 spectrometer. The magnetic field ($H$) was applied parallel to the $\langle 100 \rangle$ axis. The effect of white light illumination on IR and ESR spectra was examined.

## 3. Results and Discussion

First, in the following sub-section, we report the results of IR and ESR measurements to show the presence of divacancies and their charge state. We also correlate the annealing behavior of the IR and ESR signals with the positron trapping rate to identify the positron trapping center. Subsequently, we report the temperature dependence of positron lifetime and trapping rate in §3.2.

### 3.1 *Identification of positron trapping center*

As mentioned in §2, the Fermi level of the specimens was located at $E_V + 0.40$ eV at room temperature. Considering the fact that the donor level and first acceptor level of a divacancy are located at $E_V + 0.27$ eV and $E_C - 0.41$ eV, respectively, the charge states of divacancies are expected to be neutral. Figure 1 shows the IR spectra measured in the presence and absence of a white light illumination. The 3.3 $\mu$m absorption band is not found in the absence of white light illumination. The absorption band becomes visible in the presence of white light illumination. The above results show that divacancies are in a neutral state at thermal equilibrium and they are then optically ionized to a single-negative charge state. Figure 2 shows the ESR spectra measured in the presence and absence of white light illumination. Although no signals are found in the absence of the white light illumination, apparent signals appear when the specimen is illuminated by white light. This feature is quite similar to the photo-response observed in the IR measurement. From the $g$-values of the G6 and G7 spectra for $H /\!/ \langle 100 \rangle$,[28] a spectrum which consists of two split signals may appear at $H = 320.9$–$321.1$ mT and 319.5–320.0 mT, respectively, in the present experimental conditions. Thus, the observed signals should be assigned to the G7 spectrum. No spectra arises from the other defects were observed. Thus, it is again confirmed that neutral divacancies are the major defect species. The concentration of divacancies is estimated to be on the order of $10^{16}$ cm$^{-3}$ from the production rate.[35]

Figure 3 shows the positron lifetimes ($\tau_1$ and $\tau_2$) and intensity ($I_2$) obtained from the two-component analysis of lifetime spectra measured at 5.5 K as a function of annealing temperature. It is found that lifetime $\tau_1$ approximately agrees with that expected from the two-state trapping model. This confirms that lifetime $\tau_2$ is related to positron annihilation at vacancy-type defects. Figure 4 shows the positron trapping rate due to the defects as a function of annealing temperature, compared with the result for the IR absorption coefficient (peak at 0.34 eV) related to divacancies. These values are, normalized by the values before annealing. (The IR measurement was done in the presence of white light illumination to detect the 3.3 $\mu$m band.) The absorption coefficient decreases at around 350°C and reaches the detection limit at 400°C. This result is consistent with that obtained in a previous work.[28] The annealing behavior of the trapping rate seems to be similar to that of the IR absorption coefficient. This allows us to conclude that the second lifetime component observed after the

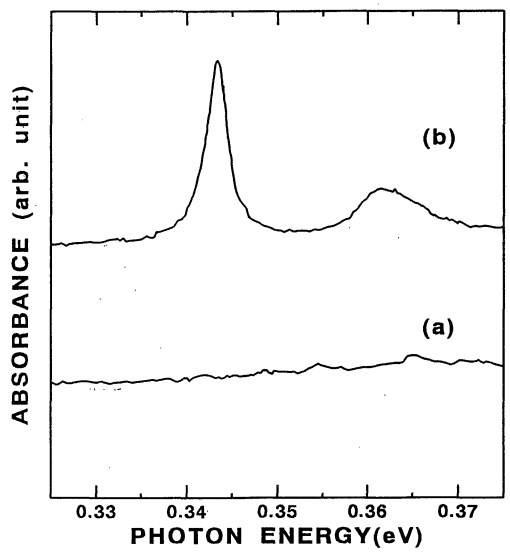


Fig. 1. Infrared absorption spectra for the specimen irradiated with 3 MeV electrons at a fluence of $7 \times 10^{17}$ e$^-$/cm$^2$ measured (a) in the absence and (b) in the presence of white light illumination at 6 K.

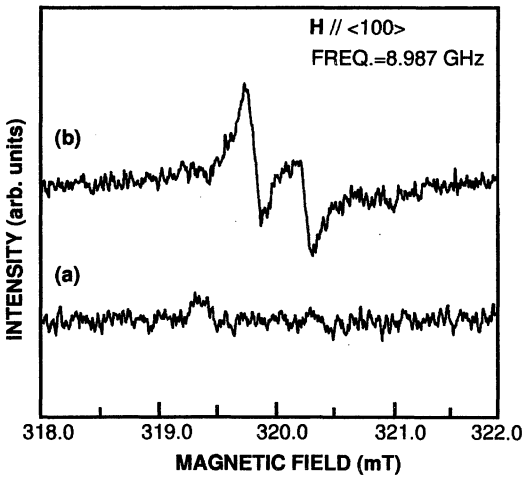


Fig. 2. Electron spin resonance spectra for the specimen irradiated with 3 MeV electrons at a fluence of $7 \times 10^{17}$ e$^-$/cm$^2$ measured (a) without and (b) with white light illumination at 20 K.

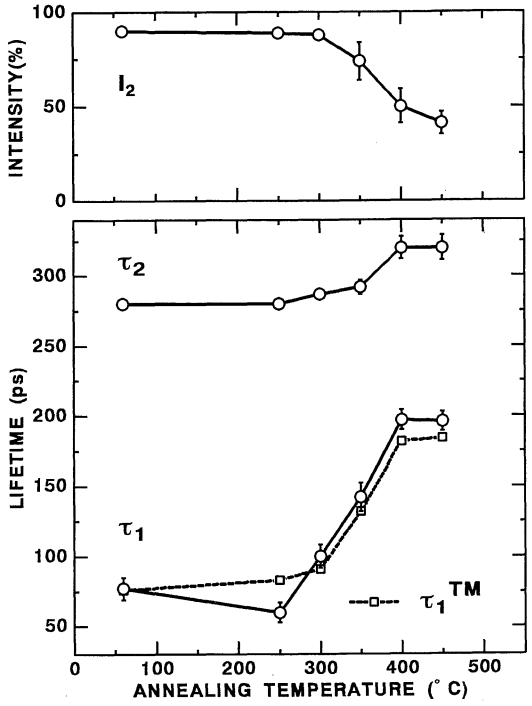


Fig. 3. Positron lifetimes ($\tau_1$ and $\tau_2$) and intensity ($I_2$) for the specimen irradiated with 3 MeV electrons at a fluence of $7 \times 10^{17}$ e$^-$/cm$^2$ at 5.5 K as a function of annealing temperature. Lifetime $\tau_1^{TM}$ denotes lifetime $\tau_1$ expected from the two-state trapping model (eq. (2)).

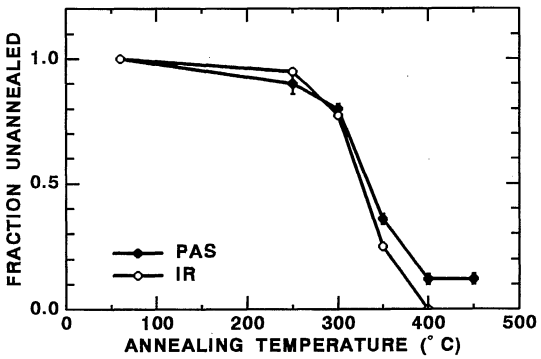


Fig. 4. Positron trapping rate which corresponds to the second lifetime component in Fig. 3 (filled circle) and infrared absorption coefficient at the 0.34 eV peak (open circle) determined from the measurement in the presence white light illumination as a function of annealing temperature. These values are normalized by the values before the annealing.

irradiation arises from divacancies. Lifetime $\tau_2$ is about 280 ps for the as-irradiated state at 5.5 K. This value is 10–15 ps less than that for neutral divacancies determined from 15–300 K in a previous study.[16] Considering the low measurement temperature range, this may be interpreted in terms of temperature-dependent lifetime as discussed in §3.2. Lifetime $\tau_2$ increases to 320 ps and the trapping rate slightly deviates from IR signal intensities after the annealing above 350°C. This indicates the formation of quadrivacancies with a disappearance of divacancies above 350°C. Lifetime $\tau_2$ = 320 ps is about 30 ps less than that for quadrivacancies at room temper-

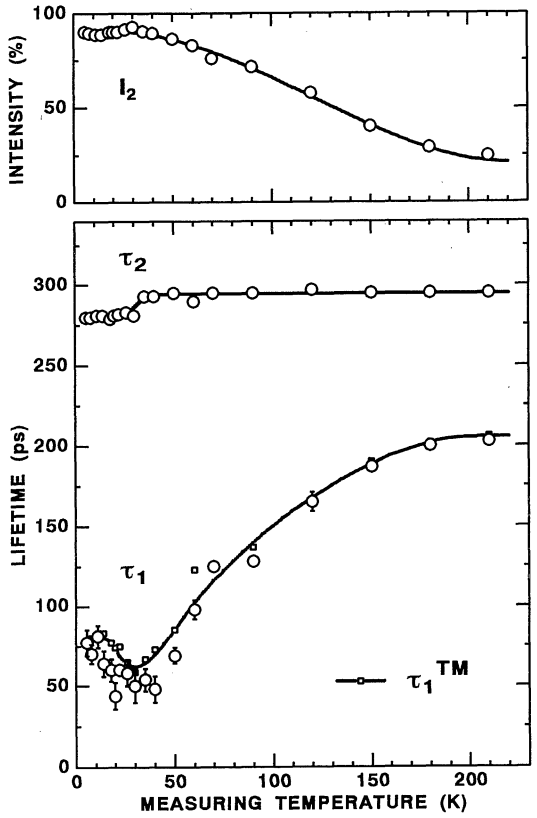


Fig. 5. Positron lifetimes ($\tau_1$ and $\tau_2$) and intensity ($I_2$) for the specimen irradiated with 3 MeV electrons at a fluence of $7 \times 10^{17}$ e$^-$/cm$^2$ as a function of measuring temperature. Lifetime $\tau_1^{TM}$ denotes the lifetime $\tau_1$ expected from two-state trapping model (eq. (2)).

ature determined in a previous study.[36] This may also be explained in terms of temperature-dependent lifetime.

From the above results, it is concluded that neutral divacancies are the major positron trapping centers in the irradiated specimen. Next, we discuss the temperature dependence of positron annihilation characteristics associated with divacancies.

### 3.2 *Temperature dependence of positron annihilation*

Figure 5 shows the positron lifetimes ($\tau_1$ and $\tau_2$) and intensity ($I_2$) for the as-irradiated specimen as a function of measuring temperature. It is found that the value and temperature dependence of the lifetime $\tau_1$ approximately agree with that expected from the trapping model. Lifetime $\tau_1$ is slightly (10–20 ps) lower than that expected from the trapping model at several points. This deviation is probably due to some uncertainties in the decomposition of lifetime spectra caused by the reduction of lifetime $\tau_1$. However, it does not indicate the existence of another defect species since lifetime $\tau_1$ does not exceed that expected from the trapping model. Thus, we concluded that the second lifetime component was related to positron annihilation at vacancies. As discussed in the preceding subsection, neutral divacancies are the major positron trapping centers in the specimen. The intensity $I_2$ increases with decreasing temperature suggesting that the positron trapping rate increases at low temperatures as shown later. Lifetime $\tau_2$ is about 280 ps at low temper-

atures but increases to 295 ps at around 30 K. The value above 30 K is comparable to the positron lifetime at neutral divacancies reported in previous works.[16,37,38] The temperature variation of lifetime $\tau_2$ at around 30 K was not clearly observed in our previous work[16] within the experimental uncertainties. The temperature-dependent positron lifetime reflects the change in the overlap between positron and electron wavefunctions at divacancies. This is probably due to the effect of lattice relaxation. The theoretical calculation by Saito and Oshiyama.[10] shows that an outward lattice relaxation is induced when a positron is trapped by a neutral divacancy and the positron lifetime increases by about 10 ps as compared to an ideal divacancy. This effect is interpreted in terms of the Coulomb repulsion between positrons and ions at vacancies. The magnitude of the lattice relaxation (breathing mode) is estimated to be ~2.8% from the change in lifetime $\tau_2$. It is likely that the lattice vibration is not sufficient to induce lattice relaxation at low temperatures. The excitation of lattice vibration at high temperature may assist the lattice relaxation and hence prolong the positron lifetime.

Figure 6 shows the trapping rate due to neutral divacancies as a function of measuring temperature. The trapping rate increases with decreasing temperature, decreases after reaching a maximum at around 30 K and increases again below 20 K. The maximum at around 30 K seems to be similar to that observed by Shimotomai *et al.* through the Doppler broadening measurement.[25] As mentioned above, the concentration of divacancies is on the order of $10^{16}\,\mathrm{cm}^{-3}$. The specific trapping rate is approximately estimated to be $\sim 2 \times 10^{15}\,\mathrm{s}^{-1}$ and $\sim 6 \times 10^{16}\,\mathrm{s}^{-1}$ at 210 K and 30 K, respectively. The present results show that the trapping rate due to neutral divacancies strongly depends on the temperature which contradicts the previous hypothesis that it is temperature independent. As mentioned in §1, the theoretical calculation by Puska *et al.* predicts that the trapping rate due to neutral vacancies is independent of temperature when the binding energy is dissipated by electron excitation.[19] Thus, the above result is hardly explained by the theory. The temperature dependence of the trapping rate shown in Fig. 6 is apparently different from the case of negatively charged vacancies with shallow levels (i.e., the trapping rate increases upon cooling and saturates at low temperatures). It is possible that the change in the trapping rate from 30 K to 210 K can be explained by the existence of some shallow trapping centers. In such a case, to explain the result below 30 K, one should assume the existence of other defects. However, it seems to be inconsistent with the conclusion of annealing experiment that divacancies are the major positron trapping centers. How do we interpret the unique temperature dependence?

The undulating temperature dependence of the trapping rate may be interpreted in terms of resonance trapping since the dependence itself seems to have features common to resonance phenomena such as neutron absorption by nuclei and particle scattering by potentials. In general, the cross section for the resonance phenomena is given by the Breit-Wigner formula[39]

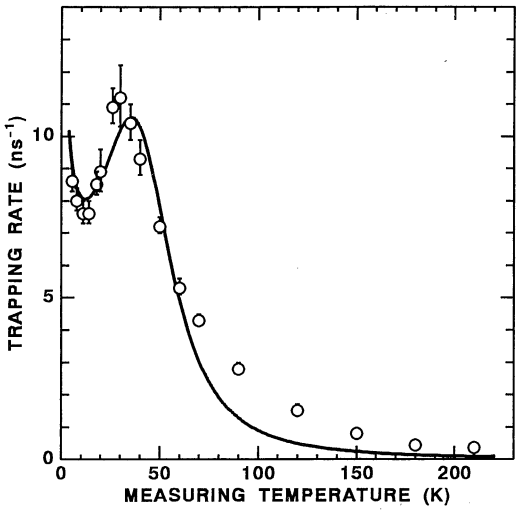


Fig. 6. Positron trapping rate which corresponds to the second lifetime component in Fig. 5 as a function of measuring temperature. Solid line shows the line fitted line using eq. (5).

$$\sigma = \pi \lambda\!\!\!^{-2} \frac{\Gamma^2}{(E - E_{\mathrm{R}})^2 + (\Gamma/2)^2}. \tag{5}$$

Here, $\lambda\!\!\!^{-}$ and $E$ are the wavelength and the energy of incident particles, respectively, $E_{\mathrm{R}}$ is the resonance energy and $\Gamma$ is the half width of the resonance which is related to the lifetime of the resonance state. The experimental result shown in Fig. 6 is likely to be reproduced using eq. (5) under the assumption that $E$ and $\lambda\!\!\!^{-}$ are regarded as the thermal energy ($\sim 3kT/2$) and thermal wavelength ($\sim 10(300/T)^{1/2}$ Å), respectively, of positrons and the trapping rate is proportional to eq. (5) and the thermal velocity of positrons ($\sigma\nu_+$). The solid line shows the best fit of the formula. The peaked behavior at 30 K and the baseline appearing below 20 K are expressed by the Lorentzian part of eq. (5) and the pre-Lorentzian part of $\nu_+\sigma$ which depends on the temperature ($\nu_+ \lambda\!\!\!^{-2} \propto T^{-1/2}$), respectively. The experimental result is well-reproduced over the entire temperature range. This implies that some type of resonance may dominate the positron trapping into neutral divacancies. From the analysis, the resonance energy and the half width were determined to be 2.6 meV and 4.2 meV, respectively. The lifetime of the resonance state is estimated to be $\sim 10^{-13}$ s from the uncertainty principle. The maximum specific trapping rate expected from eq. (5) is on the order of $10^{17}\,\mathrm{s}^{-1}$. It is close to the experimental value estimated above. Scattering resonance is known to exist for small vacancies and plays an important role in the trapping process of non-thermal positrons. However, it seems to be unsuitable here since the resonance energy is usually rather high (of the order of ~1 eV).[40] To interpret the strong temperature dependence of the trapping rate in metals,[41–43] Shirai and Takamura calculated the trapping cross section using the "cloudy-crystal-ball" model.[44] Their result shows that not only s- but also p- and d-wave resonance enhances positron trapping in the thermal energy region. On the contrary, Puska's theory shows that the resonance energy is rather high for the vacancies in

Si in the case that the trapping potential is a simple square well.[19] We inferred the possibility of resonance from the arguments concerning the lattice relaxation effect accompanying positron localization in vacancies and the electrical polarization effect of the vacancies due to the approach of positrons toward vacancies.

It is important to note that a certain amount of lattice distortion may be induced associated with positron trapping into divacancies as shown by the change in lifetime $\tau_2$ at around 30 K and this is naturally understood from the results of theoretical calculations.[7,9,10,45] It seems that the positron-lattice interaction is sufficiently strong to distort the lattice around vacancies. Presumably, the trapping potential of distorted vacancies is deeper than that of ideal vacancies since the effective volume of vacancies increases as a result of the positron trapping. A theory of extrinsic self-trapping developed by Toyozawa predicts that electrons in semiconductors are strongly localized at defects by a cooperative effect of the defect potential and electron-lattice couplings.[46] The theory is quite general and may be applicable to positron trapping into vacancies. It is likely that positron and acoustic phonon coupling is important for the extrinsic self-trapping at vacancies in homopolar semiconductors such as Si due to the absence of the Fröhlich-type interaction.

The total energies (lattice and electron energy+positron energy) of both free and trapped states can be expressed using adiabatic potentials in a configuration coordinate diagram. The equilibrium point of the trapped state may shift due to the positron lattice interaction. If we simply assume that the Hamiltonian for lattice motion is described within a harmonic approximation, equal spacing vibronic levels appear for each state. The extrinsic self-trapping theory justifies the trapping with multiphonon emission from the free state to the trapped state. Namely, the excess energy is dissipated by multiphonon emission through successive transition between vibronic levels. The trapping rate was calculated by several researchers using the adiabatic potentials for free and trapped states: $AT^n \exp(-E_A/kT)$ where $A$ is a constant and $E_A$ is the energy barrier at the crossing point of the adiabatic potentials for the free and trapped states.[47–50] The value of $n$ is $(-1/2)$ and $(-3/2)$ in the non-adiabatic and adiabatic limits, respectively.[49] Usually the experimental value of $E_A$ is in the range from several meV to 0.5 eV. The above formula suggests that (i) the trapping rate increases with temperature as a thermal activation process in which the thermal energy of positrons is comparable to the energy barrier and (ii) the exponential part of the equation approaches unity at higher temperatures and hence the trapping rate gradually decreases with temperature. The increase in the trapping rate above 20 K may be explained by (i). However, the overall temperature dependence of the trapping rate is not successfully reproduced by the thermodynamic feature. As discussed above, a positron-vacancy system is expected to have discrete vibronic levels. If one of the vibronic energy levels coincides with the energy of positrons at the conduction band, a resonance-like transition to the trapped state may occur without thermal activation to overcome the energy barrier at the crossing point of adiabatic potentials. Such a tunneling effect may be a matter of course since positrons in solids are quantum particles, i.e., waves. The excess energy of positrons may be transferred to the lattice around vacancies, i.e., the lattice is in the temporal excited state. The situation is quite analogous to the resonance trapping of neutrons by nuclei as explained by the compound nucleus theory. The excess energy may be dissipated through multi-phonon emission. It is interesting to note that the lifetime of the resonance state obtained above is comparable to the period of lattice vibration.

The effect of polarization due to the electric field of positrons themselves should also be considered. It is expected that electrically neutral defects may be polarized when charged particles approach them due to the electric field. Consequently, an attractive interaction is expected to work between neutral defects and charged particles *via* the polarization potential. The polarization potential is usually given by $-\alpha e^2/2r^4$, where $\alpha$ is the polarizability.[51,52] The polarization potential was taken into account in carrier trapping by neutral defects in the phonon cascade theory.[47,48] The theory shows that the trapping rate is proportional to $T^{-1/2}$.[51] The experimental result obtained in this work is obviously unexplained by the theory. We should mention another important aspect of the polarization effect which can cause resonance trapping. From the energy conservation law, the effective potential is given by the sum of the polarization potential and centrifugal force potential: $Eb^2/r^2$, where $b$ is the impact parameter.[39] The effective potential has a well at the central region of the defect and a finite barrier height outside the well due to the combination of the polarization and the centrifugal force potentials. When the energy of stationary state inside the potential well coincides with the energy of incident positrons, resonance trapping is expected to occur due to the tunneling effect. In such a situation, the cross section is given by eq. (5). However, it is questionable whether the change in lifetime $\tau_2$ at around 30 K is explained by the polarization effect.

## 4. Summary

In this work we determined the temperature dependence of positron lifetime and trapping rate associated with electrically neutral divacancies in Si. A unique temperature dependence of the trapping rate was observed which was different from that for negatively charged vacancies and was hardly explained by previous models. This unique temperature dependence was tentatively and qualitatively explained in terms of resonance trapping since the temperature dependence of the trapping rate seemed to be a typical example of resonance phenomena. The resonance was inferred to be originating from vibronic energy levels in the trapped state and/or to have been due to the polarization effect. To interpret the unique temperature dependence quantitatively by resonance or by other theories, further study is required.

## Acknowledgements

The authors are grateful to Professor M. Suezawa and to Dr. M. Hasegawa of Tohoku University for their help

in IR measurements and fruitful discussion on positron trapping by vacancies. The authors also thank Dr. H. Itoh and Mr. H. Sunaga of the Japan Atomic Energy Research Institute for their help in ESR measurement and electron irradiation, respectively.

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