Positron trapping at vacancies in electron-irradiated Si at low temperatures

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Experimental results on positron trapping at vacancies in electron-irradiated silicon are presented. The positron lifetimes 273±3 and 248±2 ps in pure Si and heavily-phosphorus-doped Si ([P]=10^{20} cm^{-3}) are assigned to a negative monovacancy V^- and a negative vacancy-phosphorus pair $(V\text{-P})^-$, respectively. In pure Si, positron trapping displays a strong negative temperature dependence, and the specific trapping rate reaches very large values (10^{17}–10^{18} s^{-1}) at low temperatures. In Si:P the trapping rate is independent of temperature. These different temperature behaviors are attributed to different positron-trapping mechanisms, a cascade of one-phonon transitions in pure Si, and an Auger process in Si:P.

I. INTRODUCTION

Because of their positive charge, positrons are strongly repelled by the positive-ion cores in solids. Open-volume defects such as vacancies, isolated or associated with other defects, are attractive centers, where positrons get trapped. As a result of trapping the annihilation characteristics change. Because of the reduced electron density around a vacancy the annihilation rate decreases and the electron-positron momentum distribution narrows.[1–3]

Positron annihilation at vacancy defects in semiconductors has been clearly observed. Positron trapping in silicon has been reported after irradiation and deformation.[4–10] In compound semiconductors, especially in GaAs, positron annihilation has revealed the presence of native vacancies.[11–15] Furthermore, the possibility of probing vacancy defects in the near-surface region, in thin films, and at interfaces has been demonstrated by using low-energy-positron beams.[16–18]

Annihilation characteristics give specific information on the defects involving vacancies. In semiconductors it is important to correlate this information to the defect properties known from well-established techniques which are sensitive to vacancies as well as other defects such as interstitials, antisites, and impurities. Positrons in standard experiments sample the bulk properties as, for example, electron paramagnetic resonance (EPR) or optical absorption do. The determination of the concentration of vacancy defects from annihilation parameters requires that the specific trapping rate per defect, or the trapping cross section, is known. So far the mechanisms and the cross sections of positron trapping in semiconductors are poorly known even in the case of vacancies.

In metals the trapping process is reasonably well understood.[19] In the transition to the bound state at a vacancy defect, the release of the positron binding energy is assisted by electron-hole excitation in the conduction band. Trapping is limited by the quantum-mechanical transition rate, which is independent of temperature for small defects such as a vacancy. The positron binding energy is typically a few eV, and the specific trapping rate for a monovacancy is of the order of 10^{15} s^{-1} in all metals.

In semiconductors there exists experimental evidence indicating that positron trapping is temperature dependent.[6,7,20] Specific positron-trapping rates have been estimated in a few cases. From neutron-irradiated Si Dannefaer *et al.*[5] have estimated the specific trapping rate 2×10^{14} s^{-1} for divacancies at 300 K. This is in good agreement with the value 3×10^{14} s^{-1} deduced from electron-irradiation experiments by Shimotomai *et al.*[7] From electron irradiation in GaAs Stucky *et al.*[13] found the specific trapping rate 6×10^{14} s^{-1} for As vacancies at 300 K. These values are comparable to those typically encountered for vacancies in metals. Until now, there are no theoretical calculations on positron trapping in semiconductors.

As the free-carrier capture at defect centers,[21,22] the positron trapping at vacancies is expected to vary strongly with the semiconductor, the position of the Fermi level, and temperature. The charge of the vacancy defect and its screening play a determining role in the mechanism by which the energy released in the trapping is carried away. A strong reduction in the trapping cross section is expected when a neutral defect becomes positively charged. In analogy with the carrier capture, a multiphonon or an Auger transition at a neutral defect may be replaced by a phonon cascade capture mechanism, when the defect becomes negatively charged. At low temperatures the cascade capture leads to a large increase in the trapping cross section at charged defects.

The aim of this work is to study positron-trapping mechanisms at vacancies in silicon at two different Fermi-level positions. We present experimental results on the temperature dependence of the trapping rate in electron-irradiated silicon samples. The results show that the positron trapping at vacancies occurs via different mechanisms in high-purity float-zone Si and in heavily-phosphorus-doped Si ([P]=10^{20} cm^{-3}). In pure Si the trapping is strongly temperature dependent, and the

specific trapping rate reaches giant values (10^{17}–10^{18} s^{-1}) at low temperatures. In Si:P the trapping process has characteristics similar to those in metals, i.e., the specific trapping rate is of the order of 10^{15} s^{-1}, and it is independent of temperature. We conclude that positrons are trapped at negative vacancies via a phonon cascade capture in pure Si, and at negative vacancy-phosphorus pairs via an Auger transition in Si:P.

The paper is organized as follows. In Sec. II experimental details are given. In Sec. III experimental lifetime results are presented, and in Sec. IV the positron traps are identified as monovacancies in pure Si and vacancy-phosphorus pairs in P-doped silicon. In Sec. V we estimate the specific trapping rates and attribute their different temperature dependences to different trapping mechanisms.

II. EXPERIMENT

High-purity Si and *n*-type Si heavily doped with phosphorus were studied. The high-purity samples were cut from a float-zone-refined Si ingot grown at the Centre d'Etudes Nucléaires de Grenoble. The resistivity of this material was $\rho = 10^4$ Ω cm. The residual boron and phosphorus concentrations, based on photoluminescence measurements, were $n_A = 3.3\times10^{12}$ cm^{-3} and $n_D = 1.4\times10^{12}$ cm^{-3}, respectively. This is in good agreement with the electrical measurement, which yielded $n_A - n_D = 1.5\times10^{12}$ cm^{-3}. The concentrations of oxygen and carbon were below the detection limit of 10^{15} cm^{-3}. The Si:P samples were cut from a Czochralski-grown Si ingot doped with phosphorus. The phosphorus concentration was approximately 10^{20} cm^{-3}, and the resistivity was lower than 8×10^{-4} Ω cm.

Irradiations were carried out with 1.5- and 3.0-MeV electrons in the Van de Graaf accelerators at Centre d'Etudes Nucléaires de Grenoble and Centre d'Etudes Nucléaires de Fontenay aux Roses. Irradiation temperature was 20 K and the electron current 2–4 $\mu A\,cm^{-2}$. Three pairs of pure Si samples were irradiated with 3.0-MeV electrons. The fluences were 1×10^{15}, 1×10^{16}, and 1×10^{17} e^-/cm^2. In the case of Si:P samples the irradiation energy was 1.5 MeV, and the fluences were 3×10^{16}, 3×10^{17}, and 3×10^{18} e^-/cm^2. After irradiation the samples were transferred in liquid nitrogen into the positron-lifetime spectrometer, and thus the defect structure corresponds to an annealing temperature of 77 K. Positron lifetime was measured in a liquid-helium cryostat. The temperature range studied was from 4 to 150 K, and the temperature regulation was better than ±1 K.

The positron lifetime was also measured *in situ* at 20 K immediately after electron irradiation in pure Si. The incident-electron energy was 1.5 MeV and the fluence 1×10^{17} e^-/cm^2. The samples and the irradiations are listed in Table I.

The lifetime spectrometer was a conventional fast-slow coincidence system.[1,2] The width of the resolution function was optimized for each lifetime spectrum, and it remained within ±3 ps from the mean value 276 ps for the full width at half maximum. Typically, the total number of counts in a single spectrum was 10^6. A 20-μCi ^{22}Na source evaporated on a 1-mg/cm^2 Ni foil was used. The annihilations in the source were estimated to contribute two components, 3% of 180 ps and 5.9% of 500 ps. In the *in situ* measurement the source activity was 60 μCi evaporated on a 1-μm-thick Al foil, and the source correction was 2.6% of 500 ps. After subtracting the source components the spectra were analyzed with either one or two lifetimes. The average lifetime τ was determined in terms of the lifetimes τ_1 and τ_2 and their intensities I_1 and I_2 as $\tau = I_1\tau_1 + I_2\tau_2$.

III. EXPERIMENTAL RESULTS

A. Pure silicon

Positron lifetime in pure Si samples before the electron irradiations was measured to be 221±1 ps at 300 K and 219±1 ps at 77 K. The average positron lifetimes as functions of temperature after the 3.0-MeV electron irradiationss at 20 K and annealing at 77 K are given in Fig. 1. The lifetime values measured at 4 K clearly increase with the electron fluence. After the 1×10^{15}-e^-/cm^2 irradiation the average lifetime at 4 K is 2 ps above the value measured in the unirradiated samples. After the fluences 1×10^{16} and 1×10^{17} e^-/cm^2, the increase at 4 K is 16 and 39 ps, and the lifetime is 237 and 260 ps, respectively.

Figure 1 also shows that τ decreases strongly as temperature increases. The decrease from 4 to 120 K is approximately 20 ps in these two samples. A most interest-

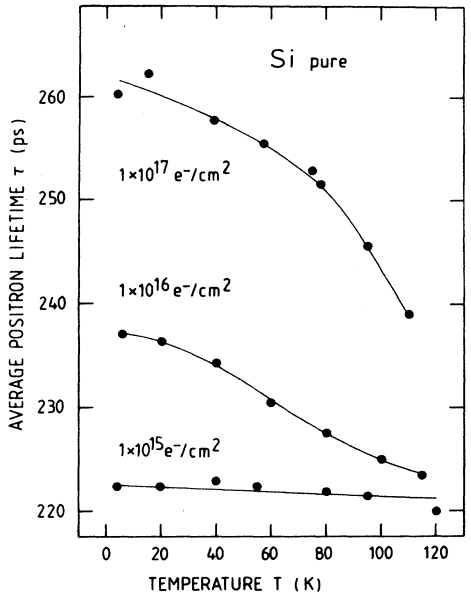

FIG. 1. The average positron lifetime τ as a function of temperature in electron-irradiated pure Si after different fluences. The variation of the lifetime is completely reversible from 4 to 120 K. The lifetime in bulk Si is 221±1 ps at 300 K and 219±1 ps at 77 K. Irradiation temperature was 20 K and the incident-electron energy 3.0 MeV.

ing feature is that this change in lifetime is completely reversible. Thus it is not an annealing effect. The first annealing stage in these samples was found to take place around 150 K.

After 1×10^{16}- and 1×10^{17}-e^-/cm^2 irradiations we find it possible to resolve two separate lifetime components without putting any constraints on the exponential fits in all the spectra, apart from the single spectrum measured at 115 K after the electron irradiation 10^{16} e^-/cm^2. The results of the decompositions are given in Figs. 2 and 3. For both fluences the long lifetime τ_2 remains constant as temperature varies from 4 to 120 K. Within the experimental errors, the value of τ_2 is the same for two samples, 273±3 and 277±3 ps, respectively. The intensity I_2 in Figs. 2 and 3 decreases as temperature increases, and this explains the decrease of the average lifetime observed in Fig. 1. The short lifetime τ_1 after 1×10^{16} and 1×10^{17}-e^-/cm^2 irradiations is about 150 and 110 ps, respectively.

Lifetime measurement carried out *in situ* at the irradiation temperature 20 K yields the average positron lifetime $\tau=241$ ps after the 1×10^{17}-e^-/cm^2 irradiation with 1.5-MeV electrons. The lifetime spectrum can be decomposed into two components. The long lifetime is $\tau_2=273\pm1$ ps, and its intensity I_2 is 77±1%. The short lifetime is $\tau_1=132\pm5$ ps. The average lifetime of 241 ps is approximately 20 ps lower than the value obtained after the 1×10^{17}-e^-/cm^2 irradiation with 3-MeV electrons and annealing at 77 K. However, it is important to notice that the long lifetime τ_2 has the same value after the 1.5- and 3.0-MeV irradiations. The lifetime τ_2 has a lower intensity I_2 after the 1.5-MeV irradiation, which explains the shorter average lifetime.

In conclusion, we find the same lifetime $\tau_2=273\pm2$ ps after electron irradiation at 20 K with or without annealing at 77 K. Moreover, this lifetime is found after 1.5- as well as 3.0-MeV irradiation.

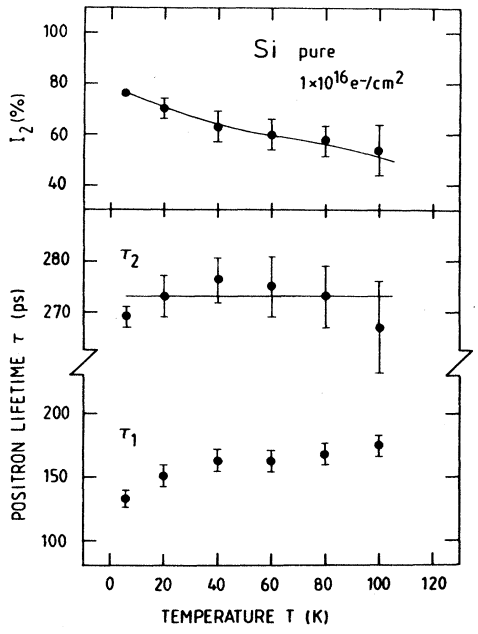

FIG. 2. Positron lifetimes τ_1 and τ_2 and the intensity I_2 as functions of temperature in pure Si after 1×10^{16}-e^-/cm^2 electron irradiation. The average lifetime τ is presented in Fig. 1. Irradiation temperature was 20 K and the incident-electron energy 3.0 MeV. The variations of the lifetime parameters are completely reversible.

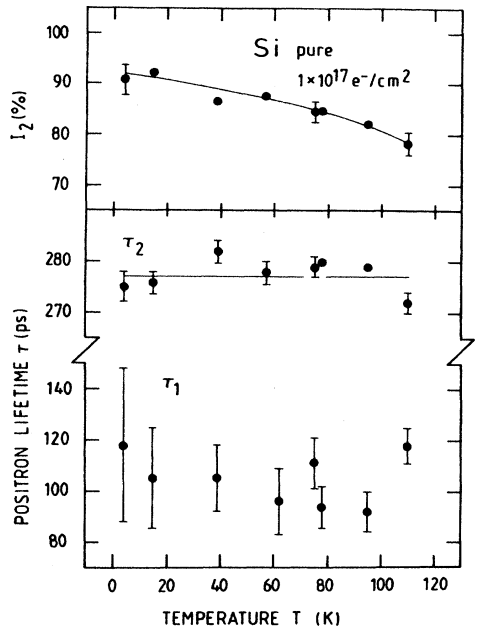

FIG. 3. Positron lifetimes τ_1 and τ_2 and the intensity I_2 as functions of temperature in pure Si after 1×10^{17}-e^-/cm^2 electron irradiation. Irradiation temperature was 20 K and the incident-electron energy 3.0 MeV. The variations of the lifetime parameters are completely reversible.

B. Phosphorus-doped silicon

Positron lifetime in phosphorus-doped Si:P was found to be 221±1 ps at 300 K. As in pure Si, the lifetime is nearly independent of temperature. From 77 to 300 K the increase is less than 2 ps. The average positron lifetimes τ measured in Si:P after the 1.5-MeV electron irradiations and annealing at 77 K are presented as functions of temperature in Fig. 4. After the lowest fluence 3×10^{16} e^-/cm^2 the lifetime is 3 or 4 ps higher than in unirradiated samples. The decomposition of the spectra was not possible ($I_2<10\%$).

With the irradiation fluence 3×10^{17} e^-/cm^2, the average lifetime reaches a value 235 ps, corresponding approximately to an increase of 15 ps. Unlike in pure Si, τ shows only a weak linear and reversible increase with temperature. Two lifetime components are resolved in this sample, and the decompositon as a function of temperature is presented in Fig. 5. The long lifetime τ_2 is now around 248 ps and it exhibits a slight increase with temperature. The intensity I_2 is approximately 90% and tends to decrease with temperature. The short lifetime τ_1

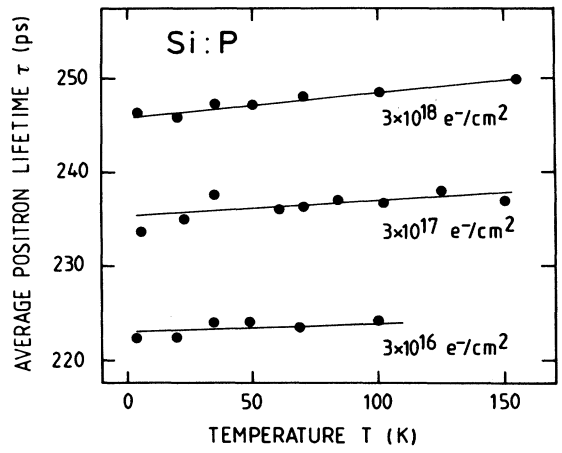

FIG. 4. The average positron lifetime τ in electron-irradiated phosphorus-doped Si ([P]$=10^{20}$ cm^{-3}) after different fluences. Irradiation temperature was 20 K and the incident-electron energy 1.5 MeV.

remains constant with a value of 130±10 ps.

The increase of the electron fluence further to 3×10^{18} e^-/cm^2 leads to saturation in positron trapping ($I_2=100\%$), and there is only one lifetime in the spectra. This lifetime is 248±2 ps, consistent with the results of the decomposition after the 3×10^{17}-e^-/cm^2 electron irradiation. There also seems to be a weak linear increase of 2×10^{-2} ps K^{-1} with temperature. This trend was confirmed by measurements at 300 K, where the lifetime was 252±1 ps.

To conclude this section we make a summary of the experimental findings as follows. The positron lifetime results exhibit two striking differences when pure Si and Si:P are compared. First, the long lifetime τ_2 induced by electron irradiation at 20 K is 273±3 ps in pure Si and 248±2 ps in Si:P. Second, the intensity I_2 shows a strong reversible negative temperature dependence below 120 K in pure Si, whereas it remains nearly constant in Si:P. The two differences are discussed below. In Sec. IV the long lifetime will be assigned to a monovacancy in pure Si and to a vacancy-phosphorus pair in Si:P. In Sec. V the different temperature dependences of I_2 will be attributed to two different positron-trapping mechanisms.

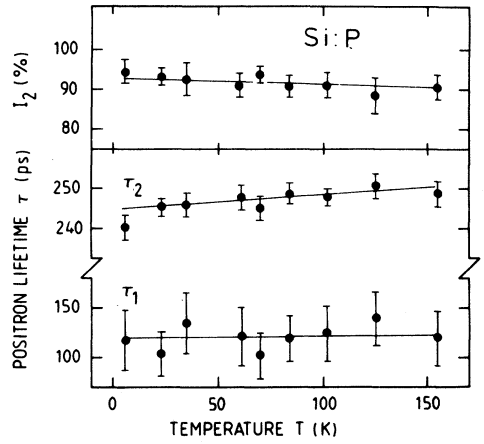

FIG. 5. Positron lifetimes τ_1 and τ_2 and the intensity I_2 as functions of temperature in phosphorus-doped Si ([P]$=10^{20}$ cm^{-3}) after 3×10^{17}-e^-/cm^2 electron irradiation. Irradiation temperature was 20 K and the incident-electron energy 1.5 MeV.

IV. IDENTIFICATION OF POSITRON TRAPS

Positron trapping at defects induced by electron irradiation is readily seen in pure Si and Si:P as the average lifetime increases appreciably after irradiation. In the following, we first recount some consequences of the trapping model[23] and then successively examine the characteristics of positron trapping in pure Si and Si:P.

A. Trapping model

When there are two modes for annihilation, i.e., positrons may annihilate from a delocalized state in bulk or as trapped at a defect, the lifetime spectrum takes the form

$$n(t)=I_1\lambda_1\exp(-\lambda_1 t)+I_2\lambda_2\exp(-\lambda_2 t) . \quad (1)$$

In terms of the two-state trapping model, the experimental annihilation rates $\lambda_1=\tau_1^{-1}$ and $\lambda_2=\tau_2^{-1}$ are related to the characteristic annihilation rates in the bulk (λ_b) and at a defect site ($\lambda_d<\lambda_b$) as follows:

$$\lambda_1=\lambda_b+\kappa \quad (2)$$

and

$$\lambda_2=\lambda_d . \quad (3)$$

Here κ is the trapping rate, which is proportional to the defect concentration c_d:

$$\kappa=\mu c_d . \quad (4)$$

The factor μ is the specific trapping rate. Equation (3) implies that the lifetime $\tau_d=\lambda_d^{-1}$ is readily determined by the experimental annihilation rate λ_2, independent of the trapping rate or the defect concentration. Furthermore, from the lifetimes τ_1 and τ_2 and their intensities I_1 and I_2 one can calculate the average lifetime,

$$\tau=I_1\tau_1+I_2\tau_2 , \quad (5)$$

which is relatively insensitive to uncertainties in the decomposition of the spectrum. In a situation in which only the trapping rate κ is subject to change, the average lifetime defines the trapping rate,

$$\kappa=\frac{\tau-\tau_b}{\tau_d-\tau}\lambda_b . \quad (6)$$

In conclusion, when there is only one kind of a defect present, it is characterized by the positron lifetime τ_2, and as this lifetime remains unchanged, the average life-

time τ yields the positron-trapping rate κ. If the defect concentration is too low ($\kappa \ll \lambda_b$), all positrons annihilate before trapping and $I_2 = 0$. On the other hand, at high defect concentrations ($\kappa \gg \lambda_b$) all positrons annihilate as trapped in defects and $I_2 = 100\%$. The comparison of the annihilation rate λ_1 calculated from Eq. (2) with the experimental one provides a check on the consistency of the two-state trapping model.

B. Vacancies in pure Si

The positron lifetime was found to be 221 ± 1 ps in pure Si before irradiation. This result is in agreement with the value 220 ps accepted as the bulk lifetime in silicon.[10] From 77 to 300 K the increase of this lifetime is less than 2 ps.

After electron irradiation, positrons are trapped at irradiation-induced defects. The defect lifetime τ_2 is the same, 273 ± 3 ps, for irradiation performed with either 1.5- or 3.0-MeV electrons. The value of τ_2 is also independent of the irradiation fluence. This strongly suggests that this lifetime is due to a well-defined defect.

The electron energies of 1.5 and 3.0 MeV are sufficient to produce both vacancies and divacancies in Si lattice. The maximum recoil energies of the knocked-on atoms are 290 and 920 eV, respectively. The mean recoil energies, however, are very close to the displacement threshold energy $E_d = 10$–20 eV needed to create a single Frenkel pair, although energetic knocked-on atoms can produce small displacement cascades including divacancies. Thus the majority of displacements leads to the formation of vacancy-interstitial pairs. However, self-interstitials are mobile in Si already at the irradiation temperature 20 K, which leads to considerable recombination of Frenkel pairs. This may change much the ratio between mono- and divacancy concentrations. The lifetime data suggest that positrons are trapped at monovacancies in pure Si samples.

Several authors have previously associated lifetimes around 270 ps with a monovacancy in Si. Fush *et al.*[4] found a lifetime of 266 ± 10 ps after 1-MeV electron irradiation at 20 K. During annealing this lifetime disappeared at 150 K, which is consistent with the temperature where vacancies are known to migrate. Dannefaer *et al.*[9] measured the same lifetime, 271 ± 2 ps, in thermal equilibrium above 1450 K and assigned it to monovacancies. Positron lifetimes in semiconductors have been calculated by Puska *et al.*[24–26] The predicted lifetime for a Si vacancy is 254–260 ps.

Lifetimes around 270 ps are clearly shorter than the lifetime associated with the divacancy in Si. The experimental lifetimes for divacancies fall in the range 318–330 ps. Dannefaer *et al.*[5] have proposed that after 330 K neutron-irradiation divacancies give rise to a 325-ps lifetime. Fush *et al.*[4] have attributed the lifetime 318 ps to divacancies in Si after 1-MeV electron irradiation and annealing above 150 K. Shimotomai *et al.*[7] have reported lifetimes of 318–327 ps after 2-MeV electron irradiation at 300 K. After similar irradiation divacancies have been clearly identified by electron-paramagnetic-resonance (EPR), electron-nuclear double-resonance (ENDOR), and deep-level transient spectroscopy (DLTS) measurements.[27–29]

We assign the lifetime 273 ps to monovacancies in Si. When this value is compared to the lifetimes of 254–260 ps calculated by Puska *et al.*,[24–26] the open volume appears to be larger than for an ideal vacancy, which suggests that the relaxation of the first-neighbor atoms of the vacancy are outwards. The lifetime 273 ps is still well below the theoretically predicted value for the divacancy. For an ideal divacancy, the theoretical lifetime is 306–309 ps,[25,26] nearly 20% longer than for the monovacancy.

Further support to the assignment of the 273-ps lifetime to monovacancies comes from the annealing properties. The annealing stage of this lifetime was observed at 150 K. This is in the temperature region where vacancies become mobile,[28] whereas divacancies are stable up to 450–500 K.[30]

In pure Si the Fermi level still remains in the middle of the energy gap after electron irradiations. Therefore, the 273-ps lifetime corresponds to the charge state occupied at this Fermi-level position. Since the early identification of the V^+ charge state of the Si vacancy, experimental evidence of three other charge states V^0, V^-, and V^{2-} has accumulated. The identification of the vacancies in electrical measurements is, however, difficult, and the ionization levels are not precisely known. Watkins and Troxell[31] have proposed a scheme for the ionization levels in which the silicon vacancy is a negative U center with the level $(0/+)$ at 0.05 eV above the top of the valence band E_v and the $(+/2+)$ level at $E_v + 0.13$ eV. The ionization levels $(-/0)$ and $(2-/-)$ lie somewhere in the energy gap above $E_v + 0.13$ eV and below $E_c - 0.17$ eV (E_c is the bottom of the conduction band). Van Vechten[32] has proposed that the $(-/0)$ level lies below the midgap at $E_c - 0.73$ eV, and that the $(2-/-)$ level is above the midgap at $E_c - 0.27$ eV. EPR and DLTS, as well as electrical measurements, indicate that a vacancy–group-V-impurity pair gives rise to the ionization levels $(-/0)$ located around $E_c - 0.45$ eV.[33–35] The assumption that the vacancy-impurity ionization levels are vacancy-like[21] leads to locate the ionization level $(2-/-)$ of the vacancy slightly above $E_c - 0.45$ eV, in good agreement with the levels proposed by Van Vechten.[32] We conclude, therefore, that the 273-ps positron lifetime is due to vacancies in the single negative charge state, i.e., V^-.

Different charge states could explain why we observe at low temperatures positron trapping only at monovacancies, although both vacancies and divacancies are present. EPR measurements have placed the ionization level $(2-/-)$ of a divacancy at $E_c - 0.4$ eV,[36] making it possible that the divacancy could be neutral or singly negatively charged when the Fermi level is in the middle in the energy gap. Based on DLTS measurements, Evwaraye and Sun[29] have proposed a scheme of ionization levels in which $(0/+)$, $(-/0)$, and $(2-/-)$ levels are located at $E_v + 0.25$ eV, $E_c - 0.41$ eV, and $E_c - 0.23$ eV, respectively. Thus the midgap position of the Fermi level would correspond to the neutral charge state of a divacancy, and we expect that positron trapping at negatively charged vacancies is much more efficient.

The decrease of the average lifetime as a function of temperature (Fig. 1) is explained by the decrease of the intensity I_2 (Figs. 2 and 3), i.e., the fraction of positrons annihilating at vacancies. Thus only the positron-trapping rate is subject to change and it may be calculated from the average lifetime according to Eq. (6). This, however, requires that the two-state trapping model is valid. Below this is checked by comparing the short lifetime τ_1 from Eq. (2) with the experimental one. For 1.5-MeV irradiation, the calculated value for τ_1 is 135 ps and agrees well with the experimental value 132±5 ps. The agreement is good also for 3.0-MeV irradiation when the fluence is 1×10^{16} e^-/cm^2, but after the higher fluence of 1×10^{17} e^-/cm^2 it is no longer satisfactory. In this sample the intensity I_2 is high (90%), and the calculated values for τ_1 are much below 100 ps. Such short lifetimes are below the limit of the experimental resolution. Further, we were unable to improve the fitting by adding a third lifetime, either free or constrained, into the analysis. In conclusion, we consider that the experimental data can be treated in terms of the two-state trapping model in all three samples.

The trapping rate κ calculated from Eq. (6) is given as a function of temperature in Fig. 6. In the figure the trapping rate in the 1×10^{16}-e^-/cm^2 irradiated sample has been scaled by a constant factor of 6.0 to compare the temperature dependences. We find an appreciable decrease in κ with temperature in both 1×10^{16}- and 1×10^{17}-e^-/cm^2 irradiated samples. Below 20 K the trapping rate κ is approximately 2×10^9 and 13×10^9 s^{-1} in the two samples, respectively. Increasing the temperature to 120 K reduces the trapping rate by a factor of 10, and the decrease is nearly linear. The change is reversible, and therefore it cannot be related to an annealing of the irradiation-induced vacancies. There is no reason to expect any change in the configuration of a vacancy in the temperature range 4–120 K in pure Si. We conclude therefore that Fig. 6 illustrates a strong decrease of the specific positron-trapping rate μ, defined in Eq. (4). It will be seen in Sec. V that the identification of the 273-ps lifetime as a negative vacancy V^- is quite consistent with the specific trapping rate estimated for this defect and with the strong reduction of μ with temperature.

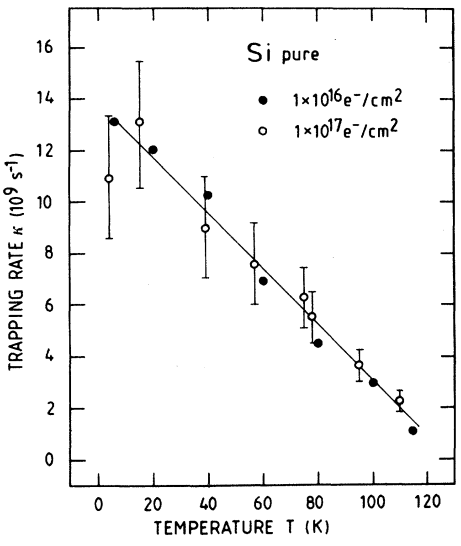

FIG. 6. Positron trapping rate κ calculated from Eq. (4) as a function of temperature in pure Si after 3.0-MeV electron irradiation at 20 K. The trapping rate corresponding to the fluence 1×10^{16} e^-/cm^2 has been scaled by a constant factor of 6.0 to compare the variation of κ with temperature. The variation is completely reversible.

C. Phosphorus-vacancy pairs in Si:P

The defect lifetime $\tau_2=248\pm2$ ps induced by 1.5-MeV electron irradiation in the P-doped samples is clearly shorter than any previously reported value for a Si vacancy. Dannefaer and Kerr[12] have observed a 240-ps lifetime in Czochralski-grown Si after heat treatment and attributed it to a vacancy-oxygen complex. In the present case phosphorus is the dominant impurity, and we therefore consider the vacancy-phosphorus pair (E-center) as the defect structure for the 248-ps lifetime. Small clusters of phosphorus atoms may exist in addition to isolated substitutional P atoms, as the concentration is as high as 10^{20} cm^{-3}. Even then the pair of a vacancy and one P atom would be the dominant defect. Pure vacancies can be ruled out since they migrate already below 200 K.[28] Such annealing is not observed for the 248-ps lifetime, but the first annealing stage occurs around 450 K in agreement with the disappearance of V-P pairs.[37]

The vacancy-phosphorus pair is the dominant defect produced by electron irradiation at room temperature in P-doped Si.[38] Here we observe them to be present after 20-K electron irradiation and annealing at 77 K. Formation of these centers may take place after increasing the temperature to 77 K or during the irradiation at 20 K. In low-resistivity n-type Si the vacancy migration energy associated with the charge state V^{2-} is only 0.18 eV,[28] and hence vacancy migration occurs already below 80 K. The probability to form V-P pairs is high due to the high phosphorus concentration and the attractive interaction between the opposite charges of the vacancies and ionized P impurities. In addition, formation of these centers already during the electron irradiation may also occur. Vacancies are not mobile at 20 K, but limited vacancy migration may take place under the irradiation conditions. This kind of a process has been suggested to be responsible for the existence of close vacancy-oxygen pairs immediately after electron irradiation at 20 K.[39] As this material was grown by the Czochralski method, oxygen is also present. However, because of the very high phosphorus content the 248-ps lifetime is interpreted as a positron annihilating at a V-P pair rather than at a site of a vacancy-oxygen pair.

The V-P pair has an ionization level ($-/0$) at 0.44 eV below the conduction band in weakly doped Si:P.[30] Due to the very high P concentration the interaction between phosphorus atoms may change the position of the ionization level. The concentration of phosphorus atoms, 10^{20} cm^{-3}, is sufficiently high to keep the Fermi level in the conduction band at about $E_c+0.07$ eV after 3×10^{18}-

e^-/cm^2 irradiation (see Sec. V B 2). Given the position of the Fermi level we can assign the 248-ps lifetime to the negatively charged $(V\text{-P})^-$ pair. The atomic configuration of the negative charge state is not known, as this center cannot be observed with EPR. However, by extending the structural model of the neutral $(V\text{-P})^0$ pair,[38] we reach the conclusion that the positron sees the Si vacancy as V^{2-}. The positron lifetime changes with the charge state of a defect only when the charge-state transition induces a distortion around the lattice site.[24,26] We observe a strong reduction of the lifetime in $(V\text{-P})^-$ compared to the lifetime in an isolated vacancy V^-. This suggests an inward relaxation at the vacancy site when it is doubly negative. In Sec. V it will be seen that the electron-positron screening effect in Si:P may also reduce the positron lifetime in a vacancy.

Previously, Mascher *et al.*[40] associated the V-P pair to a lifetime of 270 ps measured in the same P-doped (10^{20} cm^{-3}) Si material as ours after 40-MeV proton irradiation. This difference could be due to a different charge state. However, a question arises whether the defect responsible for the 270-ps lifetime is a pure V-P pair. The migration energy of the E center is 0.95–1.25 eV depending on the charge state,[37] but the 270-ps lifetime was still observed after annealing above 1200 °C. As proton irradiation produces displacement spikes, the 270-ps defect might be also a multiple vacancy associated to phosphorus atoms.

The average lifetime as well as the lifetime τ_2 in Figs. 4 and 5 were found to be independent of temperature. Therefore one expects to find a positron-trapping rate which remains constant. This is illustrated in Fig. 7, where κ calculated from Eq. (6) is depicted in the temperature range 4–150 K. The trapping rate is $(7\pm1)\times10^9$ s^{-1}. Additional measurements at 230 and 300 K indicated that the trapping rate is still at the same level. The fact that no annealing occurred in these samples below 450 K clearly indicates that the concentration of positron traps remains unchanged. Therefore the specific positron-trapping rate into $(V\text{-P})^-$ pairs turns out to be independent of temperature below 300 K.

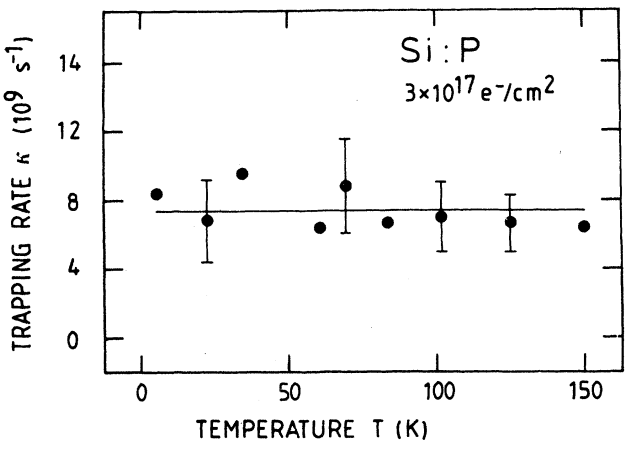

FIG. 7. Positron trapping rate κ in phosphorus-doped Si ([P]$=10^{20}$ cm^{-3}) after 1.5 MeV electron irradiation at 20 K. The electron fluence was 3×10^{17} e^-/cm^2.

In summary, we have identified the positron traps as negatively charged vacancies V^- in pure Si and as negatively charged vacancy-phosphorus pairs $(V\text{-P})^-$ in Si:P. We have also reached the conclusion that the specific trapping rate into a vacancy V^- displays a strong negative temperature dependence between 4 and 120 K in pure Si and remains constant from 4 to 300 K in the case of $(V\text{-P})^-$ pairs in Si:P.

V. POSITRON TRAPPING

A. Specific trapping rate

The specific positron-trapping rate μ in Eq. (4) can be written in terms of the trapping cross section σ as

$$\mu=v\sigma\ , \tag{7}$$

where v is the thermal velocity of a positron. This form is practical in comparing positron-trapping cross section with the cross sections for carrier capture. The estimation of μ (or σ) from the experimental trapping rate κ is straightforward, when the concentration of the defects trapping positrons is known. The defect concentration induced by electron irradiation is

$$\frac{dc_d}{d\phi}=\frac{\Sigma}{N_A}\ , \tag{8}$$

where Σ is the defect-production rate, ϕ is the integrated flux, and N_A is the atomic density. Complications arise from determining the defect-production rate Σ in silicon, as recombination of the vacancy-interstitial pairs occurs already during irradiation even at 20 K. In silicon Σ is highly dependent on the type and concentration of impurities.[39] In the following we first neglect the recombination and later try to assess it using existing experimental defect-production rates.

The total displacement rate, neglecting all the recombination effects, gives an overestimate and an upper limit for the defect-production rate Σ and consequently, a lower limit for the specific trapping rate. We have accomplished this estimation by applying the McKinley-Feshbach approximation for the electron-atom scattering cross section and using the total displacement probability similar to that in the Kinchin-Pease model with a cutoff at the threshold displacement energy E_d.[41] For E_d we have adopted the value 21 eV. The vacancy-production rate Σ so obtained is 2.6 and 3.6 cm^{-1} for 1.5- and 3.0-MeV electrons, respectively. This estimation of Σ, together with the experimental trapping rate κ, results in the specific positron-trapping rate μ presented in Table I (μ, no recombination). In the case of pure Si samples, where κ depends on temperature, μ is calculated at 20 K. In Si:P κ and μ are independent on temperature. In both types of silicon samples we get $\mu=10^{14}$–10^{15} s^{-1}, which is equal to the values typically encountered in metals. Thus the specific trapping rates for vacancies in silicon are at least as high as in metals. It can be even much higher, when the recombination is taken into account, as will be

seen below.

Recombination of interstitial atoms with vacancies reduces the final number of displaced atoms. In silicon this effect is pronounced due to the athermal interstitial migration taking place down to at least 0.5 K (Refs. 42 and 43) during electron irradiation. As originally proposed by Watkins[39] to explain results of EPR measurements, vacancy-interstitial recombination occurs unless the interstitial atoms find some other sinks than the vacancies. In *p*-type Si the acceptor atoms act as traps for interstitials. The vacancy-production rate increases linearly with the doping level, until it saturates at the acceptor concentrations of 10^{15}–10^{16} cm^{-3}.[39] The highest values in *p*-type Si for 1.5-MeV electron irradiations below 20 K are in the range 0.1–1 cm^{-1}.[39,44] There appears to be no evidence for interactions of self-interstitials with donor impurities. Therefore in *n*-type Si with very few interstitial sinks the vacancy-production rate may be as low as 0.001–0.01 cm^{-1}.[39,44]

Kouimtzi and Banbury[44] have reported a production rate of 0.002 cm^{-1} for 1.5-MeV electron irradiation at 4 K in B-doped Si having an acceptor concentration of 4×10^{12} cm^{-3}. This concentration is comparable to that in our pure Si material ($n_A=3\times10^{12}$ cm^{-3}), and we adopt the vacancy-production rate $\Sigma=0.002$ cm^{-1} for pure Si. For 3.0-MeV electrons a simple scaling with the ratio of the total number of displacements calculated above yields a vacancy-production rate $\Sigma=0.003$ cm^{-1}. These very low values indicate that the recombination of vacancy-interstitial pairs is nearly complete, only 0.1% of vacancies survive.

Estimation of the recombination effects in our Si:P samples is more difficult. There are three types of potential traps for interstitials. First, as Czochralski-grown material the oxygen content is high, about 10^{16} cm^{-3}. Infrared adsorption studies indicate that oxygen is an effective trap for interstitials, but still the cross section seems to be much lower than for group-III acceptor atoms at low temperatures.[39] Second, due to the high phosphorus concentration of 10^{20} cm^{-3}, Si:P samples are expected to contain pairs and small clusters of phosphorus atoms. Such clusters may be able to trap self-interstitials in silicon. Third, the residual acceptors are traps for interstitials. Altogether, we may assume that the total concentration of traps for self-interstitials is at the level of 10^{15}–10^{16} cm^{-3} or higher, which in *p*-type Si is sufficient to saturate the vacancy-production rate into the range 0.1–1 cm^{-3}. As an order-of-magnitude estimate we adopt for Si:P the vacancy production rate $\Sigma=0.3$ cm^{-1}. This value means that 10% of vacancies survive during recombination.

The specific positron-trapping rates and the trapping cross sections, based on the experimental defect-production rates discussed above, are listed in Table I (μ, with recombination). Two points can be noted. First, in pure Si the level of the specific trapping rate is 10^{17}–10^{18} s^{-1} at 20 K. This is a giant value compared to the trapping rates in metals, and it is strongly temperature dependent. Also, the corresponding values for the trapping cross section, 10^{-11}–10^{-12} cm^2, are comparable to the giant cross sections for carrier capture.[21,22] Second, in Si:P positron trapping has characteristics similar to those in metals. The specific trapping rate μ is approximately 10^{15} s^{-1} and it is constant from 4 to 300 K.

B. Trapping mechanisms

Capture of free carriers at defects in semiconductors occurs via radiative and nonradiative mechanisms. Nonradiative mechanisms can be classified into two main categories depending on whether they are phonon assisted or involve excitations of electrons (Auger processes).[21,22,45] Similar nonradiative mechanisms are expected to be available for the trapping of free positrons at defects. Radiative mechanisms are ruled out in the case of positrons as they occur in a time scale of 10^{-8} s, which is 2 orders of magnitude longer than the positron lifetime.

TABLE I. Samples and electron irradiations at 20 K. The defect lifetime τ_2, specific trapping rate μ, and trapping cross section σ are given at 20 K. The specific trapping rate μ is estimated (a) from the total-displacement rate (no recombination), and (b) from the experimental vacancy-production rates (with recombination). The values of σ are based on the values of μ with recombination. For the vacancy-production rates used to estimate the specific trapping rate, see the discussion in Sec. V A.

Sample	E_{irr} (MeV)	Fluence (e^-/cm^2)	τ_2 (ps)	μ^a (s^{-1})	μ^b (s^{-1})	σ^b (cm^2)
Pure	1.5	1×10^{17}	273±1	2×10^{14}	3×10^{17}	2×10^{-12}
Pure[c]	3.0	1×10^{15}				
Pure	3.0	1×10^{16}	273±3	1×10^{15}	2×10^{18}	1×10^{-11}
Pure	3.0	1×10^{17}	277±3	4×10^{14}	1×10^{18}	7×10^{-12}
P-doped[c]	1.5	3×10^{16}				
P-doped	1.5	3×10^{17}	248±3	2×10^{14}	2×10^{15}	1×10^{-14}
P-doped[d]	1.5	3×10^{18}	248±1			

[a]No recombination.
[b]With recombination.
[c]No trapping is observed.
[d]Trapping is in saturation.

Below we discuss separately the trapping mechanisms in pure Si and Si:P.

1. *Cascade trapping in pure Si*

In pure Si the specific trapping rate into vacancies is characterized by (i) extremely high values at low temperatures reaching 10^{17}–10^{18} s^{-1}, and (ii) a strong decrease with temperature from 4 to 120 K. Giant carrier-capture rates of the order of 10^{16}–10^{18} s^{-1} have been observed in Si and Ge, and they have been explained by a capture process at a charged defect involving the emission of a phonon cascade.[46] The cascade model for electrons assumes a series of closely spaced states near the conduction band. A carrier is captured by one of the upper excited states and it descends from one state to another at lower energy by emitting one or a very few phonons at each step.

The conditions, at which the cascade model can be applied, are well fulfilled for positrons in pure Si. Positron traps are negative centers, V^-; the trapping rate is very high and it displays a strong negative temperature dependence, as predicted by this mechanism at the low-temperature limit.[46,47]

Within a semiclassical approach of the cascade process, the carrier-capture cross section varies with temperature as T^{-n}. According to Abakumov and Yassievich,[47] $n=1$ when the thermal energy kT is smaller than the kinetic energy of a carrier having the sound velocity, i.e., $kT \ll 2$ K in Si. For $kT > 60$ K the trapping cross section decreases as T^{-3}. Gibb *et al.*[48] have extended the cascade model to situations involving deep levels. They suggest a model in which the electron is first captured by a cascade process to the energy state E_1, and the subsequent step to the ground state occurs at the rate μ_2. Energy E_1 is the lowest state reached by the cascade process. According to this two-stage model, in the low-temperature limit the capture cross section is the same as in the cascade capture. At higher temperatures the thermal reemission back to the conduction band becomes larger than the final capture to the ground state, and the capture rate μ is

$$\mu \propto \mu_2(T) T^{-3/2} \exp(E_1/kT) \ . \tag{9}$$

For example, from 100 to 200 K, electron-capture cross section at selenium (Se^{2+}) in Si can be fit in a cascade model with the power law T^{-n} with $n \approx 3.2$ as well as in the two-stage capture model of Eq. (9) with $E_1 = 14$ meV.[49]

The initial positron trapping occurs at a highly excited Rydberg-like state around a charged vacancy. In the first stage the positron descends through a ladder of closely spaced states emitting phonons of increasing energy at each step. The energy released in the final transition down to the deep ground state in the vacancy is about 1 eV and too high to be carried out by one-phonon emission. However, it is possible to observe an increase in the positron lifetime (221→273 ps) only, when the trapped positron has reached its ground state in the vacant lattice cell. In an excited Rydberg-like state the positron scans mainly the bulk and has the lifetime 221 ps. Thus the trapping process consists of two stages. A multiphonon emission or an Auger transition is necessary to take the positron to the ground state. Both these processes are slow compared to the cascade process, but fast compared to the positron lifetime.

Puska *et al.*[24] used the linear-muffin-tin-orbital atomic-sphere-approximation (LMTO ASA) Green's-function method to calculate the positron and electron single-particle states at vacancies in various semiconductors. Their results showed that the positron is more bound than the outer electrons. In Si the positron binding energy varies from 1.0 to 1.6 eV depending on the charge state of the vacancy and is typically 1.5 times higher than the binding energy of the less bound electron. Therefore, two Auger processes may occur. The bound electron carrying away the energy released by the positron is excited into a Rydberg-like state of the vacancy or is ejected into the conduction band. Even the excitation of a valence electron to the conduction band cannot be ruled out.

In Fig. 8 we show the positron-trapping rate in a $\ln\kappa$-versus-$(1/T)$ plot. One can see that above 60 K the positron data fits the law $\kappa \propto \exp(E_1/kT)$ with $E_1 = 20 \pm 2$ meV. This energy corresponds to a Rydberg-like state with the quantum number $n \approx 3$ for the positron trapped around a V^- vacancy. It is comparable to the electron captured by Se^{2+} with $E_1 = 14$ meV corresponding to the Rydberg state of $n=2$ or 3.[49] If the trapping cross section is fitted to the T^{-n} law in the same temperature range, from 60 to 120 K, one finds $n=3.1$, in good agreement with $n=3$ predicted by Abakumov and Yassievich for the cascade process.

The transition rate from the state E_1 to the ground state can be estimated in the following simple way. The transition rate $\mu_2(T)$ competes with annihilation from state E_1. We do not observe annihilations from this state. This means that the transition rate $\mu_2(T)$ is at least about 10 times faster than the annihilation rate in the

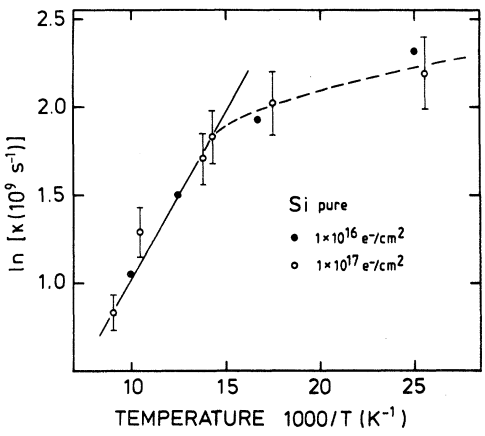

FIG. 8. Temperature dependence of the positron trapping rate κ at negative vacancies V^- in pure Si after 3.0-MeV electron irradiation at 20 K. The trapping rate corresponding to the fluence 1×10^{16} e^-/cm^2 has been scaled by the same constant factor of 6.0 as in Fig. 6.

bulk, i.e., $\mu_2(T) > 5\times10^{10}$ s^{-1}. Such high transitions rates are possible, because the positron wave function in the state E_1 is already fairly localized in the vicinity of the vacancy. The classical radius of the $n=3$ Rydberg state for a positron in Si is about 40 Å.

It is interesting that the positron-trapping rate does not fit the predicted temperature dependence below 60 K, because the carrier cascade model is supposed to work especially well in the low-temperature region. In semiconductors, most of the studies of the carrier-capture rate are performed above 100 K. The origin of the discrepancy in the temperature behavior is not yet understood, but may indicate that for the positron a full quantum-mechanical treatment of the trapping process is necessary. However, we may conclude that the cascade process explains qualitatively the positron trapping at negative vacancies in pure Si.

2. *Trapping via Auger process in Si:P*

The positron-trapping rate in Si:P is quite similar to that in metals. This is not entirely unexpected because Si crystals doped with phosphorus to 10^{20} cm^{-3} exhibit metallic properties.[50] The critical concentration n_t for the metal-insulator transition in Si:P is 3.75×10^{18} cm^{-3}, in good agreement with the theoretical value

$$n_t^{1/3} a_0^* \approx 0.25 \ , \tag{10}$$

where a_0^* is the effective Bohr radius for the electron.[51] The donor levels of P atoms are no more discrete but form a band (see, e.g., Mott[52] and Pantelides *et al.*[53] and references therein). At 0 K the crystal has its valence bands fully occupied and the conduction band is filled up to the Fermi level with the 10^{20} cm^{-3} electrons from P donors. A simple parabolic band can be assumed to calculate the Fermi energy. With the effective mass of $1.062m_0$ (Ref. 54) the Fermi level lies at 0.071 eV above the bottom of the conduction band.

In Si:P the Thomas-Fermi screening length is $\lambda_{TF}\approx4$ Å, only about 10 times longer than its typical value in metals. Thus the screening of the positron charge in this material is close to the metallic limit and more efficient than in pure Si. This changes the positron lifetime in a vacancy. Puska[55] has calculated the lifetime in an As vacancy V^{2-} at the metallic limit of screening, and found a 12-ps decrease. The difference is expected to be roughly the same for a silicon vacancy. The positron lifetime in a $(V\text{-P})^-$ pair is approximately 25 ps lower than in a vacancy V^- in pure Si. We may attribute about 5–10 ps of this difference to the screening in Si:P, and the rest is due to the different charge state of the vacancy. By extending the configuration model of the neutral vacancy-phosphorus pair $(V\text{-P})^0$ proposed by Watkins[28] to the negative $(V\text{-P})^-$ pair, we reach the conclusion that the positron sees a vacancy, which has three pairs of localized electrons. This means that the positron sees a V^{2-} vacancy in Si:P instead of a V^- vacancy in pure Si. Positron lifetimes are rather insensitive to the charge state as long as no relaxation occurs,[24,26] and therefore we can conclude that the first-neighbor atoms of the vacancy are relaxed inwards in $(V\text{-P})^-$ compared with V^-. Such a tendency corresponds to that predicted by Samara.[56]

Although the positron trapping in Si:P occurs at a negatively charged vacancy, the cascade process is no longer possible because the screening of the Coulomb potential $(Ze/r)\exp(-r/\lambda_{TF})$ is very efficient. The effective Bohr radius [$Z=1$ for $(V\text{-P})^-$] for the positron is 6.2 Å. Substituting this value into Eq. (10) we see that the positron can no longer be bound to a Rydberg-like state, when the conduction-electron density is higher than 7×10^{19} cm^{-3}.

As seen in Sec. IV, the positron-trapping rate in Si:P remains constant at least up to 300 K. This temperature independence *a priori* rules out the capture mechanism via multiphonon emission, because the capture rate of this process is temperature dependent.[22,57–59] The positron-trapping mechanisms which may yield a capture rate independent of temperature in Si:P are (i) the capture via electron-hole excitation in the conduction band as in metals, and (ii) the capture via Auger processes. Depending on the energy E_r released in positron capture, various Auger processes may take place. If E_r is high, $E_r > E_g$, the three following Auger processes are possible: (1) a valence electron is ejected into the conduction band, (2) a valence electron is ejected into a localized state at a deep trap, or (3) a localized electron at a deep trap is ejected into the conduction band. For $E_r < E_{gap}$ the band-band Auger transition is no longer possible, and the processes involving localized states at deep traps may occur depending on the required ionization energies and momentum conservation.

Here we are dealing with positron trapping at negatively charged vacancies in the vacancy-impurity pairs $(V\text{-P})^-$. Puska *et al.*[24,25] have calculated the positron binding energies and lifetimes at vacancies. The theoretically predicted binding energies are 1.0 eV for isolated V^- vacancies and 1.5 eV for isolated V^{2-} vacancies. The positron binding energy at V-P pairs are expected to be of the same order. For example, the positron binding energy at V_{As}-As_{Ga} complexes is slightly higher (0.2 eV) than in isolated pure V_{As} vacancy. The energy released in positron trapping at vacancies in Si:P is thus higher than the optical band gap, $E_g + E_F$. At 20 K, the photoluminescence experiments indicate that the optical gap is approximately 1.1 eV and that the energy gap E_g in phosphorus-doped Si ($[P]=10^{20}$ cm^{-3}) is smaller by 0.145 meV than the energy gap of 1.17 eV in pure Si.[54,60] The three Auger processes quoted above therefore seem possible.

The question arises, whether electron-hole creation in the conduction band or the Auger process may account for the specific trapping rate value of 2×10^{15} s^{-1} in Si:P. For carrier capture it is accepted that an Auger transition may yield capture rates comparable to the rates obtained in multiphonon emission processes. Capture rates as high as 5×10^{15} s^{-1} have been explained by the multiphonon emission process in GaP.[59] However, the experimental data on the Auger process are less firm and the theoretical values appear to be very sensitive to the choice of the wave functions used to describe the free- or bound-carrier states.[61] Jaros[62] has proposed that many of the capture cross sections as high as 10^{-13}–10^{-16} cm^2, which exhibit only weak temperature dependence, might

be explained by this mechanism.

We have roughly estimated that neither the electron-hole excitation in the conduction band nor the band-band Auger process can yield trapping rates as high as 2×10^{15} s^{-1}. Thus an Auger transition is likely to involve localized states in the case of positron trapping at the $(V\text{-P})^-$ pair, which contains up to six localized electrons.

In conclusion, in Si:P the insensitivity of the positron trapping rate to temperature is typical of an Auger process. However, the specific trapping rate in the range 10^{14}–10^{15} s^{-1} would lead to conclude that the Auger process is unusually efficient in a $(V\text{-P})^-$ pair.

IV. CONCLUSIONS

In this paper we have studied positron-trapping mechanisms in semiconductors by investigating the temperature dependence of positron trapping in electron-irradiated silicon at different Fermi-level positions.

In pure Si the positron lifetime 273±3 ps is attributed to negatively charged monovacancies V^-. The trapping rate is strongly temperature dependent and decreases by an order of magnitude between 4 and 120 K. In heavily phosphorus-doped Si ($[P]=10^{20}$ cm^{-3}) the lifetime of trapped positrons is 248 ps. This lifetime is attributed to negatively charged vacancy-phosphorus pairs $(V\text{-P})^-$. The difference between the two lifetimes indicates that the lattice relaxation associated with the V^{2-} vacancy in the V^{2-}-P^+ complex is inward compared with an isolated V^-.

The specific trapping rates are difficult to estimate because of the recombination during low-temperature irradiation. However, the results tend to show that the specific trapping rate at V^- in pure Si reaches a giant value of 10^{17}–10^{18} s^{-1} at 20 K. The very large trapping cross section and the strong temperature dependence point out that positron trapping occurs via the phonon-cascade mechanism.

In heavily doped n-type Si:P the specific trapping rate is of the order of 10^{15} s^{-1} and independent of temperature, as in metals. The doping level is so high that the crystal has metallic properties. Due to the high carrier concentration the long-range Coulomb interaction is screened out, and the phonon-cascade mechanism is not possible for positron trapping. We have attributed the trapping to the Auger process, where localized electrons at V^{2-} are excited to the conduction band.

In summary, positron trapping at vacancies in semiconductors is as complex as carrier capture. Different trapping mechanisms occur depending on the charge state of the defects and the Fermi level of the sample. The value of the specific trapping rate may vary several orders of magnitude.

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[1] *Positrons in Solids,* Vol. 12 of *Topics in Current Physics,* edited by P. Hautojärvi (Springer-Verlag, Heidelberg, 1979).

[2] *Positron Solid State Physics,* Proceedings of the LXXXIII International School of Physics "Enrico Fermi," Varenna, 1983, edited by W. Brandt and A. Dupasquier (North-Holland, Amsterdam, 1983).

[3] *Positron Annihilation,* edited by P. C. Jain, R. M. Singru, and K. P. Gopinathan (World Scientific, Singapore, 1985).

[4] W. Fush, V. Holzhauer, S. Mantl, F. W. Richter, and R. Sturm, Phys. Status Solidi B **89**, 69 (1978).

[5] S. Dannefaer, G. W. Dean, D. P. Kerr, and B. G. Hoggs, Phys. Rev. B **14**, 2709 (1976).

[6] S. Dannefaer, S. Kupca, B. G. Hogg, and D. P. Kerr, Phys. Rev. B **22**, 6135 (1980).

[7] M. Shimotomai, Y. Ohgino, H. Fukushima, Y. Nagayasu, T. Mihara, K. Inoue, and M. Doyama, in *Defects and Radiation Effects in Semiconductors,* Inst. Phys. Conf. Ser. No. 59 (Institute of Physics, London, 1981), p. 241.

[8] S. Dannefaer, N. Fruensgaard, S. Kupca, B. G. Hogg, and D. Kerr, Can. J. Phys. **61**, 451 (1983).

[9] S. Dannefaer, P. Mascher, and P. Kerr, Phys. Rev. Lett. **56**, 2195 (1986).

[10] S. Dannefaer, Phys. Status Solidi A **102**, 481 (1987).

[11] G. Dlubek, O. Brümmer, F. Plazaola, and P. Hautojärvi, J. Phys. C **19**, 331 (1986).

[12] S. Dannefaer and D. Kerr, J. Appl. Phys. **60**, 591 (1986).

[13] M. Stucky, C. Corbel, B. Geffroy, P. Moser, and P. Hautojärvi, in *Defects in Semiconductors,* Materials Science Forum, edited by H. J. von Bardeleben (Trans Tech, Aedermannsdorff, 1986), Vols. 10–12, p. 265.

[14] G. Dlubek and R. Krause, Phys. Status Solidi A **102**, 443 (1987).

[15] C. Corbel, M. Stucky, P. Hautojärvi, K. Saarinen, and P. Moser, Phys. Rev. B **38**, 8192 (1988).

[16] P. Hautojärvi, P. Huttunen, J. Mäkinen, and A. Vehanen, in *Defects in Electronic Materials,* Vol. 104 of *Materials Research Society Symposia Proceedings,* edited by M. Stavola, S. J. Pearson, and G. Davies (Materials Research Society, Pittsburgh, 1987), p. 105.

[17] A. Uenodo, S. Tanigawa, K. Suzuki, and K. Watanabe, Appl. Phys. Lett. **53**, 473 (1988).

[18] P. Schultz, E. Tandberg, K. G. Lynn, B. Nielsen, T. E. Jackman, M. W. Denhoff, and G. C. Aers, Phys. Rev. Lett. **61**, 187 (1988).

[19] R. M. Nieminen and M. J. Manninen, in *Positrons in Solids,* Ref. 1, p. 145; R. M. Nieminen, in *Positron Solid State Physics,* Ref. 2, p. 359.

[20] W. Fush, U. Holzhauer, and F. W. Richter, Appl. Phys. **22**, 415 (1980).

[21] M. Jaros, *Deep Levels in Semiconductors* (Hilger, Bristol, 1982).

[22] B. K. Ridley, *Quantum Processes in Semiconductors* (Clarendon, Oxford, 1982).

[23]R. N. West, Adv. Phys. **22**, 263 (1973); *Positrons in Solids,* Ref. 1, p. 89.
[24]M. J. Puska, O. Jepsen, O. Gunnarsson, and R. M. Nieminen, Phys. Rev. B **34**, 2695 (1986).
[25]M. J. Puska, S. Mäkinen, M. Manninen, and R. M. Nieminen, Phys. Rev. B (to be published).
[26]M. Puska and C. Corbel, Phys. Rev. B **38**, 9874 (1988).
[27]E. G. Sieverts, S. H. Muller, and C. A. J. Amerlaan, Phys. Rev. B **18**, 6834 (1978).
[28]G. D. Watkins, in *Deep Centers in Semiconductors,* edited by S. T. Pantelides (Gordon and Breach, New York, 1986), p. 147.
[29]A. O. Evwaraye and E. Sun, J. Appl. Phys. **47**, 3776 (1976).
[30]L. C. Kimerling, in *Radiation Effects in Semiconductors,* Inst. Phys. Conf. Ser. No. 31 (Institute of Physics, London, 1977), p. 221.
[31]G. D. Watkins and J. R. Troxell, Phys. Rev. Lett. **44**, 593 (1980).
[32]J. A. Van Vechten, Phys. Rev. B **33**, 2674 (1986).
[33]M. Hirata, N. Hirata, and H. Saito, J. Appl. Phys. Jpn. **5**, 252 (1966).
[34]E. L. Elkin and G. D. Watkins, Phys. Rev. **174**, 881 (1968).
[35]A. Chantre, M. Kechouane, and D. Bois, Physica B+C **116B**, 547 (1983).
[36]G.D. Watkins and J. W. Corbett, Phys. Rev. **138**, A543 (1965).
[37]L. C. Kimerling, H. M. De Angelis, and J. W. Diebold, Solid State Commun. **16**, 171 (1975).
[38]G. D. Watkins and J. W. Corbett, Phys. Rev. **134**, A1359 (1964).
[39]G. D. Watkins, in *Lattice Defects in Semiconductors,* Inst. Phys. Conf. Ser. No. 23 (Institute of Physics, London, 1975), p. 1.
[40]P. Mascher, D. Kerr, and S. Dannefaer, Phys. Rev. B **35**, 3043 (1987).
[41]J. Bourgoin and M. Lannoo, *Point Defects in Semiconductors II* (Springer-Verlag, Heidelberg, 1983).
[42]K. L. Brower, Phys. Rev. B **1**, 1908 (1970).
[43]R. E. McKeighen and J. S. Koehler, Phys. Rev. B **4**, 462 (1971).
[44]S. D. Kouimtzi and P. C. Banbury, J. Phys. C **14**, 3701 (1981).
[45]J. S. Blakemore, *Semiconductor Statistics* (Pergamon, Oxford, 1962).
[46]M. Lax, Phys. Rev. **119**, 1502 (1960).
[47]V. N. Abakumov and I. N. Yassievich, Fiz. Tekh. Poluprovodn. **12**, 3 (1978) [Sov. Phys.—Semicond. **12**, 1 (1978)].
[48]R. M. Gibb, G. J. Rees, B. W. Thomas, B. L. H. Wilson, B. Hamilton, D. R. Wight, and N. F. Mott, Philos. Mag. **36**, 1021 (1977).
[49]H. G. Grimmeis, E. Jansen, and B. Skarstam, J. Appl. Phys. **51**, 3740 (1980).
[50]T. F. Rosenbaum, R. F. Milligan, M. A. Paalanen, G. A. Thomas, and R. N. Bhatt, Phys. Rev. B **27**, 7509 (1983).
[51]N. F. Mott, *Metal-Insulator Transitions* (Taylor and Francis, London, 1974).
[52]N. F. Mott, in *Localization and Interaction in Disordered Metals and Doped Semiconductors,* edited by D. M. Filayson (Edinburgh University Press, Trowbridge, 1986), p. 29.
[53]S. T. Pantelides, A. Selloni, and R. Car, Solid State Electron. **28**, 17 (1985).
[54]J. Wagner, in *Localization and Interaction in Disordered Metals and Doped Semiconductors,* edited by D. M. Filayson (Edinburgh University Press, Trowbridge, 1986), p. 343.
[55]M. J. Puska, in *Positron Annihilation,* Proceedings of the 8th International Conference on Positron Annihilation, edited by L. Dorikens-Vanpraet, M. Dorikens, and D. Segers (World Scientific, Singapore, in press).
[56]G. A. Samara, Phys. Rev. B **37**, 8523 (1988).
[57]C. H. Henry and D. V. Lang, Phys. Rev. B **15**, 989 (1977).
[58]B. K. Ridley, J. Phys. C **11**, 2323 (1978).
[59]D. V. Lang, in *Deep Centers in Semiconductors,* edited by S. T. Pantelides (Gordon and Breach, New York, 1986), p. 409.
[60]J. Wagner, Solid State Electron. **28**, 25 (1985).
[61]F. A. Riddoch and M. Jaros, J. Phys. C **13**, 6181 (1980).
[62]M. Jaros, Solid State Commun. **25**, 1071 (1978).