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A POSITRON LIFETIME STUDY OF DEFECTS IN PLASTICALLY DEFORMED SILICON

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Abstract. Deformation-induced defects in Si have been studied using positron lifetime measurement. Two lifetime components related to dislocations and large vacancy clusters were detected after the deformation. Annealing experiments showed that the dislocation-related component consisted of further two components. One annihilated after the annealing at around 900° C. The other remained even at 1100° C. The latter component was attributed to dislocations themselves. Positron trapping rate due to dislocations was proportional to T^{-1} between 100 and 300K and saturated below 50K. These temperature characteristics were interpreted in terms of shallow trapping levels originating from dilatational strain field around dislocations and one dimensional character of dislocation.

Introduction

It is known that many ESR and DLTS active centers exists in plastically deformed Si [1]. They are attributed to point defects and their agglomerates but not dislocations themselves since most centers disappear after the annealing at rather low temperature (<800° C).

Previous positron studies [2,3] showed that two kinds of positron trapping centers related to large vacancy clusters and vacancy-like parts on dislocations were introduced by deformation. Although dislocations are also expected to act as positron trapping centers, it has not been confirmed yet. Present results allows us to conclude that dislocations in Si work as positron trapping and annihilation centers.

Experimental

Samples were prepared from floating-zone-grown Si crystals doped with phosphorus (2×10^{15}cm^{-3}; Si:P) or boron (4×10^{14}cm^{-3}; Si:B1, 1×10^{16}cm^{-3}; Si:B2). They were subjected to compressive deformations along [123] direction at 800° C in a vacuum. The dislocation density N_d was determined from etch-pit density. The Fermi level E_F was determined from the Hall effect measurement. Isochronal and isothermal annealings were done in appropriate conditions.

Positron lifetime measurement was carried out using a positron source (^{22}NaCl ~4×10^5 Bq) and a conventional spectrometer between 15 and 300K. Lifetime spectra were resolved into two or three lifetime components using a fitting program of PATFIT-88 [4]: Spectrum was fitted by the relation $L(t)=(I_1/\tau_1)\exp(-t/\tau_1)+(I_2/\tau_2)\exp(-t/\tau_2)+(I_3/\tau_3)\exp(-t/\tau_3)$, in the case of three-component analysis. Here, τ_i ($i=1,2,3$) are the lifetimes and I_i are the intensities ($I_1+I_2+I_3=1$). If the two defects trapping model [5] is a good approximation, the lifetimes τ_i should be $\tau_1=(\tau_B^{-1}+\kappa_2+\kappa_3)^{-1}$, $\tau_2=\tau_{D1}$ and $\tau_3=\tau_{D2}$. Here, τ_B is the positron lifetime in the bulk which was determined to be 220±2 ps from the measurement of undeformed Si, τ_{D1} and τ_{D2} are the positron lifetimes at defects denoted by D1 and D2, respectively. κ_2 and κ_3 are the net positron trapping rates due to the defects D1 and D2, respectively: $\kappa_2=(I_2/I_1)\{\tau_B^{-1}+(1-I_3)/\tau_2+I_3/\tau_3\}^{-1}$ and $\kappa_3=(I_3/I_1)\{\tau_B^{-1}+I_2/\tau_2+(1-I_2)/\tau_3\}^{-1}$. The trapping rates are proportional to the concentrations of defects. The validity of the analysis based on the trapping model can be checked by the relation for τ_1.

Results and Discussion

Figure 1 shows the results of three-component analysis of lifetime spectrum for the Si:P sample. The lifetime spectra of other samples were also analyzed as well. Table I summarizes the results of the analyses together with the dislocation densities and the Fermi levels. Each lifetime τ_1 agrees with that expected from the trapping model. Thus, second and third lifetime components are related to annihilations at defects. Two lifetime components ~285 ps and 544 ps related to defects were obtained for the Si:P sample. The former component was also obtained for the Si:B1 sample, but the latter not. Although the mean lifetime (τ_M) is longer than the bulk lifetime, no second and third components were obtained for the Si:B2 sample. This will be discudded later.

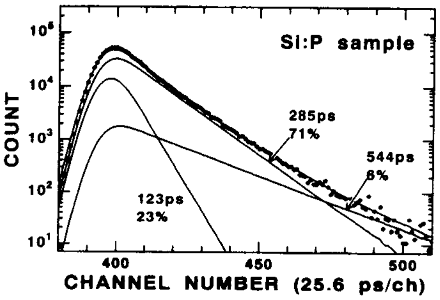

Figure 1 Lifetime spectrum for the Si:P sample. Solid lines show the results of three-component analysis.

Figure 2 shows the lifetimes τ_1 and τ_2, intensities I_2 and I_3 for the Si:P sample as a function of annealing temperature. (Annealing time is 30min) Since the lifetime τ_3 scattered around 544 ps, it was fixed to 544 ps to minimize statistic uncertainties in the analysis. The lifetime τ_1 agrees with that expected from the trapping model. The lifetime τ_2 decreases from ~285 ps to ~ 240 ps at around 900° C. The intensity I_3 becomes weak above 1000° C, while I_2 is still strong even at 1100° C. Since the intensity is not proportional to the defect concentration, we determined the trapping rate. Figure 3 shows the annealing behaviors of the trapping rate κ_2 which corresponds to the second lifetime component. It decreases with the decrease in the lifetime τ_2 but remains even at 1100° C. Above results suggest that the second lifetime component consists of further two components; one disappears at around 900° C and the other remains even at 1100° C. The lifetime at the latter center is ~240 ps. That at the former is roughly estimated to be ~300 ps from the change of lifetime and trapping rate. Similar result was obtained for the Si:B1 sample. We discuss second and third lifetime components separately in the following.

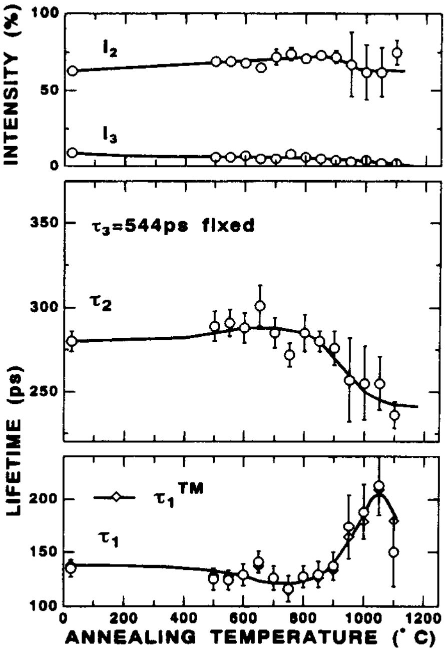

Figure 2 Lifetimes and intensities as a function of annealing temperture. τ_1^{TM} denotes the lifetime τ_1 expected from the trapping model.

Second lifetime component: As mentioned above, second lifetime component consists of further two components:

$$\tau_2\sim 285\text{ ps}\left\{\begin{array}{l}\tau_{2A}\sim 300\text{ ps}\\ \tau_{2B}\sim 240\text{ ps}\end{array}\right.$$

The lifetime τ_{2A}~300 ps indicates that the size of open volume associated with the defects are comparable to that of a divacancy in Si. However, isolated divacancies hardly survive at 800° C where the deformation was taken place. This leads us to a model that

Table I Dislocation densities, the Fermi levels and the results of analysis of lifeitme spectra. τ_1^{TM} and τ_M denote the lifeitme τ_1 expected from the trapping model and mean lifetime, respectively.

Sample	N_d (cm^{-2})	E_F (eV)	τ_1 (ps)	τ_2 (ps)	τ_3 (ps)	I_2 (%)	I_3 (%)	τ_1^{TM} (ps)	τ_M (ps)
Si:P	$2.4x10^8$	E_C-0.27	123	285	544	71	6	118	263
Si:B1	$1.1x10^8$	E_V+0.27	173	285	...	55	...	174	235
Si:B2	$1.6x10^8$	E_V+0.16	225	...	...	...	...	...	225

this center is some vacancy-like parts on dislocations as suggested by Krause et al. [3]. It is proposed [6-8] that the anti-phase defects called solitons may exist on reconstructed dislocation cores. Soliton-vacancy complexes were also proposed to be electrically active centers on dislocation cores. From a geometrical view point, the open volumes of soliton-vacancy complexes on 30˚ and 90˚ partial dislocations seem to be comparable to those of a monovacancy or a divacancy in Si. Thus, such defects are expected to act as the positron trapping centers giving rise to the lifetime $\tau_{2A} \sim 300$ ps. The Si:K1/K2 ESR centers were proposed to be vacancy-like parts on dislocation [1]. The activation energy for the disappearance of the lifetime component $\tau_{2A} \sim 300$ ps was determined to be ~3.5eV from the isothermal annealing experiment. It is much higher than that of Si:K1/K2 centers ~1.3eV determined by Wöhler et al. [9]. Thus, the lifetime component $\tau_{2A} \sim 300$ ps is not related to the Si:K1/K2 centers.

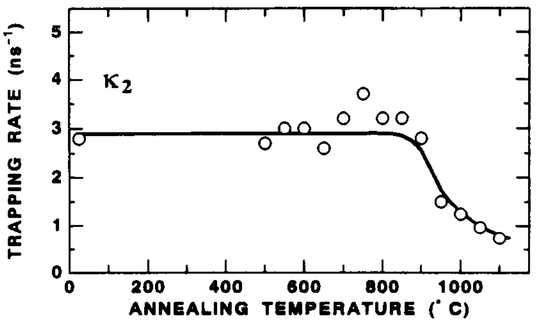

Figure 3 Positron trapping rate κ_2 corresponds to second lifetime component in Fig.2 as a function of annealing temperature.

The lifetime component $\tau_2 \sim 285$ ps is observed for the Si:P and Si:B1 samples as shown in Table I. Although such a lifetime component was not analyzed for the Si:B2 sample, the mean lifetime was longer than the bulk lifetime suggesting the lifeitme at trapping centers is slightly longer than the bulk lifetime, say 230-240 ps. These shows that the defects giving rise to the lifetime $\tau_{2A} \sim 300$ ps work as effective trapping centers in the former two samples, but not in the latter sample. We interpreted this in terms of the effect of the Fermi level. Namely, the defect giving rise to the lifetime $\tau_{2A} \sim 300$ ps has a donor level between $E_V+0.16$ eV and $E_V+0.27$ eV, and hence its charge state changes from neutral which can trap a positron to positive which can not trap a positron, or vice versa, depending on the Fermi level. The theoretical study by Heggie and Jones [8] shows that the donor levels of the single dangling bonds of soliton-vacancy complexes on the 30˚ and 90˚ partial dislocations should appear in the lower half of the band gap and two different charge states, neutral and positive, are available. This also supports the above argument.

Previous ESR and DLTS studies [1] show that the point defects and their agglomerates introduced by deformation completely disappear due to the annealing up to 900˚ C. The lifetime component $\tau_{2B} \sim 240$ ps shows a remarkably high thermal stability as compared to such defects. The electron microscopy observation [10] shows that dot-like defects, stacking faults and faulted dipoles disappears after the annealing at 900˚ C and only straight dislocations remain. Hence, we propose that the lifetime $\tau_{2B} \sim 240$ ps is related to dislocations themselves, and not point defects. The lifetime is in the medium between that at a monovacancy and the bulk lifetime. From a geometrical view point, the diameter of open cylinder involving the core of a 90˚ partial dislocation seems to be similar to that of a monovacancy. The atomic density at the core of a 30˚ partial dislocation seems to be comparable to that of bulk. Thus, it may be reasonable to think that the lifetime ~240 ps is a weighted average among such types of dislocations.

To clarify the interaction between a positron and trapping centers, we measured the temperature dependences of positron lifetime and trapping rate below 300K. Here, we focused on the positron lifetime and trapping rate associated with dislocations. Figure 4 shows the temperature dependences of lifetime τ_1 and τ_2, and intensities I_2 and I_3 for the Si:P sample which was annealed at 900˚ C for 800min prior to the measurement. The lifetime τ_2 is nearly constant around 240 ps between 15 and 300K. It suggests that the open volume of dislocation cores is insensitive to the temperature. The size of open volume of a dislocation core may be determined by the balance between the energy gain due to the reconstructions of dangling bonds and the increase in the elastic strain energy due to lattice relaxations. Probably, such

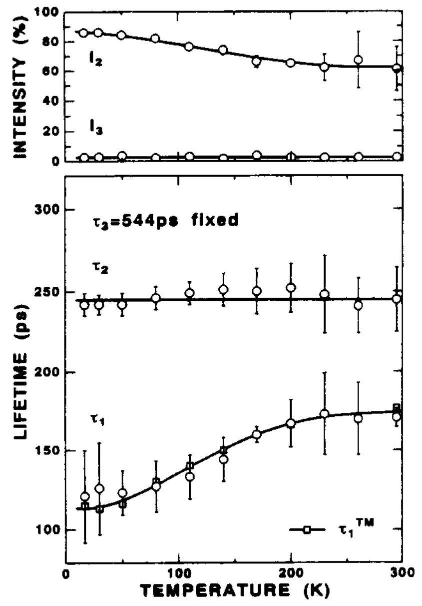

Figure 4 Temperature dependences of lifetimes and intensities for the Si:P sample annealed at 900° C for 800min.

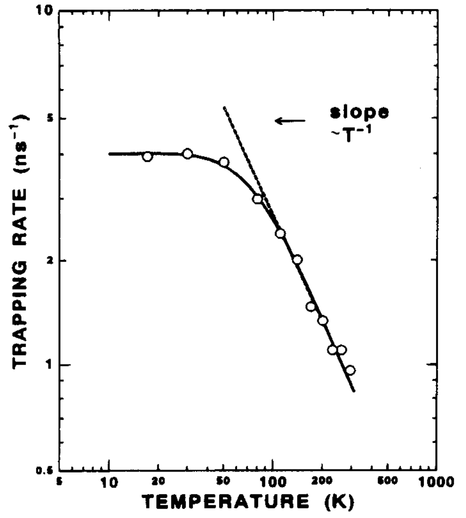

Figure 5 Temperature dependence of trapping rate κ_2 corresponds to the second lifetime component in Fig.4.

energies are nearly independent of temperature due to the bonding character of dislocation core.

Figure 5 shows the dependence of trapping rate κ_2 responsible for the lifetime τ_2 on temperature. The trapping rate increases upon cooling and saturates at low temperature. The effective trapping radius of dislocations at 15K was estimated to be ~20Å in accordance with Cotterill et al. [11]. It is much larger than the spatial extent of the dislocation cores. The temperature dependence of trapping rate shown in Fig.5 is interpreted in terms of shallow trapping level: A positron is at first trapped by the shallow level around dislocation and subsequently transfered to a relatively deep state in the dislocation core. The net trapping rate for such a two-step trapping may be given by $\kappa=\kappa_0\eta/(\eta+\delta)$, where κ_0 is the trapping rate by the shallow level, δ is the detrapping rate from the shallow level and η the transition rate from the shallow level to the deep level [12]. Here, detrapping from the deep state to free state is neglected. Manninen and Nieminen [13] gave the ratio of the detrapping and trapping rates for a dislocation as

$$\frac{\delta}{\kappa_0} = \frac{m^* k_B T}{2 N_d \hbar^2 erf\left(\sqrt{E_b / k_B T}\right)} \exp(-E_b / k_B T), \qquad (1)$$

where m* is the effective mass of a positron which is almost equal to the static mass in the case of Si [14], N_d is the dislocation density and E_b is the magnitude of energy level. The pre-exponential factor relates to the effective density of state. The solid line in Fig.5 shows the fitting line using Eq.(1). The experimental result is well-reproduced with the above model. The energy level E_b was determined to be ~11 meV. Such shallow level may be induced from the deformation potential due to the dilatational strain field around dislocations. Several theoretical works [15-18] show that the weakly-bound states for an electron and a hole appear due to such potential. Probably, a long-range attraction also exists, and shallow trapping levels are induced.

The trapping rate due to dislocations is proportional to $\sim T^{-1}$ in the temperature range between 100 and 300K as shown in Fig.5. It is explained as the pre-exponential factor of Eq.(1) is approximately proportional to T in that temperature range. (Variation of error function is small.) It is interesting to note that the trapping rates of negatively charged vacancies which have the shallow trapping levels due to the Coulomb attraction are proportional to $\sim T^{-3/2}$ in the temperature range between 100 and 300K [19]. Such a temperature dependence comes from the fact that the pre-exponential factor of δ/κ_0, namely the term related to density of state, is proportional to $T^{3/2}$. Thus, the different temperature dependence of the trapping rate between dislocations (line defect) and small vacancies (point defect) can be explained as the difference of density of states depending on the geometrical dimensions of the defects.

Third lifetime component: Obviously, the lifetime $\tau_3 \sim 544$ ps is related to large vacancy clusters. The exess vacancies are generated due to the non-conservative motion of jogs on dislocations. The jogs are introduced by the cutting between dislocations on the different slip planes. Probably, vacancies produced at jogs in spatially localized regions easily grow to large vacancy clusters. The lifetime >500 ps observed in the previous works were attributed to hexavacancies or cluster larger than ten-vacancy [2,3]. A theoretical calculation [20] shows that the lifetime at a hexavacancy may be $\sim$400 ps which are much shorter than 544 ps. Thus, we think that the vacancy clusters giving rise to the lifetime 544 ps are larger than hexavacancy. However, it is difficult to determine the size of vacancy cluster exactly from the present theory since it could not produce the lifetime exceed 500 ps.

Third lifetime component $\sim$544 ps was observed for the Si:P sample, but not for boron-doped samples. This is probably explained as the effect of the Fermi level as mentioned above.

Summary

Two kinds of positron trapping centers related to dislocations and large vacancy clusters were found after plastic deformation. The dislocation-related component consisted of further two components: The vacancy-like parts on dislocations and dislocations themselves. Dislocations have shallow trapping levels originating from their dilatational strain field. The temperature dependence of the trapping rate was found to reflect one dimensional character of dislocations.

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