Materials Science Forum
ISSN: 1662-9752, Vols. 175-178, pp 327-330
doi:10.4028/www.scientific.net/MSF.175-178.327

Online: 1994-11-24

Materials Science Forum Vols. 175-178 (1995) pp. 327-330

POSITRON 2D-ACAR STUDY ON DIVACANCIES IN Si

T. Chiba[1], A. Kawasuso[1], M. Hasegawa[2], M. Suezawa[2], T. Akahane[1] and K. Sumino[2]

[1] National Institute for Research in Inorganic Materials, Namiki 1-1, Tsukuba-shi, Ibaraki 305, Japan

[2] Institute for Materials Research, Tohoku University, Sendai 980, Japan

Keywords: Si, Semiconductor, Divacancy, Defect, Positron Annihilation, 2D-ACAR, Positron Trapping

ABSTRACT

We investigated divacancies of charge states, V_2^0, V_2^- or V_2^{2-} in FZ Si introduced by electron irradiation using measurements of the 2 dimensional angular correlation of positron annihilation radiations (2D-ACAR) at subambient temperatures. Bulk (untrapped) annihilation components of irradiated specimens were estimated referring to anisotropies of 2D-ACAR distributions of the specimens and of unirradiated Si. Intensities of the remaining trapped components agreed well with the results of our former lifetime measurements. However the relaxation of V_2^{2-} at higher temperatures inferred by the lifetime measurements was not confirmed. Anisotropy of 2D-ACAR distribution of trapped positrons in V_2^- was obtained from a specimen with oriented divacancies.

Charge state of divacancy in Si can be controlled exclusively to be one of V_2^+, V_2^0, V_2^- or V_2^{2-} by an appropriate combination of dopant species, their concentrations, fluences of 15 MeV electron irradiation and subsequent heat treatments.[1-3] Following the positron lifetime study,[4-14] we measured 2D-ACAR of FZ Si with V_2^0, V_2^- and V_2^{2-} and of unirradiated FZ Si at 295K, 200K, 100K and 15K, with the projection directions being [100], [011] and [111] for 295K and 15K, and [011] for intermediate temperature measurements. Characteristics of the specimens are shown in Table. 1. From the Hall effect measurements we confirmed that the charge states of all the specimens do not change at low temperatures.[14]

The purpose of the present work was to get further information about the lattice relaxation around V_2^{2-} detected as an increase of trapped lifetime with temperature,[14] and to get anisotropies of 2D-ACARs of trapped positrons, which should contain information of electronic states of divacancies.

2D-ACAR distribution can be decomposed into a centrally symmetric isotropic part and an anisotropy. We found for all the samples we measured the anisotropies do not change their shapes beyond the uncertainty of the measurements, but only differ in their

Table 1 Characteristics of specimens.

Specimen Charge state	Dopant conc. (cm^{-3})	Fluence (e/cm^2)	V_2 conc. (cm^{-3})	Annealing (°C×hrs.)	Fermi level at 300K (eV)
V_2^0	B: 4.0×10^{14}	3×10^{17}	3×10^{16}		$E_v+0.40$
V_2^{-1}	P: 1.7×10^{16}	5×10^{17}	5×10^{15}	250 × 1	$E_c-0.34$
V_2^{-2}	P: 1.7×10^{16}	3×10^{16}	8×10^{14}	150 × 0.5	$E_c-0.17$

328 Positron Annihilation - ICPA-10

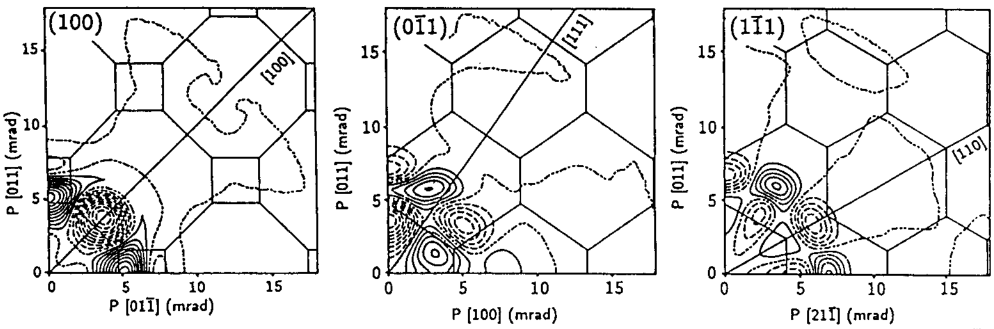

Fig. 1 Anisotropies of 2D-ACAR of unirradiated pure FZ Si projected along [100], [0$\bar{1}$1] and [1$\bar{1}$1] directions. Contour spacing is 0.87% of the [100] projection peak. Solid lines: positive, broken lines: negative and chain lines: zero contour heights (same for other anisotropies).

amplitudes. Therefore, we think the anisotropies come from the positrons annihilating in the bulk of the specimens. With reference to the anisotropies of the unirradiated Si, which are shown in Fig. 1, we get the bulk annihilation component of each specimen at each temperature so as to reproduce the amplitude of the anisotropy. Subtracting this bulk component the remaining distribution, corresponding to the trapped component, was found to be centrally symmetric for each measurement.

According to the trapping model the intensity of the trapped ACAR component is given by $\kappa/(\lambda_B+\kappa)$, and the trapped lifetime component, $I_2=\kappa/(\lambda_B+\kappa-\lambda_D)$, where λ_B is the bulk annihilation rate, λ_D, the annihilation rate in the trap and κ, the trapping rate. In Fig. 2 intensities of defect components, $\kappa/(\lambda_B+\kappa)$, obtained by the ACAR and lifetime measurements [14] are compared. Assuming that $\lambda_B=(222ps)^{-1}$ we get κ from the trapped component of ACAR, which agrees fairly well with the result of the lifetime measurement.

While both of λ_D from the lifetime measurement and FWHM of the trapped component of the ACAR are considered to represent, in some ways, the size of the trapping center, i.e., divacancy, these two parameters, however, are found to show different temperature dependence as depicted in the middle and upper parts of Fig. 2. The steepest decrease of λ_D of V_2^{-2} with increasing temperature is interpreted to represent lattice relaxation near V_2^{-2} due to the occupancy of two excess electrons in the anti-bonding states and Coulomb repulsion between them.[14] However, the steepest decrease of the FWHM of the defect ACAR was found for V_2^0. The FWHM of V_2^{-2} shows only a small decrease and does not simply support the lifetime data interpretation. More work including theoretical calculations [15–17] are needed to solve this apparent discrepancy between the lifetime and the ACAR results. The ACAR results can provide

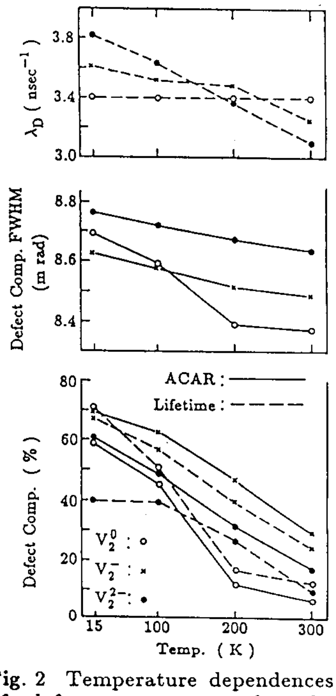

Fig. 2 Temperature dependences of defect components by the ACAR and lifetime measurements, FWHM of reduced 1D-ACAR of defect components and trapped annihilation rates for V_2^0, V_2^- and V_2^{2-}.

Materials Science Forum Vols. 175-178 329

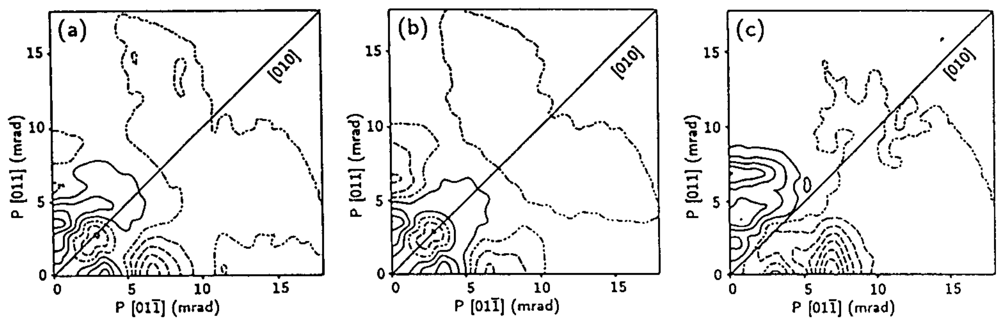

Fig. 3 Anisotropies of trapped 2D-ACAR components of oriented V_2^{-1} specimen. (a): Anisotropy after [011] and [01$\bar{1}$] foldings. (b): Anisotropy after [011], [01$\bar{1}$] and [010] foldings. (c): Anisotropy for N (see text). Contour spacing is 0.15% of the trapped 2D-ACAR peak.

different information not obtained by lifetime studies.

The apparent isotropy of the trapped ACAR component also poses problems. In order to investigate whether this is caused by the cancellation among four possible orientations of divacancies, we measured a specimen with oriented divacancies. By heating the V_2^- specimen to 170° C for 1 hour under compressive stress of 150 kgw/cm^2 along [011] direction, then cooling to room temperature and releasing the stress, the population of the divacancies of the orientations within the (011) plane, namely [1$\bar{1}$1] and [11$\bar{1}$] was increased about 50% relatively to the divacancies off the (011) plane, along [111] and [$\bar{1}$11].[1] This inequivalence can be detected by the 2D-ACAR measurement with [100] projection direction. Then [011] and [01$\bar{1}$] directions are not equivalent. Following the same procedure described above we got trapped components at 15K, 100K, 200K and 295K. These show very small tetragonal symmetries. We summed all of these trapped components to have better statistics. Then we got an anisotropy shown in Fig. 3 (a). We denote the anisotropy from the divacancies lying in the (011) plane ([1$\bar{1}$1] and [11$\bar{1}$]) by $N_{//}$ and the anisotropy from the divacancies off the (011) plane ([111] and [$\bar{1}$11]) by $N_{\perp}$. Fig. 3 (a) corresponds to $1.2\ N_{//} + 0.8\ N_{\perp} = 0.4\ N_{//} + 0.8\ (N_{//} + N_{\perp})$. We folded the anisotropy of Fig. 3 (a) along [010] and got Fig. 3 (b), which corresponds $N_{//} + N_{\perp}$. Then we subtracted 2 times Fig. 3 (b) from 2.5 times Fig. 3 (a) to get Fig. 3 (c), which corresponds to $N_{//}$. The amplitudes of the anisotropies relative to the 2D-ACAR peak heights are very small, 1.4% for (a), 0.9% for (b) and 1.8% for (c) of Fig. 3. For comparison the anisotropies of pure Si shown in Fig. 1 are 16.9% for [100], 12.3% for [0$\bar{1}$1] and 8.8% for [1$\bar{1}$1] projections. It is noted that this anisotropy is still a combination of those from divacancies of two orientations, [1$\bar{1}$1] and [11$\bar{1}$], but because these divacancies are reflection symmetric with respect to the (100) plane (perpendicular to the 2D-ACAR projection direction), they should show the same anisotropies. We hope that the anisotropy shown in Fig. 3 (c) has an important information of the electronic structure of the divacancy, V_2^-, and encourages further study including theoretical calculations.[15–17]

Similarly by adding all the trapped components for each of the V_2^0, V_2^- and V_2^{2-} specimens we got anisotropies which barely exceed the experimental uncertainties and correspond to Fig. 3 (b) for these specimens. These are shown in Fig. 4. The anisotropy amplitudes relative to the trapped 2D-ACAR peaks are 1.0% for V_2^0, 0.8% for V_2^{-1} and 0.8% for V_2^{-2} specimens. Though the three anisotropies look similar, we cannot discuss the similarities or differences of these anisotropies because an important part can be cancelled

330 *Positron Annihilation - ICPA-10*

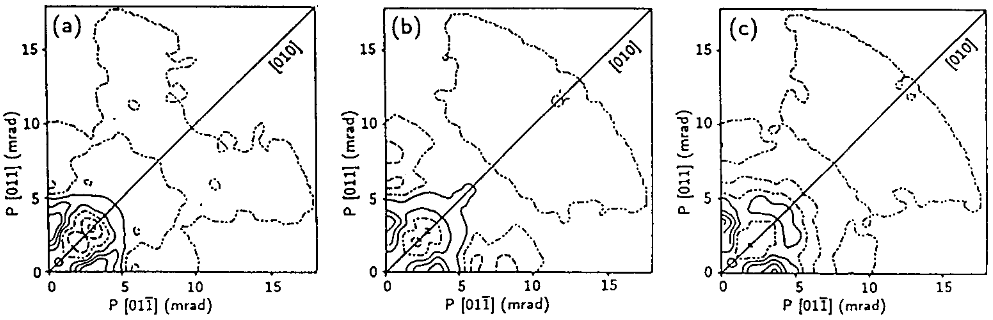

Fig. 4 Anisotropies of trapped 2D-ACAR components. (a): V_2^0, (b): V_2^{-1}, (c): V_2^{-2}. Contour spacing is 0.15% of the trapped 2D-ACAR peak.

out in these combined anisotropies. However, we can conclude that the apparent isotropy of the trapped 2D-ACAR components are caused by the cancellation among four possible orientations of divacancies.

Quite recently the 2D-ACAR measurements have been successfully applied to study defects in GaAs.[18,19] The 2D-ACAR techniques will prove its increasing importance in defect studies.

Acknowledgments

We thank Dr. K. Masumoto and the technical staff of the Laboratory of Nuclear Science, Tohoku University for their help in electron irradiation. We are grateful to Prof. A.A. Manuel of the University of Geneva for sending the manuscripts of their papers prior to publication.

References

1) G.D. Watkins and J.W. Corbett: Phys. Rev. **138** (1965) A543.
2) A.O. Evwaraye and E. Sun: J. Appl. Phys. **47** (1976) 3776.
3) G. A. Samara: Phys. Rev. **B39** (1989) 12764.
4) S. Dannefaer, G.W. Dean, D.P.Kerr and B.G. Hogg: Phys. Rev. **B14** (1976) 2709.
5) S. Dannefaer, S. Kupca, B.G. Hogg and D.P.Kerr: Phys. Rev. **B22** (1980) 6153.
6) W. Fuhs, U. Holzhauer, S. Mantl, F.W. Richter and R. Strum: Phys. Stat. Sol. **(b)89** (1978) 69.
7) M. Shimotomai, Y. Ohgino, H. Fukushima, Y. Nagayasu, T. Mihara, K. Inoue and M. Doyama: Inst. Phys. Conf. Ser. No.59 (1981) p.241.
8) Motoko-Kwete, D. Segers, M. Dorikens, L. Dorikens-Vanpraet, P. Claws and I. Lemahieu: Appl. Phys. **A49** (1989) 659.
9) Motoko-Kwete, D. Segers, M. Dorikens, L. Dorikens-Vanpraet and P. Claws: Phys. Stat. Sol. **(a)122** (1990) 129.
10) P. Mascher, S. Dannefaer and D. Kerr: Phys. Rev. **B40** (1989) 11764.
12) C. Corbel, M. Stucky, P. Hautojarvi, K. Saarinen and P. Moser: Phys. Rev. **B38** (1988) 8192.
13) J. Makinen, P. Hautojarvi and C. Corbel: J. Phys. Condens. Matter **4** (1992) 5137.
14) A.Kawasuso, M.Hasegawa, M.Suezawa, S.Yamaguchi and K.Sumino: Hyperfine Interactions (in press); and to be submitted.
15) M.J. Puska and C. Corbel: Phys. Rev. **B38** (1988) 9874.
16) O. Sugino and A. Oshiyama: Phys. Rev. **B42** (1990) 11869.
17) M. Saito, A. Oshiyama and S. Tanigawa: Phys. Rev. **B44** (1991) 10601.
18) R. Ambigapathy, A.A. Manuel, P. Hautojarvi, K. Saarinen and C. Corbel: submitted to Phys. Rev. **B.**
19) A.A. Manuel, R. Ambigapathy, P. Hautojarvi and C. Corbel: to be published in J. Physique (France).

Positron Annihilation - ICPA-10
10.4028/www.scientific.net/MSF.175-178

Positron 2D-ACAR Study on Divacancies in Si
10.4028/www.scientific.net/MSF.175-178.327