Identification of open-volume defects in disordered and amorphized Si: A depth-resolved positron annihilation study

G. Amarendra,* R. Rajaraman, G. Venugopal Rao, K. G. M. Nair, and B. Viswanathan
Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam-603 102, India

R. Suzuki, T. Ohdaira, and T. Mikado
Quantum Radiation Division, Electrotechnical Laboratory, 1-1-4, Umezono, Tsukuba, Ibaraki-305, Japan
(Received 29 November 2000; published 23 May 2001)

Depth-resolved positron beam studies have been carried out on Ar-irradiated Si using Doppler S parameter and lifetime measurements. Si samples have been irradiated with 140-keV Ar ions to a dose of 2×10^{13} and 5×10^{16} Ar/cm^2, respectively, so as to produce disordered and amorphous states in near-surface regions. The observed features of the defect sensitive line shape S parameter indicate the presence of small vacancylike defects in the disordered sample and higher-order vacancy clusters in an amorphous sample. Pulsed positron beam lifetime results indicate that the disordered Si sample exhibits lifetime distribution ascribable to mostly divacancies. In the case of an amorphous sample, the lifetime distribution is broad with larger lifetime values indicating the presence of a distribution of large vacancy clusters or nanovoids. By using theoretical lifetime values for Si reported in the literature, an empirical fit to the lifetime variation as a function of vacancy cluster size is obtained. By comparing the experimental lifetime distribution with this data, the vacancy cluster size distribution in disordered and amorphous Si is deduced. In disordered Si, divacancies are found to be the dominant defects species followed by small concentration of V_3. In amorphous Si, nanovoids in the size range of four to seven vacancy clusters are present with V_5 and V_6 clusters being the dominant defect species. The implication of these results is discussed in light of recent computer-simulation studies.

DOI: 10.1103/PhysRevB.63.224112 PACS number(s): 61.43.Dq, 61.72.−y, 61.80.Fe, 78.70.Bj

I. INTRODUCTION

Study of amorphous semiconductors and Si in particular, has been an area of active research over the last few decades.[1] There is a renewed interest in ion and electron-beam induced amorphization in Si.[2–4] Recently, a process of maskless fabrication of silicon devices has been proposed using focused ion beam for patterning on Si wafers.[5] In this paper, it is reported that subsurface defects induced by the ion beam gives rise to preferential electrodeposition of Au only at the irradiated regions. It is interesting to note that a minimum ion dose giving rise to a critical concentration of defects is required to achieve Au electrodeposition. Using an ion or electron beam, selective depth regions of the sample can be disordered, i.e., crystalline state containing lattice defects, or amorphized,[2–4] i.e., the irradiation-induced defect concentration is so large that it gives rise to lattice instability leading to amorphous state. In the disordered state, the existence of crystalline state with the presence of defects can be inferred from structural sensitive techniques like Raman spectroscopy, x-ray scattering, ion channeling, and electron microscopy. On the other hand, in amorphous state these experimental techniques will indicate the loss of long-range order and crystallinity. The absence of a crystalline peak and the appearance of shifted broad maximum in Raman spectroscopy and similar features in x-ray scattering and electron microscopy, can be used to identify the existence of an amorphous phase. There is a broad understanding that in Si, ion irradiated with low doses, monovacancies are not stable at room temperature and only divacancies may be observed. On the other hand, the nature of vacancylike defects in amorphous Si is still elusive. It may be pointed out that the existence, accumulation, and overlap of defects is a key ingredient in both homogeneous and heterogeneous models of amorphization.[1–4] With respect to the structure of amorphous Si, continuous random network (CRN) model of tetrahedrally coordinated Si atoms with varying bond lengths and bond angles has been the workhorse.[1] There are also other models[6] invoking the existence of five, six, and seven membered rings within the CRN. On the other hand, *ab initio* density-functional based molecular dynamics and Hartree-Fock calculations[7] for crystalline Si have indicated that six-vacancy cluster (V_6) is energetically the most stable defect, followed by V_5 and V_4 clusters. With respect to amorphous Si, it is expected that there will be open-volume defects, since the density of amorphous Si is less than that of crystalline Si. However, there have been very few experimental studies addressed to the identification of vacancy-type defects and their size distribution, which would throw more light on the nature of structural defects in amorphous Si.

Positron annihilation spectroscopy is a powerful tool to study the open-volume defects in materials.[8–11] There have been extensive studies on irradiation effects in crystalline Si using positron annihilation (for a review see Refs. 10 and 11). With respect to amorphous Si, Dannefaer *et al.*[12] have reported depth averaged conventional positron lifetime results on thermally evaporated and sputtered amorphous Si thin films deposited on a Si substrate, where lifetime values in the range of 400–500 ps were observed. The emergence of variable low-energy positron beams[9] enables depth resolved defect studies at near-surface and interfacial regions of thin-film samples. There have been a few reports[13,14] using a positron beam based doppler S-parameter to study amorphized Si samples. A series of Si samples, amorphized by different

 ©2001 The American Physical Society

methods, have been studied[13] to probe neutral and negatively charged Si dangling bonds. In this paper, only the glow discharged sample has been found to contain nanovoids but their size could not be estimated from *S*-parameter measurements. In another doppler and lifetime study on self-ion irradiated Si,[14] defects in ion-beam induced epitaxially grown layer and at an amorphous crystalline (a/c) interface have been studied. They have observed lifetimes attributable to only divacancies in ion-beam amorphized region and large vacancy clusters ($\tau \sim 398$ ps) in a depth region beyond the a/c interface. Recently, Brusa *et al.*[15] have reported positron beam *S*-parameter measurements on Si samples irradiated with He ions to different doses. The state of the samples, as to whether it is disordered or amorphous, is not known in this paper.

In the present paper a combined study of depth resolved positron Doppler *S*-parameter and lifetime measurements is reported on Ar-irradiated Si samples. We have chosen two irradiation doses such that the low dose sample is disordered, while the high dose sample is amorphous. We present the positron annihilation results on these two samples so as to illustrate the difference in open-volume defects, namely, vacancy clusters in these two distinct irradiated states. By comparing our experimental positron annihilation results with the available *ab initio* calculations, we make an attempt, for the first time, to identify the vacancy cluster size distribution in the disordered and amorphous state of Si. The implication of the present results is discussed in the light of recent computer simulations on amorphous Si. A preliminary report of these results has been presented earlier in a conference.[16]

II. EXPERIMENTAL DETAILS

Si(111) wafers of 500 μm thickness were cleaned in 1:1 hydrofluoric acid and demineralized water for removing the surface oxide layers and irradiated with 140-keV Ar ions to a dose of 2×10^{13} and 5×10^{16} Ar/cm^2. These irradiations were carried out with low Ar-ion-beam current ($\sim$200 nA) with Si samples mounted on a large Cu holder. The temperature monitored during irradiation was $\sim$300 K. From the TRIM code calculations[17] of 140-keV Ar ions in Si, it is found that the maximum lattice damage occurs at a depth of $\sim$100 nm, while the damage distribution extends up to about 260 nm. We have chosen the above two doses based on our earlier positron beam, Raman, and ion channeling studies on Si irradiated to different Ar doses,[18] which indicated the critical threshold dose for amorphization to be 5×10^{13} Ar/cm^2. Thus, in the present paper, the low dose sample is disordered (hence forth referred to as *d*-Si), while the high dose sample is amorphous (referred to as *a*-Si). Raman and ion channeling studies[18] on the high dose sample have confirmed that the sample is amorphous and the extent of amorphized region is deduced to be $\sim$320 nm from ion channeling results. Doppler broadening measurements as a function of positron beam energy E_p have been carried out at room temperature on irradiated and unirradiated samples using a magnetically guided positron beam.[19] From these measurements, a line shape *S* parameter,[9–11] sensitive to vacancylike defects, is deduced. The measured *S* parameter is normalized with respect to the bulk *S*-parameter value of the unirradiated sample. The experimental *S* parameter vs E_p curves are fitted using the VEPFIT program[20] by treating the irradiated sample as a combination of defected and undefected layers and the respective *S* parameters deduced. An intense variable energy pulsed positron beam, generated by an electron LINAC at Electrotechnical laboratory,[21] was used for the positron lifetime measurements. Positron lifetime spectra of irradiated and reference samples were measured at room temperature at selected depth regions of the sample by measuring the time interval between the timing signal of the pulsed positron beam and the timing signal of annihilation γ ray. The time resolution full width at half-maximum of this lifetime spectrometer is $\sim$280 ps and all the spectra were acquired with a total counts of $\sim10^6$. The experimental lifetime spectra were analyzed using the PATFIT program,[22] which gives discrete lifetime components and the CONTIN program,[23] which gives continuous lifetime distribution. The lifetime values deduced by the former program are found to be slightly larger than the mean values of the lifetime distribution obtained using the latter program for both *d*-Si and *a*-Si samples. The extent of smoothening in the CONTIN program is kept the same for all the lifetime spectra.

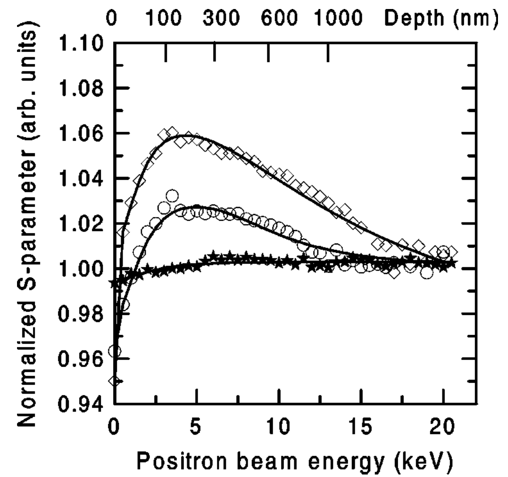

FIG. 1. Normalized *S*-parameter vs positron beam energy E_p for unirradiated Si (stars), *d*-Si (open circles), and *a*-Si (open diamonds) samples. The solid line through the data points is a fit obtained using VEPFIT analysis. Mean implantation depth of positron beam is indicated on the top axis.

III. RESULTS

Figure 1 shows the variation of the normalized *S* parameter as a function of E_p for unirradiated and irradiated Si samples. As compared to the unirradiated sample, the *S* parameter of the *d*-Si sample increases, reaches a maximum around E_p of 3 keV, corresponding to a depth scale of 100 nm and subsequently decreases gradually and reaches unirradiated values. The depth location of the peak *S* parameter, which signals the location of maximum lattice damage, is consistent with TRIM code estimates. The variation of the *S* parameter for the *a*-Si sample is qualitatively similar to that of *d*-Si. However, it is found that the peak value of the *S*

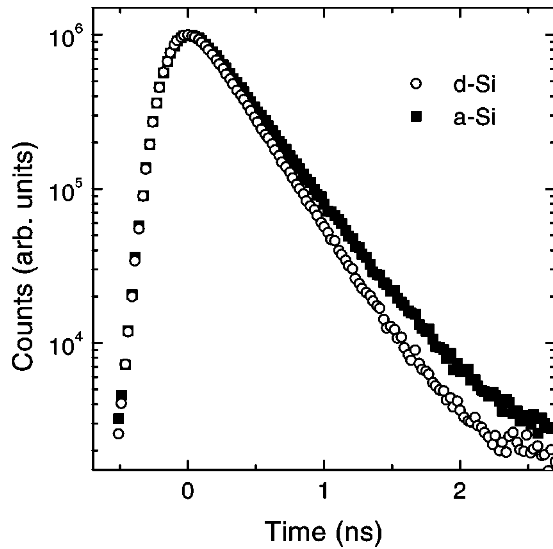

FIG. 2. Measured lifetime spectra for d-Si (open circles) and a-Si (filled squares) obtained at positron beam energy of 5 keV, which corresponds to a depth of $\sim$225 nm.

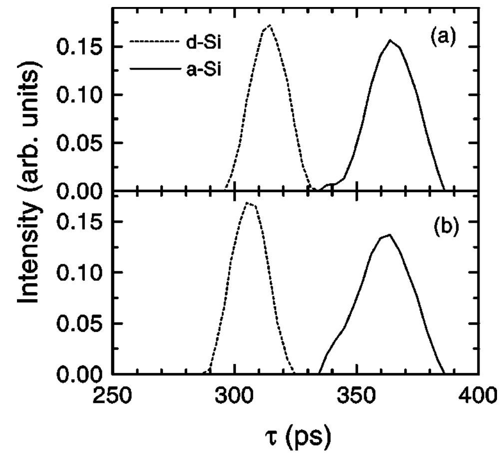

FIG. 3. Positron lifetime distribution in terms of intensity vs lifetime for d-Si and a-Si samples obtained at E_p of (a) 3 keV (depth $\sim$100 nm) and (b) 4 keV (depth$\sim$150 nm).

parameter and the width of $S(E_p)$ curve are larger for a-Si as compared to d-Si. The solid line through the data points is a result of the VEPFIT analysis. For the d-Si, the resolved normalized S parameters are 1.035 ± 0.002 (defected layer) and 1.000 ± 0.002 (undefected layer). With respect to the a-Si sample, the resolved S parameters are 1.070 ± 0.002 and 1.001 ± 0.002 for the defected and undefected layers, respectively. *Ab initio* calculations of Doppler line shape parameter were reported as a function of vacancy clusters size in Si.[24] The reported S parameter values are 1.018 for V_1, 1.045 for V_2, 1.053 for V_3, 1.067 for V_4, and 1.081 for V_5. Experimental S parameters in the range of 1.02 to 1.047, have been reported for divacancies in the literature.[10] Based on the comparison of the present results with calculated and experimental S-parameter values, it can be inferred that divacancies are the dominant defects in the d-Si sample, while bigger vacancy clusters, possibly around a size range of V_4, could be present in the a-Si sample.

So as to obtain a better identification of vacancy-type defects, positron lifetime measurements have been carried out on the same samples. Figure 2 shows the lifetime spectra measured at E_p of 5 keV (depth$\sim$225 nm) corresponding to d-Si and a-Si samples. As seen from the figure, the slope of the lifetime spectrum of a-Si is larger than that of d-Si. The PATFIT program could fit only a single lifetime component to the data and the deduced lifetime values are 318 ± 2 ps and 366 ± 2 ps for d-Si and a-Si, respectively. Positron lifetimes for various vacancy clusters in crystalline Si have been reported using *ab initio* calculations.[24–27] These indicate values in the range of 254–279 ps for monovacancies and 299–309 ps for divacancies. Experimental positron lifetime values in the range of 295–325 ps have been reported for divacancies in Si.[10,11,28] Based on this comparison, the present lifetime values in d-Si suggest that vacancy clusters, mostly divacancies, are present in the sample. The larger lifetime value in a-Si indicates that average vacancy cluster size is larger than that of divacancies. So as to obtain vacancy size distribution in these samples, we present positron lifetime distribution results obtained using the CONTIN program at two depth intervals. Figure 3 shows the deduced positron lifetime distribution in d-Si and a-Si samples, obtained at (a) E_p of 3 keV, corresponding to a depth of $\sim$100 nm, at the peak damaged region and (b) E_p of 4 keV corresponding to a depth of $\sim$150 nm. The lifetime distributions of d-Si and a-Si samples, corresponding to a depth of $\sim$150 nm [Fig. 3(b)], are similar to those of $\sim$100 nm depth, with a marginal shift towards lower values. As can be seen from Fig. 3(a), the d-Si sample exhibits a narrow lifetime distribution in the range of 295–330 ps, with a maximum around 315 ps. The lifetime values of d-Si indicate that the dominant defect species are divacancies. In the case of a-Si sample, the positron lifetime distribution is broader with a maximum around 365 ps and the distribution ranges from 340 to 385 ps. Broader lifetime distribution suggests that vacancy clusters of different sizes are present in the sample.

To convert this experimental lifetime distribution into vacancy cluster size distribution, we need to compare this with the calculated lifetimes for various vacancy clusters in Si. A summary of various *ab initio* lifetime values reported in the literature[24–27] is shown in Table I. All the above calculations were made for crystalline Si and the observed scatter in the computed lifetime for a given vacancy cluster may be attributed due to the specific formalism used and the inclusion or exclusion of lattice relaxation around the defect. At the outset it may be pointed out that in the absence of any lifetime calculations for amorphous Si, we can only resort to comparison of our experimental results with the calculated values for crystalline Si. Due to large scatter in the calculated lifetime values for a given cluster, it will be difficult to make meaningful identification of vacancy clusters by comparing our experimental data with these values. Further, it is known that as vacancy cluster size increases, the local electron density sensed by the positron decreases, giving rise to an increase in the observed lifetime values.[8–10] In view of this, the *ab initio* lifetime values have been fitted in terms of positron

TABLE I. Summary of reported lifetime values (ps) for various vacancy clusters V_n in Si. The lifetime values obtained using empirical relation, Eq. (1) are also shown. The individual lifetime values (Refs. 24–27) are indicated as data points in Fig. 4.

Lifetime (ps)	Bulk	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8
Range of lifetime values reported (Refs. 24–27)	215 to 221	254 to 279	299 to 309	320 to 330	325 to 354	345 to 376	348 to 375		387 to 399
Lifetime values from Eq. (1)	218	266	299	323	342	357	369	379	387

lifetime τ vs number of vacancies N_v in the cluster using the following empirical relation:

$$\tau = C + \frac{A N_v}{(B + N_v)}. \tag{1}$$

The best fit with the lowest χ^2 is chosen and the deduced constants are A (in ps) $=266.57$, $B=4.60$, and C (in ps) $=218$. Figure 4 shows the plot of various calculated lifetime values and the variation of τ as per Eq. (1). As can be seen from Fig. 4, we obtain a smooth variation of lifetime as a function of vacancy cluster size and these values are shown in the last row of Table I. However, so as to deduce the cluster size distribution from the plot shown in Fig. 3, we need to have a band of lifetime values to assign an area corresponding to each vacancy cluster. For this purpose, we have adopted the following criterion. The lower range of lifetime value for a vacancy cluster of size N is set corresponding to the value of $(N-0.5)$, while the higher limit is taken to be that of $(N+0.5)$. By comparing the experimental lifetime distribution curve shown in Fig. 3, with the lifetime values as per the above criterion, the area under the lifetime distribution curve corresponding to each vacancy cluster, has been deduced. This analysis has been carried out for selected depth regions and the data is presented corresponding to sample depth of ~ 150 nm [lifetime spectrum shown in Fig. 3(b)] in Fig. 5, in terms of the relative intensity of clusters versus the number of vacancies in the cluster. For the case of the d-Si sample, the most dominant defects are divacancies and a small concentration of trivacancies are also seen. On the other hand, the cluster size distribution of an a-Si sample ranges from four to seven vacancies. In this distribution, V_5 is found to be the dominant defect species, followed by V_6, V_4, and V_7. Within the uncertainties of the analysis, it can be stated that the cluster size distribution in a-Si is dominated by V_5 and V_6 clusters. This plot establishes that d-Si contains mostly divacancies, while a-Si has a broad size distribution of nanovoids with V_5 and V_6 being the dominant clusters. At deeper depths (beyond ~ 200 nm), it is found that lifetime distribution shifts to lower values indicating that the mean of cluster size distribution is shifting to lower sizes. The reduction in lifetime at deeper depths could possibly

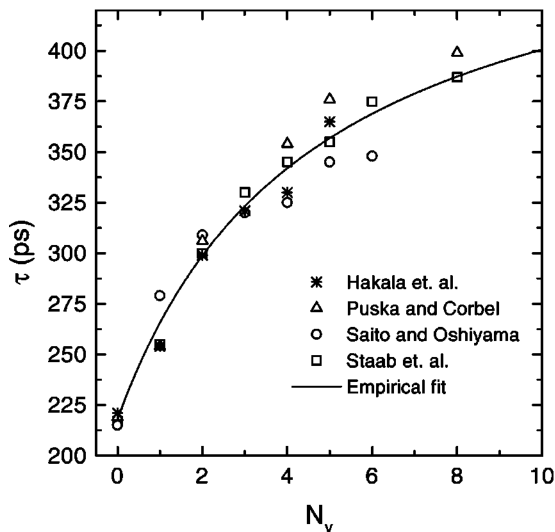

FIG. 4. Variation of positron lifetime τ as a function of number of vacancies N_v in the cluster. Lifetime values reported by various authors are indicated as data points and the solid line is an empirical fit obtained using Eq. (1) for these data.

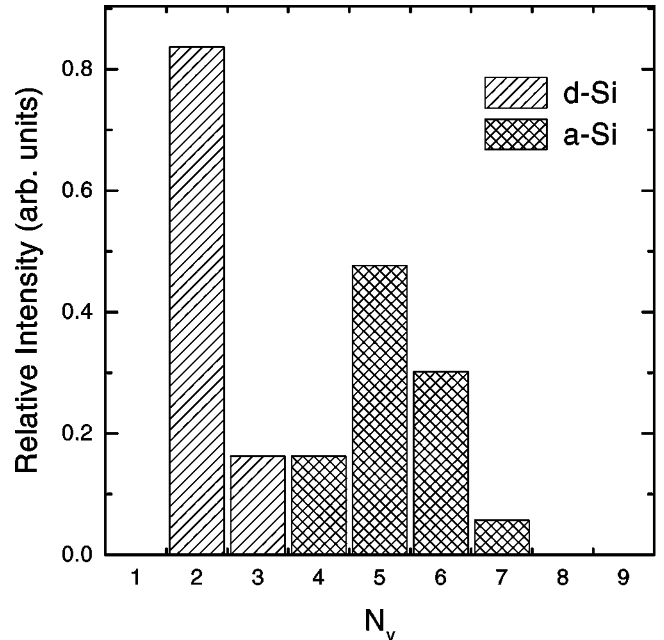

FIG. 5. Vacancy cluster size distribution in terms of relative intensity of clusters vs number of vacancies in the cluster N_v, deduced from experimental lifetime data for d-Si and a-Si samples, corresponding to E_p of 4 keV (depth$\sim$150 nm).

also arise due to Ar decoration of nanovoids. Self-ion irradiation studies on Si may resolve this aspect.

IV. DISCUSSION

Given the fact that positron annihilation studies can only provide information about vacancy defects, our discussion pertains only to the identification of these in d-Si and a-Si. *Ab initio* and molecular-dynamics energy calculations for various vacancy clusters in crystalline Si (Ref. 7) reveal that V_6 (energy gain upon addition of monovacancy, $\Delta E \sim -6.5$ eV) is the most stable defect in crystalline Si followed by V_5 ($\Delta E \sim -5$ eV), V_4 ($\Delta E \sim -4.7$ eV), V_3 ($\Delta E \sim -2$ eV), and V_2 ($\Delta E \sim -2.2$ eV). It is plausible that even though energetically larger clusters are more stable, unless the irradiation-induced defect concentration is large enough to give rise to overlap and agglomeration of small vacancy clusters, these larger clusters may not form. Thus, for the d-Si sample, in which the irradiation dose is less than the amorphization threshold dose, mostly divacancies V_2 with a small concentration of V_3 are found. Previous conventional positron lifetime studies have also indicated a lifetime component in the range of 295–325 ps ascribable due to the presence of divacancies in Si.[10,11,28] There is also corroborative evidence towards the existence of divacancies from other techniques like infrared absorption spectroscopy.[29]

The implications of the present results on a-Si sample are discussed in the light of recent computer-simulation results[30] on ion-beam-induced amorphization in Si. Simulation results indicate that upon amorphization, the atomic coordination varies from 3 to 6, with a mean coordination of four. Further, they indicate the presence of significant concentrations of five-member and three-member atomic rings with a distribution of bond lengths and bond angles. These results, viewed in the framework of CRN of tetrahedrally bonded a-Si, would suggest the existence of either free vacancies or vacancy clusters in the amorphous matrix. Our experimental results on a-Si rule out the existence of monovacancies or divacancies, while there are vacancy clusters with a size distribution ranging from four to seven vacancies per cluster. Further, clusters containing five (V_5) and six (V_6) vacancies are found to be the dominant defect species. Taking the bond lengths for a-Si from these computer-simulation results, we estimate that the size of the V_5 defect (a central Si vacancy together with its four neighbors being vacant) to be ~ 1 nm and similar size for V_6. *Ab initio* and molecular-dynamics energy calculation,[7] as stated earlier, indicate that V_6 is the most stable defect followed by V_5 with a typical size of ~ 1 nm. On the other hand, the present experimental results indicate that V_5 is the most dominant cluster followed by V_6 in a-Si, suggesting that they are energetically stable in amorphous state. From the calculations,[7] the planar ring structure for V_5 and V_6 is found to be more energetically stable than the three-dimensional structure. However, from our present experimental results, it will not be possible to comment on this aspect. A recent simulation study[31] of vibrational and thermodynamic properties of a-Si, shows that the presence of localized low-energy vibrational excitations, produced by nanovoids of different sizes (0.5–1.5 nm) manifests itself as a sharp peak in the observed specific heat at low temperatures. The present results of existence of nanovoids in the amorphous state of Si are in accordance with the above simulation findings. We believe that the identification of cluster size distribution as well as typical size of nanovoids in a-Si, could be useful inputs for evolving more realistic models of the amorphous state of Si.

Finally, we would like to comment on the comparison of the present results on ion-beam-induced a-Si with those reported earlier on a-Si prepared by different methods. A range of S-parameter values reported for glow discharge and thermally evaporated a-Si thin films[13] is an indication that the defect distribution in these different amorphous films is not the same. Conventional positron lifetime measurements[12] reported on sputtered and evaporated a-Si films, indicate lifetime values of 400–500 ps. The authors[12] have attributed these lifetime values to be arising from five vacancy clusters. However, a comparison of those experimental lifetime values[12] with the values shown in Table I would suggest that nanovoids of size bigger than V_{10}, were present in those samples. This may be an indication of the fact that even though techniques like x-ray, electron microscopy, and channeling studies indicate that the a-Si samples prepared by different methods have amorphous structure, the intrinsic vacancy cluster size distribution may be different depending on the method of preparation. Positron beam annihilation studies on various a-Si thin films, employing continuous lifetime analysis, can throw more light on this aspect. The empirically fit positron lifetime vs the vacancy cluster size relation reported here, could be useful for future studies in this direction.

V. SUMMARY

Depth-resolved positron annihilation studies on Ar-irradiated Si have been reported for disordered and amorphous Si samples. The experimental results are compared with the available *ab initio* calculations towards defect identification and the size distribution of vacancy clusters deduced from this comparison. The low dose sample, which is disordered (d-Si) is found to contain mostly divacancies. The high dose sample, which is amorphous (a-Si) is found to contain nanovoids with size ranging from four to seven vacancy clusters. A combination of five and six vacancy clusters is found to be the dominant open-volume defects in the amorphous state of Si. The present experimental results are consistent with the recent computer-simulation results.

ACKNOWLEDGMENTS

One of the authors (G.A.) is grateful to the Science and Technology Agency (STA), Japan for awarding short-term financial support to carry out the lifetime experiments at ETL, Japan. The authors thank Dr. A.K. Arora for various useful discussions.

[*]Email address: amar@igcar.ernet.in

[1] *Amorphous Semiconductors*, edited by M . H. Brodsky (Springer-Verlag, Berlin, 1979); *Current Topics in Amorphous Materials*, edited by Y. Sakurai, Y. Hamakawa, T. Masumoto, K. Shirae, and K. Suzuki (Elsevier Science, Amsterdam, 1993).
[2] R.D. Goldberg, J.S. Williams, and R.G. Elliman, Phys. Rev. Lett. **82**, 771 (1999); T. Motooka, S. Harada, and M. Ishimaru, *ibid.* **78**, 2980 (1997).
[3] S. Takeda and J. Yamasaki, Phys. Rev. Lett. **83**, 320 (1999).
[4] T. Henkel, V. Heera, R. Kogler, W. Skorupa, and M. Seibt, J. Appl. Phys. **82**, 5360 (1997).
[5] P. Schmuki and L.E. Erickson, Phys. Rev. Lett. **85**, 2985 (2000).
[6] D.E. Polk, J. Non-Cryst. Solids **5**, 365 (1971); D.E. Polk and D.S. Boudreaux, Phys. Rev. Lett. **31**, 92 (1973); P. Steinhardt, R. Alben, and D. Weaire, J. Non-Cryst. Solids **15**, 199 (1974).
[7] J.L. Hastings, S.K. Estreicher, and P.A. Fedders, Phys. Rev. B **56**, 10 215 (1997).
[8] *Positron Solid State Physics*, edited by W. Brandt and A. Dupasquier (North-Holland, Amsterdam, 1983).
[9] P.J. Schultz and K.G. Lynn, Rev. Mod. Phys. **60**, 701 (1988).
[10] *Positron Annihilation in Semiconductors*, edited by R. Krause-Rehberg and H. S. Leipner (Springer-Verlag, Berlin, 1998).
[11] P. Asoka-Kumar, K.G. Lynn, and D.O. Welch, J. Appl. Phys. **76**, 4935 (1994).
[12] S. Dannefaer, D. Kerr, and B.G. Hogg, J. Appl. Phys. **54**, 155 (1983).
[13] M.P. Petkov, T. Marek, P. Asoka-Kumar, K.G. Lynn, R.S. Crandall, and A.H. Mahan, Appl. Phys. Lett. **73**, 99 (1998).
[14] J. Xu, E.G. Roth, O.W. Holland, A.P. Mills, Jr., and R. Suzuki, Appl. Phys. Lett. **74**, 997 (1999).
[15] R.S. Brusa, G.P. Karwasz, N. Tiengo, A. Zecca, F. Corni, R. Tonini, and G. Ottaviani, Phys. Rev. B **61**, 10 154 (2000).
[16] G. Amarendra, R. Rajaraman, G. Venugopal Rao, K. G. M. Nair, B. Viswanathan, R. Suzuki, T. Ohdaira, and T. Mikado, in *Proceedings of the 12th International Conference on Positron Annihilation* (ICPA-12), edited by W. Triftshauer, G. Kogel, and P. Sperr (Scitec Publications, Munich, Germany, 2000); Mater. Sci. Forum **363–365**, 129 (2001).
[17] *The Stopping and Range of Ions in Solids*, edited by J. F. Ziegler, J. P. Biersack, and U. Littmark, (Pergamon, New York, 1985).
[18] G. Amarendra, G. Venugopal Rao, A.K. Arora, K.G.M. Nair, T.R. Ravindran, K. Sekar, B. Sundaravel, and B. Viswanathan, J. Phys.: Condens. Matter **11**, 5875 (1999).
[19] G. Amarendra, B. Viswanathan, G. Venugopal Rao, J. Parimala, and B. Purniah, Curr. Sci. **73**, 409 (1997).
[20] A. Van Veen, H. Schut, J. de Vries, R. A. Hakvoort, and M. R. IJpma, in *Slow Positron Beams for Solids and Surfaces*, edited by P. J. Schultz, G. R. Massoumi, and P. J. Simpson (AIP, New York, 1990), p. 171.
[21] R. Suzuki, Y. Kobayashi, T. Mikado, H. Ohgaki, M. Chiwaki, T. Yamazaki, and T. Tomimasu, Jpn. J. Appl. Phys., Part 2 **30**, L532 (1991).
[22] P. Kirkegaard, M. Eldrup, O.E. Mogensen, and N.J. Pedersen, Comput. Phys. Commun. **23**, 307 (1981).
[23] R.B. Gregory, J. Appl. Phys. **70**, 4665 (1991).
[24] M. Hakala, M.J. Puska, and R.M. Nieminen, Phys. Rev. B **57**, 7621 (1998).
[25] M.J. Puska and C. Corbel, Phys. Rev. B **38**, 9874 (1988).
[26] M. Saito and A. Oshiyama, Phys. Rev. B **53**, 7810 (1996).
[27] T.E.M. Staab, M. Haugk, A. Sieck, Th. Frauenheim, and H.S. Leipner, Physica B **273-274**, 501 (1999).
[28] W. Fuhs, U. Holzhauer, S. Mantl, F.W. Richter, and R. Sturm, Phys. Status Solidi B **89**, 69 (1978); P. Mascher, S. Dannefaer, and D. Kerr, Phys. Rev. B **40**, 11 764 (1989); see Chap. 4 in Ref. 10.
[29] A. Kawasuso, M. Hasegawa, M. Suezawa, S. Yamaguchi, and K. Sumino, Mater. Sci. Forum **175-178**, 423 (1995).
[30] K.M. Beardmore and N. Gronbech-Jensen, Phys. Rev. B **60**, 12 610 (1999).
[31] S.M. Nakhmanson and D.A. Drabold, Phys. Rev. B **61**, 5376 (2000).