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Determination of S-parameter for Unimplanted and Ion-implanted 3C-SiC and 6H-SiC Using Diffusion Trapping Model

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Authors' contributions

This work was carried out in collaboration between all authors. Author SBS identified the problem, explained mechanism and concluded the findings. Author MKR solved the diffusion equation, set up rate equations for different trapping sites and calculated the S-parameter for variable positron energy, author VR elucidated results, compared outcome and verified the model. All authors read and approved the final manuscript.

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ABSTRACT

The mechanism of slow positrons has been discussed in terms of diffusion of positrons at the surface of SiC and trapping in to as-grown and irradiation induced defects. The one dimensional diffusion equation has been solved and the rate equations have been set up to describe the various processes supposed to occur when a thermalized positron encounters the SiC surface. The above model has been used to obtain the S-parameter as a function of positron energy in unimplanted and in Al^+, N_2^+ and P^+ implanted 3C-SiC and 6H-SiC. The calculated results have been compared

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with the experimental data. The S-parameter in unimplanted SiC decreases rapidly at low positron energy and becomes nearly constant at high energies suggesting that at low energy the trapping of positrons in shallow defects is important while at high energy the bulk effect dominates. In case of ion-implanted SiC, the S-parameter initially increases up to ≈3 keV and then decreases at higher energies. Thus, at very low positron energy the trapping of positrons into divacancies could be clearly distinguished. The trapping rate into divacancies is found to be proportional to the fluence used to irradiate the sample.

Keywords: Positron annihilation; defects; surfaces; diffusion; silicon carbide.

1. INTRODUCTION

Silicon carbide (SiC) is regarded as a promising material for high-temperature, high-power, high-frequency, and radiation-resistant devices because it has high thermal stability and conductivity. The material has outstanding electronic properties such as an extremely high breakdown field, high electron saturation drift velocity and excellent radiation resistance [1-3]. In order to improve the device performance, it is necessary to characterize thoroughly the starting material with respect to its electrical and optical properties as well as to establish a microscopic understanding of defects. Ion implantation seems to be the only localized doping method for SiC, but this technique introduces radiation damage and easily causes amorphization [4-6]. Ion-implantation at elevated temperatures (hot implantation) is known to reduce damage and enhance the activation of impurities, but it also introduces extended defects such as dislocation loops, which degrade the electrical properties [7,8].

In recent years, positron annihilation spectroscopy (PAS) has assumed great significance to investigate the electronic and defect properties of solids. The technique has been widely applied to investigate the as-grown defects and irradiation-induced defects in SiC. Dannefaer et al. [9] presented positron lifetime and Doppler broadening data on electron-irradiated 6H-SiC which shows that both neutral carbon and silicon vacancies are formed in n-type materials, but in p-type materials no vacancy responses could be found. Polity et al. [10] correlated isochronal annealing investigations in electron-irradiated 6H-SiC with temperature dependent measurements of positron lifetime. It turned out that the positron trapping at temperatures up to 300 K was dominated by trapping in shallow positron traps. These defects were already present in the unirradiated materials and could be attributed to the antisite defects. They concluded that the annealing of the irradiation-induced monovacancies and divacancies took a continuous course up to 1740 K.

Uedono et al. [11] determined the depth distributions and species of defects from measurements of Doppler broadening spectra of annihilation radiation and lifetime spectra of positrons for 6H-SiC implanted with 200 keV P^+ at a dose of 1×10^{15} cm^{-2}. They found vacancy-type defects in the subsurface region (<100 nm) at high concentration even subsequent to an annealing at 1700ºC. Brauer et al. [12] investigated the radiation damage caused by the implantation of 200 keV Ge^+ ions into 6H-SiC by employing the monoenergetic positron beam technique. Specimens exposed to seven ion fluences ranging from 10^{16} to 10^{19} m^{-2}, together with unirradiated samples, were studied. Their positron measurements and the theoretical calculations suggest that the main defect produced due to the irradiation is the divacancy. However, Si monovacancies were also found to be created.

Ling et al. [13] performed positron emission measurements and effect of annealing on positron work function in both n-type and p-type 4H-SiC and 6H-SiC. They concluded that SiC is very attractive material for use in primary moderation and secondary re-moderation, as it has high conversion efficiency and does not require any pre-treatment e.g. 2000ºC annealing as is required for W parameter. Wang et al. [14] investigated defect formation and annealing behavior in as-grown and electron irradiated 6H-SiC slow positron beam. It has been observed that after 10 MeV electron irradiation of the n-type 6H-SiC the positron effective diffusion length decreased from 86.2 nm to 39.1 nm indicating defect creation in n-type SiC. However, in the p-type 6H-SiC irradiated by 10 MeV electrons, the change is very small. This may be because of the opposite charge of the vacancy defects. Pogrebnjak et al. [15] observed average lifetime as function of positron energy and mean implantation depth in n-type Si with and without oxygen layer and in n-type and p-type SiC with an oxygen layer of different thickness. The authors have demonstrated the dependence of the mean positron lifetime in p-type SiC after Al^+ implantation and subsequent annealing on mean implantation depth. Saturated positron lifetime of 218 ps was observed in SiC implanted with Al^+ at positron implantation energies for 2 to ~ 10 KeV. The results of these measurements are very similar to the calculated lifetime values of 216 ps obtained from Ref. [12]. Analogous conclusions were observed in an earlier study done by Triftshauser et al. [16].

The above studies suggest that in case of ion-implanted SiC large experimental data are available in the literature. However, only little theoretical work has been done to understand the mechanism of slow positron annihilation particularly the nature and concentration of defects in unimplanted and ion-implanted SiC. Normally the slow positron data are evaluated by employing the VEPFIT or POSTRAP codes. The VEPFIT programme developed by van Veen et al. [17] is a package for the evaluation of slow positron beam data. A Gaussian curve as an analytic function of the defect profile can be taken as a programme input. Both Gaussian and a step function of the defect concentration may reflect the experimental data approximately. The POSTRAP [18] programme includes defects and the effect of electric field on positron diffusion. It allows arbitrary forms of the positron implantation profile. Aers et al. [19] presented POSTRAP6 is a defect profiling programme used to calculate the fractions trapped in different regions of a sample. Thus, one can calculate the fractions annihilated at the surface in defect less regions or while trapped at defect sites. Often it cannot be decided which function is the better choice to represent the real defect profile. This is due to the broad implantation profile of the positron and the positron diffusion which is itself a function of the defect concentration. The present work is aimed at understanding the diffusion of positrons at the surface of SiC and trapping into as-grown and irradiation induced defects. The rate equations have been set up to describe the various processes supposed to occur when a thermalized positron encounters the SiC surface. We have particularly considered the dependence of the diavacency concentration on the fluence of the Al^+, N_2^+ and P^+ implantation in the above samples. The model has been used to calculate the Doppler broadening line shape parameter (S-parameter) and the results have been compared with the experimental data.

2. FORMULATION OF THE MODEL

Consider the case of slow positrons incident on SiC surface. After losing their kinetic energy, the penetrated positrons may either directly annihilate with surrounding electrons or certain fractions of positrons may diffuse back to the surface and escape into the vacuum. The positrons are known to localise in defects. We have, therefore, considered the trapping of positrons in shallow defects, and divacancies. The motion of positrons at SiC surface is governed by

$$\frac{\partial u(r,t)}{\partial t} = D_+\nabla^2 u(r,t) - \lambda_{eff}\,u(r,t) - \frac{\partial}{\partial r}\left[v_d\,u(r,t)\right] \tag{1}$$

where D_+ is the positron diffusion coefficient and $u(r,t)$ is the positron density as a function of both time and position. λ_{eff} is the effective annihilation rate of positron in a truly diffusion state and v_d is the field dependent drift velocity. We describe the motion of positrons implanted in the semi-infinite medium with a given implantation profile using the one dimensional diffusion equation [20].

$$D_+\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\left[v_d\,u(x,t)\right] - \lambda_{eff}\,u(x,t) = \frac{\partial u(x,t)}{\partial t} \tag{2}$$

The diffusion equation is solved, subject to the boundary conditions:

$$u(0,t) = 0 \qquad \text{(absorbing boundary)} \tag{3}$$

$$u(x,0) = C_0(x) \qquad \text{(implantation profile)} \tag{4}$$

Considering the Gaussian derivative type of implantation profile

$$C_0(x) = \frac{2x}{x_0^2}\exp\left[-\left(\frac{x}{x_0}\right)^2\right] \quad (5)$$

where x_0 and the mean implantation depth *'a'* of the positron as a result of inelastic interactions with SiC molecules could be expressed by the formula:

$$x_0 = \frac{2a}{\sqrt{\pi}} \quad \text{and} \quad a = AE^m \quad (6)$$

E(keV) being the energy of the incident positron. The value of m is taken to be equal to 1.6 as per experimental observations and *A = 400/ρ (Å/keV^m)* [20]. The dispersion of the depth profile increases quickly as the positron energy increases. In other words, the resolution defining the depth decreases quickly as the distance increases from the surface.

The solution of equation (2) so obtained is given by

$$u(x,t) = \sum_n A_n \sin\left(\pm\frac{n\pi x}{a}\right)\exp\left[k_1 x - \left(D_+ p^2 + \lambda_{eff}\right)t\right] \quad (7)$$

where,

$$k_1 = \frac{v_d}{2D_+} \quad , \quad p^2 = \frac{\mathrm{n}^2\pi^2}{a^2} + \frac{v_d}{2D_+} \quad (8)$$

and

$$A_n = \frac{2}{\pi}\int_0^a C_0(x)\sin\left(\pm\frac{n\pi x}{a}\right)\exp-(k_1 x)\,dx \quad (9)$$

The desired rate of positrons reaching the surface

$$N(t) = D_+\frac{\partial u(x,t)}{\partial x}\Big|_{x=0} \quad (10)$$

Thus, we get

$$N(t) = \sum_n B_n \exp(-b_n t) \quad , \quad (11)$$

where

$$B_n = \frac{\mathrm{D}_+\pi^2 n}{a^4}\int_0^a x\sin\left(\pm\frac{n\pi x}{a}\right)\exp-\left(\frac{x^2}{a^2} + k_1 x\right)dx \quad (12)$$

and

$$b_n = \frac{\mathrm{D}_+\pi^2 n^2}{a^2} + \lambda_{eff} \quad (13)$$

When a beam of monoenergetic positrons is implanted from a vacuum to an unirradiated SiC specimen, the four possible locations for the positron before the annihilation are (i) the bulk matrix, (ii) a defect, such as shallow defects (iii) on the surface, or (iv) the vacuum. We have considered the case of both unirradiated and ion irradiated SiC samples. In case of an irradiated sample the positrons will also be trapped in divacancies for higher dose of radiation. The rate equations describing all these processes as encountered by the positrons at the SiC surface are written as follows [21]:

$$\frac{\partial n_b(t)}{\partial t} = -\lambda_b n_b(t) - N(t) \tag{14}$$

$$\frac{\partial n_s(t)}{\partial t} = -\alpha_s n_s(t) + N(t) \tag{15}$$

where escape rate at the surface is

$$\alpha_s = \lambda_s + \alpha_{st} + \alpha_{1v} + \alpha_{2v} \tag{16}$$

$$\frac{\partial n_{st}(t)}{\partial t} = -\alpha_{sd} n_{st}(t) + \alpha_{st} n_s(t) \tag{17}$$

$$\frac{\partial n_{sd}(t)}{\partial t} = -\lambda_{st} n_{sd}(t) + \alpha_{sd} n_{st}(t) \tag{18}$$

$$\frac{\partial n_{2v}(t)}{\partial t} = -\alpha_{v2} n_{2v}(t) + \alpha_{2v} n_s(t) \tag{19}$$

$$\frac{\partial n_{v2}(t)}{\partial t} = -\lambda_{2v} n_{v2}(t) + \alpha_{v2} n_{2v}(t) \tag{20}$$

In the above equations n_b, n_s, n_{st}, n_{2v} represents the fraction of positrons in bulk state, in surface state and trapped into shallow defects and divacancies respectively. n_{sd}, n_{v2} represents the fraction that detrapped from shallow defects and divacancies. α_{ij} are the transition rates from i^{th} state to j^{th} state and λ_j are the annihilation rates in the respective states. Equations (14–20) have been solved using appropriate initial conditions and using equation (11) for *N(t)*.

3. CALCULATION OF S-PARAMETER IN SIC

The relation for the S-parameter in the SiC can be obtained from the following:

$$S = S_b \int_0^\infty \lambda_b n_b(t)dt + S_s \int_0^\infty \lambda_s n_s(t)dt + S_d \int_0^\infty \lambda_d n_d(t)dt \tag{21}$$

where S_b, S_s and S_d represent the value of S-parameter in the bulk, surface and defects states respectively. The third term in the above equation is the contribution to the S-parameter from trapping of positrons into defects states. Let us first consider the case of unirradiated SiC. Here the main defect is shallow traps. Thus, for as-grown SiC we write

$$S_d \int_0^\infty \lambda_d n_d(t)dt = \mathrm{S}_d \int_0^\infty \lambda_{st} n_{sd}(t)dt \tag{22}$$

The above integrals have been evaluated using equations (14-20). Thus, we get the S-parameter for unimplanted SiC

$$S = S_b + \sum_{\mathrm{n}=0}^{\infty} \frac{\mathrm{B_n}}{\mathrm{b_n}} \left(S_s \frac{\lambda_s}{\alpha_s} + S_d \frac{\alpha_{st}}{\alpha_s} - S_b \right) \tag{23}$$

We next consider the case of irradiated SiC. In this case the irradiation induces divacancies also in addition to the shallow traps. Thus, in the case of irradiated SiC, the third term in equation (21) becomes

$$S_d \int_0^\infty \lambda_d n_d(t)dt = \mathrm{S_d}\left[\int_0^\infty \lambda_{1v} n_{v1}(t)dt + \int_0^\infty \lambda_{2v} n_{v2}(t)dt\right] \tag{24}$$

The S-parameter in irradiated SiC becomes

$$S = S_b + \sum_{\mathrm{n}=0}^{\infty} \frac{\mathrm{B_n}}{\mathrm{b_n}}\left[S_s \frac{\lambda_s}{\alpha_s} + S_d\left(\frac{\alpha_{st}}{\alpha_s} + \frac{\alpha_{2v}}{\alpha_s}\right) - S_b\right] \tag{25}$$

The different positron trapping and detrapping rates used in equations (21-25) are evaluated as follow. To obtain the trapping rate α_{st} we understand that such a rate must be proportional to the vacancy concentration available for trapping. Thus,

$$\alpha_{st} = \mu_{st} C_{st} \tag{26}$$

where C_{st} is the shallow defect concentration and μ_{st} is the trapping coefficient [22]. The concentration of divacancies is known to be proportional to the fluence, f [23], the positron trapping rate into divacancies could be written as [20]

$$\alpha_{2v} = \sigma_2 \frac{Z}{2} f \tag{27}$$

where σ_2 is the trapping coefficient, Z is the coordination number of lattice and f is the fluence used to irradiate the specimen. The thermally activated detrapping rate from i^{th} state is given by [24]

$$\alpha_{ji} = \sigma_i T^{3/2} \exp\left[-\left(\frac{E_{bi}}{K_b T}\right)\right] \tag{28}$$

where, E_{bi} is the binding energy of the positrons into the i^{th} state with pre-exponential factor σ_i.

4. MODEL VERIFICATION

Employing the procedure as described above, the Doppler broadening line shape parameter (S-parameter) has been calculated as a function of incident positron energy in unimplanted and ion-implanted 3C-SiC and 6H-SiC. The parameters used in the calculation are listed in Table 1. Most of these have been taken from the experimental results. A few constants have been estimated to give good results.

The calculated results of S-parameter in unimplanted 3C-SiC and 6H-SiC have been plotted in Figs. 1 and 2. In these figures the experimental results taken from Uedono et al. [25,11] are also shown for comparison. The S-parameter in unirradiated SiC decreases with the increase in the incident positron energy. The decrease is fast at low energy and becomes nearly constant at high energies.

Table 1. Values of different parameters used in the calculation of S-parameter along with the references from which they are taken

Parameter	3C-SiC	Ref.	6H-SiC	Ref.
τ_b [ps]	138	[26]	141	[26]
τ_{st} [ps]	142	[10]	144	[10]
τ_{2v} [ps]	254	[12]	266	[11]
S_b	0.4606	[25]	0.4572	[11]
S_s	0.4817	[25]	0.4847	[*]
S_d	0.4936	[*]	0.4967	[*]
ρ [g cm^{-3}]	3.217	[*]	3.217	[12]
L_+ [nm](unimplanted)	253	[*]	253	[11]
L_+ [nm](implanted)	3.5	[*]	3.5	[11]
E_{st} [eV]	0.165	[10]	0.169	[10]
E_{2v} [eV]	3.48	[12]	3.53	[*]
μ_{st} [s^{-1}]	6.69×10^{16}	[*]	6.9×10^{16}	[10]

*Present work

This is due to the fact that at low positron energy, positrons are trapped in near surface defects i.e. the shallow defects. Thus, with increase in positron energy the S-parameter decreases and tends to approach a constant value after ≈20 keV. This suggests that at high energy all positrons are implanted into bulk and annihilate without diffusing back to the surface.

The positron diffusion length L_+ is limited due to the finite lifetime of positrons in defect free bulk, τ_b, is given by $L_+ = \sqrt{\tau_b D_+}$ [20]. In present calculation the L_+ and S-parameter for the annihilation of positrons in the bulk state S_b are taken 253 nm and 0.4572 respectively [11] that is typical for defect free semiconductors (~ 200 nm) [21].

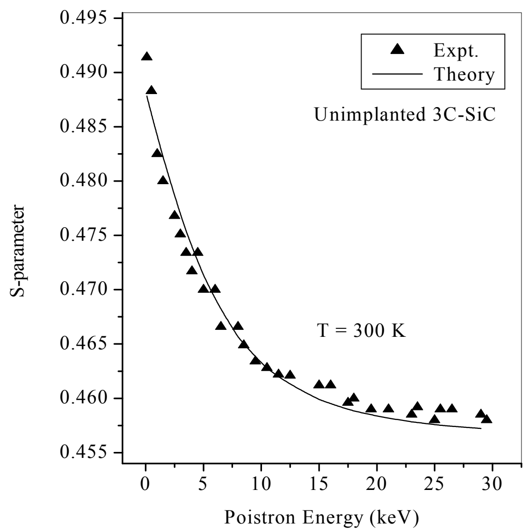

Fig. 1. Comparison of the calculated S-parameter in unimplanted 3C-SiC as a function of incident positron energy with the experimental results of Uedono et al. [25]

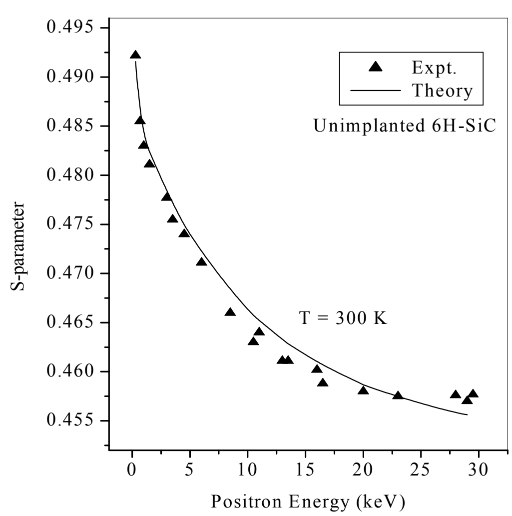

Fig. 2. Comparison of the calculated S-parameter in unimplanted 6H-SiC as a function of incident positron energy with the experimental results of Uedono et al. [11]

Next, we considered the case of Al^+, N_2^+ and P^+ -implantation at a high dose i.e. 1×10^{15} cm^{-2} in 3C-SiC and 6H-SiC. The calculated results of S-parameter as a function of incident positron energy corresponding to different types of ion implantation have been plotted in Figs. 3-5 along with the experimental results of Uedono et al. [25,11]. These figures show that in case of high dose ion implantation, the S-parameter initially increases at low energy i.e. up to E ≈3 keV and then decreases and tends to assume constant at high energy i.e. E > 20 keV. This increase in S-parameter at low positron energy is due to the trapping of positrons into divacancies created by high fluence of ions. The calculation shows that the concentration of divacancies increases in the specimen up to ≈170 nm from the surface due to irradiation by high fluence [25,11]. At higher positron energy i.e. >3 keV, the decrease in S-parameter is due to the trapping of positrons into the shallow defects and after E ≈20 keV, the bulk annihilation dominates.

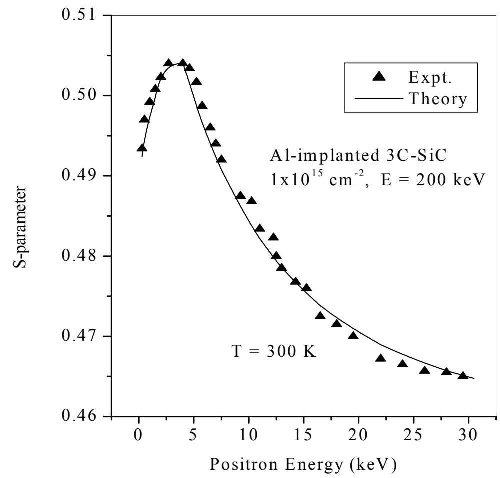

Fig. 3. Comparison of the calculated S-parameter as a function of incident positron energy in 3C-SiC implanted by 200 keV Al^+ ion at a dose of 1×10^{15} cm^{-2} with the experimental results of Uedono et al. [25]

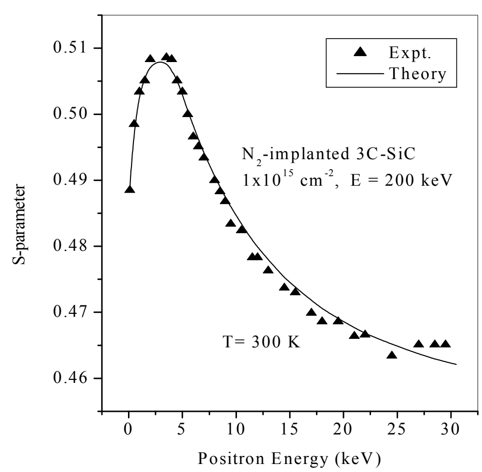

Fig. 4. Comparison of the calculated S-parameter as a function of incident positron energy in 3C-SiC implanted by 200 keV N_2^+ ion at a dose of 1×10^{15} cm^{-2} with the experimental results of Uedono et al. [25]

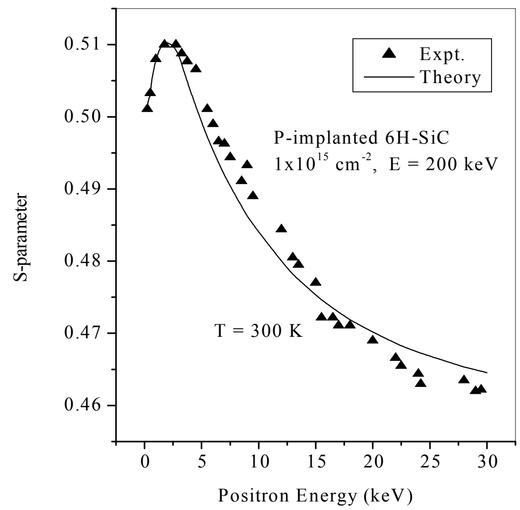

Fig. 5. Comparison of the calculated S-parameter as a function of incident positron energy in 6H-SiC implanted by 200 keV P^+ ion at a dose of $1{\times}10^{15}$ cm^{-2} with the experimental results of Uedono et al. [11]

The positron diffusion length in ion implantation SiC at low positron energies is taken 3.5 nm from experimental observations [11]. In contrast with as-grown SiC the higher value of S-paramenter estimated in ion-implanted SiC and decrease in diffusion length near the surface indicates the trapping of positrons in ion induced defects. The derived value of S-parameter for annihilation of positrons trapped by the near the surface defects induced due to irradiation represented by this model. The binding energy of positrons in shallow defects in as-grown SiC and in divacancies induced due to irradiation is estimated 0.165 eV and 3.48 eV respectively agrees with the observations of Ref. [10,12]. The present calculation also suggests that the trapping rate into divacancies is proportional to the fluence used to irradiate the specimen (equation 27).

5. CONCLUSION

The above calculations of S-parameter in unimplanted and ion-implanted 3C-SiC and 6H-SiC leads to the following conclusions:

(i) The S-parameter in unirradiated SiC decreases with the increase in the incident positron energy. The decrease is fast at low energy and becomes nearly constant at high energies. Thus, at low energy positron trapping in shallow defects is important while at high energy the bulk effect dominates.

(ii) In case of ion-implanted SiC at a dose of $1{\times}10^{15}$ cm^{-2}, the S-parameter initially increases up to ≈3 keV and then starts decreasing. Thus, at very low positron energy (near the surface ≈170 nm) the trapping of positrons into divacancies could be clearly distinguished. The trapping rate into divacancies is found to be proportional to the fluence used to irradiate the sample.

(iii) The present calculation shows that the nature and concentration of near surface defects due to irradiation in SiC could be understood by means of diffusion trapping model.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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