1

## 2    Determination of S-parameter for unimplanted and ion-
## 3    implanted 3C-SiC and 6H-SiC using diffusion trapping model

4    **Abstract**. The mechanism of slow positrons has been discussed in terms of diffusion of
5    positrons at the surface of SiC and trapping in to as-grown and irradiation induced defects. The
6    one dimensional diffusion equation has been solved and the rate equations have been set up to
7    describe the various processes supposed to occur when a thermalized positron encounters the
8    SiC surface. The above model has been used to obtain the S-parameter as a function of positron
9    energy in unimplanted and in $Al^+$, $N_2^+$ and $P^+$ implanted 3C-SiC and 6H-SiC. The calculated
10   results have been compared with the experimental data. The S-parameter in unimplanted SiC
11   decreases rapidly at low positron energy and becomes nearly constant at high energies
12   suggesting that at low energy the trapping of positrons in shallow defects is important while at
13   high energy the bulk effect dominates. In case of ion-implanted SiC, the S-parameter initially
14   increases up to ≈3 keV and then decreases at higher energies. Thus, at very low positron energy
15   the trapping of positrons into divacancies could be clearly distinguished. The trapping rate into
16   divacancies is found to be proportional to the fluence used to irradiate the sample.

### 17    1. Introduction

18   Silicon carbide (SiC) is regarded as a promising material for high-temperature, high-power, high-
19   frequency, and radiation-resistant devices because it has high thermal stability and conductivity. The
20   material has outstanding electronic properties such as an extremely high breakdown field, high
21   electron saturation drift velocity and excellent radiation resistance [1-3]. In order to improve the
22   device performance, it is necessary to characterize thoroughly the starting material with respect to its
23   electrical and optical properties as well as to establish a microscopic understanding of defects. Ion
24   implantation seems to be the only localized doping method for SiC, but this technique introduces
25   radiation damage and easily causes amorphization [4-6]. Ion-implantation at elevated temperatures
26   (hot implantation) is known to reduce damage and enhance the activation of impurities, but it also
27   introduces extended defects such as dislocation loops, which degrade the electrical properties [7,8].
28   In recent years, positron annihilation spectroscopy (PAS) has assumed great significance to
29   investigate the electronic and defect properties of solids. The technique has been widely applied to
30   investigate the as-grown defects and irradiation-induced defects in SiC. Dannefaer et al. [9] presented
31   positron lifetime and Doppler broadening data on electron-irradiated 6H-SiC which shows that both
32   neutral carbon and silicon vacancies are formed in n-type materials, but in p-type materials no vacancy
33   responses could be found. Polity et al. [10] correlated isochronal annealing investigations in electron-
34   irradiated 6H-SiC with temperature dependent measurements of positron lifetime. It turned out that the
35   positron trapping at temperatures up to 300 K was dominated by trapping in shallow positron traps.
36   These defects were already present in the unirradiated materials and could be attributed to the antisite
37   defects. They concluded that the annealing of the irradiation-induced monovacancies and divacancies
38   took a continuous course up to 1740 K.
39   Uedono et al. [11] determined the depth distributions and species of defects from measurements of
40   Doppler broadening spectra of annihilation radiation and lifetime spectra of positrons for 6H-SiC
41   implanted with 200 keV $P^+$ at a dose of $1 \times 10^{15}$ $cm^{-2}$. They found vacancy-type defects in the

42  subsurface region (<100 nm) at high concentration even subsequent to an annealing at 1700 °C. Brauer
43  et al. [12] investigated the radiation damage caused by the implantation of 200 keV Ge$^+$ ions into 6H-
44  SiC by employing the monoenergetic positron beam technique. Specimens exposed to seven ion
45  fluences ranging from $10^{16}$ to $10^{19}$ m$^{-2}$, together with unirradiated samples, were studied. Their
46  positron measurements and the theoretical calculations suggest that the main defect produced due to
47  the irradiation is the divacancy. However, Si monovacancies were also found to be created.

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

65  The above studies suggest that in case of ion-implanted SiC large experimental data are available in
66  the literature. However, only little theoretical work has been done to understand the mechanism of
67  slow positron annihilation particularly the nature and concentration of defects in unimplanted and ion-
68  implanted SiC. Normally the slow positron data are evaluated by employing the VEPFIT or
69  POSTRAP codes. The VEPFIT programme developed by van Veen et al. [17] is a package for the
70  evaluation of slow positron beam data. A Gaussian curve as an analytic function of the defect profile
71  can be taken as a programme input. Both Gaussian and a step function of the defect concentration may
72  reflect the experimental data approximately. The POSTRAP [18] programme includes defects and the
73  effect of electric field on positron diffusion. It allows arbitrary forms of the positron implantation
74  profile. Aers et al. [19] presented POSTRAP6 is a defect profiling programme used to calculate the
75  fractions trapped in different regions of a sample. Thus, one can calculate the fractions annihilated at
76  the surface in defect less regions or while trapped at defect sites. Often it can not be decided which
77  function is the better choice to represent the real defect profile. This is due to the broad implantation
78  profile of the positron and the positron diffusion which is itself a function of the defect concentration.
79  The present work is aimed at understanding the diffusion of positrons at the surface of SiC and
80  trapping into as-grown and irradiation induced defects. The rate equations have been set up to describe
81  the various processes supposed to occur when a thermalized positron encounters the SiC surface. We
82  have particularly considered the dependence of the diavacancy concentration on the fluence of the Al$^+$,
83  N$_2^+$ and P$^+$ implantation in the above samples. The model has been used to calculate the Doppler
84  broadening line shape parameter (S-parameter) and the results have been compared with the
85  experimental data.

## 2. Formulation of the Model

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

92
$$\frac{\partial u(r,t)}{\partial t} = D_+\nabla^2 u(r,t) - \lambda_{eff}u(r,t) - \frac{\partial}{\partial r}[v_d u(r,t)] \qquad (1)$$

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

97
$$D_+\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}[v_d u(x,t)] - \lambda_{eff}u(x,t) = \frac{\partial u(x,t)}{\partial t} \qquad (2)$$

98 The diffusion equation is solved, subject to the boundary conditions:
99 $\quad u(0,t) = 0 \qquad\qquad$ (absorbing boundary) $\qquad\qquad (3)$
100 $\quad u(x,0) = C_0(x) \qquad\qquad$ (implantation profile) $\qquad\qquad (4)$
101 Considering the Gaussian derivative type of implantation profile

102
$$C_0(x) = \frac{2x}{x_0^2}\exp\left[-\left(\frac{x}{x_0}\right)^2\right] \qquad (5)$$

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

105
$$x_0 = \frac{2a}{\sqrt{\pi}} \qquad\text{and}\qquad a = AE^m \qquad (6)$$

106 $E(keV)$ being the energy of the incident positron. The value of m is taken to be equal to 1.6 as per
107 experimental observations and $A = 400/\rho$ ($\mathring{A}/keV^m$) [20]. The dispersion of the depth profile increases
108 quickly as the positron energy increases. In other words, the resolution defining the depth decreases
109 quickly as the distance increases from the surface.
110 $\quad$ The solution of equation (2) so obtained is given by

111
$$u(x,t) = \sum_n A_n \sin\left(\pm\frac{n\pi x}{a}\right)\exp\left[k_1 x - \left(D_+p^2 + \lambda_{eff}\right)t\right] \qquad (7)$$

112 where,

113
$$k_1 = \frac{v_d}{2D_+} \qquad,\qquad p^2 = \frac{n^2\pi^2}{a^2} + \frac{v_d}{2D_+} \qquad (8)$$

114 and

115
$$A_n = \frac{2}{\pi}\int_0^a C_0(x)\sin\left(\pm\frac{n\pi x}{a}\right)\exp-(k_1 x)\,dx \qquad (9)$$

116
117 The desired rate of positrons reaching the surface

118
$$N(t) = D_+\frac{\partial u(x,t)}{\partial x}\Big|x = 0 \qquad (10)$$

119 Thus, we get

120
$$N(t) = \sum_n B_n \exp(-b_n t) \qquad, \qquad (11)$$

121 where

122
$$B_n = \frac{D_+\pi^2 n}{a^4}\int_0^a x\sin\left(\pm\frac{n\pi x}{a}\right)\exp-\left(\frac{x^2}{a^2} + k_1 x\right)dx \qquad (12)$$

123 and

124
$$b_n = \frac{D_+ \pi^2 n^2}{a^2} + \lambda_{eff} \tag{13}$$

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

131
$$\frac{\partial n_b(t)}{\partial t} = -\lambda_b n_b(t) - N(t) \tag{14}$$

132
$$\frac{\partial n_s(t)}{\partial t} = -\alpha_s n_s(t) + N(t) \tag{15}$$

133 where escape rate at the surface is

134
$$\alpha_s = \lambda_s + \alpha_{st} + \alpha_{1v} + \alpha_{2v} \tag{16}$$

135
$$\frac{\partial n_{st}(t)}{\partial t} = -\alpha_{sd} n_{st}(t) + \alpha_{st} n_s(t) \tag{17}$$

136
$$\frac{\partial n_{sd}(t)}{\partial t} = -\lambda_{st} n_{sd}(t) + \alpha_{sd} n_{st}(t) \tag{18}$$

137
$$\frac{\partial n_{2v}(t)}{\partial t} = -\alpha_{v2} n_{2v}(t) + \alpha_{2v} n_s(t) \tag{19}$$

138
$$\frac{\partial n_{v2}(t)}{\partial t} = -\lambda_{2v} n_{v2}(t) + \alpha_{v2} n_{2v}(t) \tag{20}$$

139     In the above equations $n_b$, $n_s$, $n_{st}$, $n_{2v}$ represents the fraction of positrons in bulk state, in surface
140 state and trapped into shallow defects and divacancies respectively. $n_{sd}$, $n_{v2}$ represents the fraction that
141 detrapped from shallow defects and divacancies. $\alpha_{ij}$ are the transition rates from $i^{th}$ state to $j^{th}$ state and
142 $\lambda_j$ are the annihilation rates in the respective states. Equations (14–20) have been solved using
143 appropriate initial conditions and using equation (11) for $N(t)$.

144     **3. Calculation of S-parameter in SiC**
145 The relation for the S-parameter in the SiC can be obtained from the following:

146
$$S = S_b \int_0^\infty \lambda_b n_b(t) dt + S_s \int_0^\infty \lambda_s n_s(t) dt + S_d \int_0^\infty \lambda_d n_d(t) dt \tag{21}$$

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

151
$$S_d \int_0^\infty \lambda_d n_d(t) dt = S_d \int_0^\infty \lambda_{st} n_{sd}(t) dt \tag{22}$$

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

154
$$S = S_b + \sum_{n=0}^\infty \frac{B_n}{b_n} \left( S_s \frac{\lambda_s}{\alpha_s} + S_d \frac{\alpha_{st}}{\alpha_s} - S_b \right) \tag{23}$$

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

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

159 The S-parameter in irradiated SiC becomes

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

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

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

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

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

169 where $\sigma_2$ is the trapping coefficient, Z is the coordination number of lattice and $f$ is the fluence used to
170 irradiate the specimen. The thermally activated detrapping rate from i[th] state is given by [24]

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

172 where, $E_{bi}$ is the binding energy of the positrons into the ith state with pre-exponential factor $\sigma_i$.
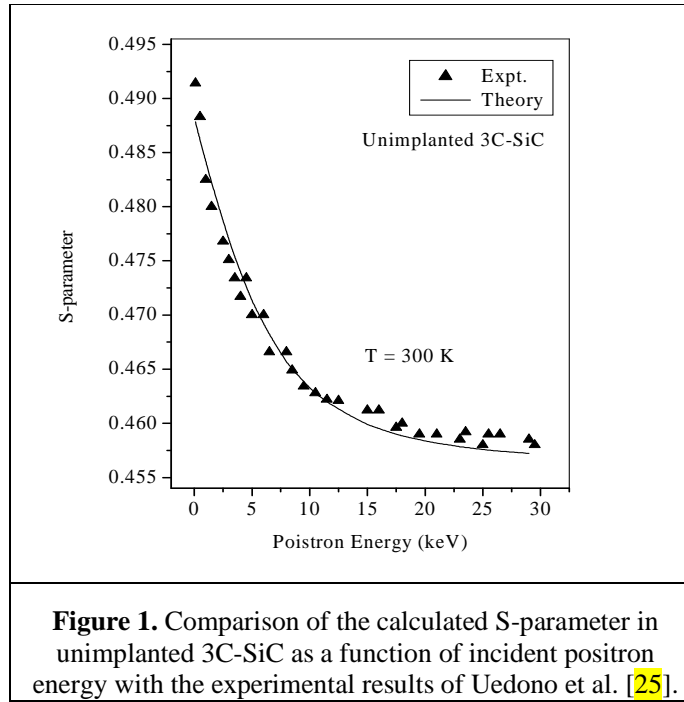
173 **4. Model Verification**
174 Employing the procedure as described above, the Doppler broadening line shape parameter (S-
175 parameter) has been calculated as a function of incident positron energy in unimplanted and ion-
176 implanted 3C-SiC and 6H-SiC. The parameters used in the calculation are listed in Table 1. Most of
177 these have been taken from the experimental results. A few constants have been estimated to give
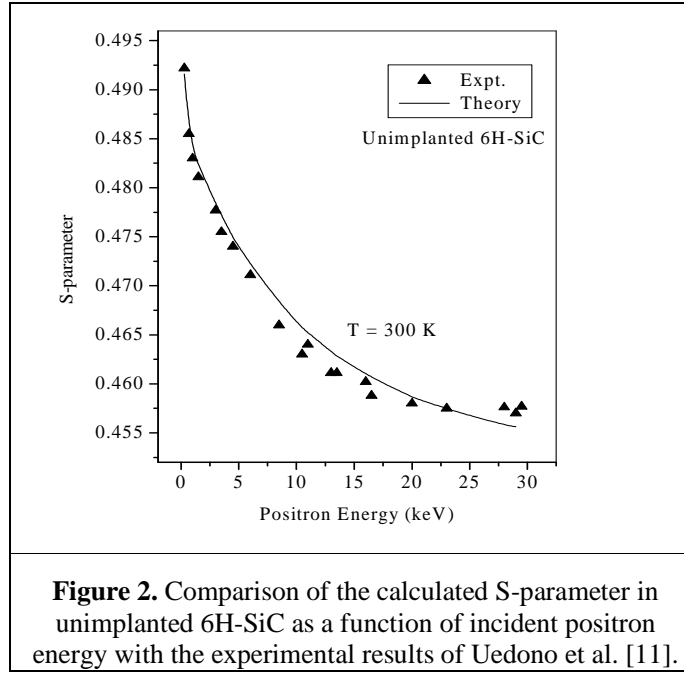178 good results.
179

| 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.** |
| $\tau_b$ [ps] | 138 | [26] | 141 | [26] |
| $\tau_{st}$ [ps] | 142 | [10] | 144 | [10] |
| $\tau_{2v}$ [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 | [*] |
| $\rho$ [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 | [*] |

| $\mu_{st}$ $[s^{-1}]$ | $6.69{\times}10^{16}$ | [*] | $6.9{\times}10^{16}$ | [10] |
|---|---|---|---|---|
| *Present work | | | | |

180
181    The calculated results of S-parameter in unimplanted 3C-SiC and 6H-SiC have been plotted in
182    Figs. 1 and 2. In these figures the experimental results taken from Uedono et al. [25,11] are also shown
183    for comparison. The S-parameter in unirradiated SiC decreases with the increase in the incident
184    positron energy. The decrease is fast at low energy and becomes nearly constant at high energies. This
185    is due to the fact that at low positron energy, positrons are trapped in near surface defects i.e. the
186    shallow defects. Thus, with increase in positron energy the S-parameter decreases and tends to
187    approach a constant value after ≈20 keV. This suggests that at high energy all positrons are implanted
188    into bulk and annihilate without diffusing back to the surface.
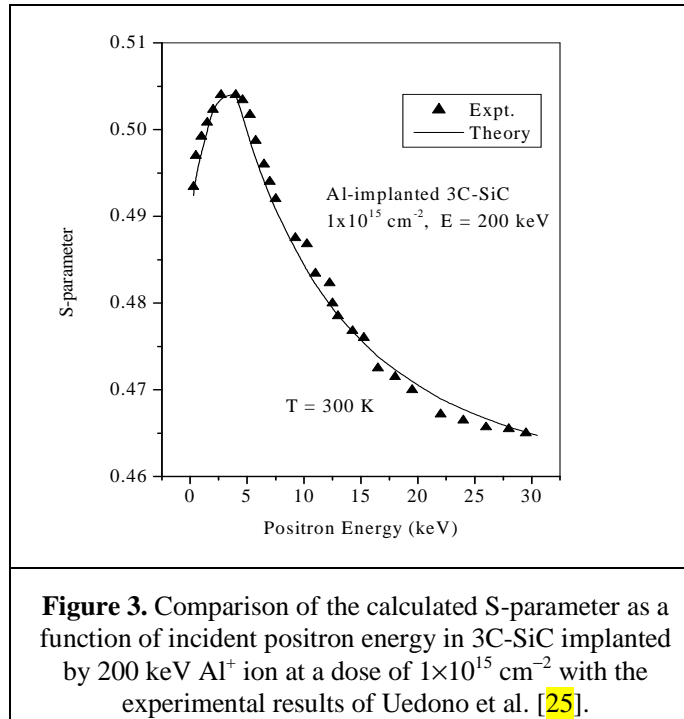189    The positron diffusion length $L_+$ is limited due to the finite lifetime of positrons in defect free bulk,
190    $\tau_b$, is given by $L_+ = \sqrt{\tau_b D_+}$ [20]. In present calculation the $L_+$ and S-parameter for the annihilation of
191    positrons in the bulk state $S_b$ are taken 253 nm and 0.4572 respectively [11] that is typical for defect
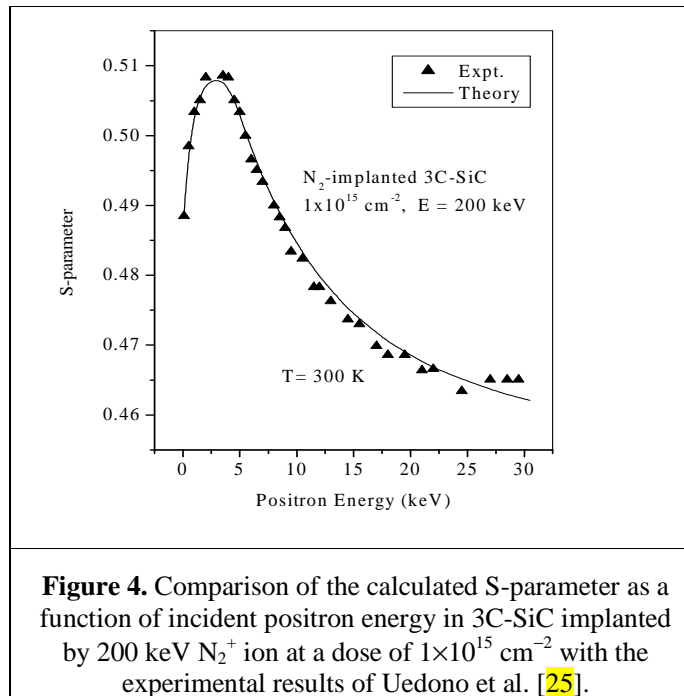192    free semiconductors (~ 200 nm) [21].
193
194



**Figure 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].

195
196

**Figure 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].

197
198
199    Next, we considered the case of Al$^+$, N$_2$$^+$ and P$^+$ -implantation at a high dose i.e. $1\times10^{15}$ cm$^{-2}$ in 3C-
200    SiC and 6H-SiC. The calculated results of S-parameter as a function of incident positron energy
201    corresponding to different types of ion implantation have been plotted in Figs. 3-5 along with the
202    experimental results of Uedono et al. [25,11]. These figures show that in case of high dose ion
203    implantation, the S-parameter initially increases at low energy i.e. up to E $\approx$3 keV and then decreases
204    and tends to assume constant at high energy i.e. E > 20 keV. This increase in S-parameter at low
205    positron energy is due to the trapping of positrons into divacancies created by high fluence of ions.
206    The calculation shows that the concentration of divacancies increases in the specimen up to $\approx$170 nm
207    from the surface due to irradiation by high fluence [25,11]. At higher positron energy i.e. >3 keV, the
208    decrease in S-parameter is due to the trapping of positrons into the shallow defects and after E $\approx$20
209    keV, the bulk annihilation dominates.
210        The positron diffusion length in ion implantation SiC at low positron energies is taken 3.5 nm from
211    experimental observations [11]. In contrast with as-grown SiC the higher value of S-paramenter
212    estimated in ion-implanted SiC and decrease in diffusion length near the surface indicates the trapping
213    of positrons in ion induced defects. The derived value of S-parameter for annihilation of positrons
214    trapped by the near the surface defects induced due to irradiation represented by this model. The
215    binding energy of positrons in shallow defects in as-grown SiC and in divacancies induced due to
216    irradiation is estimated 0.165 eV and 3.48 eV respectively agrees with the observations of Ref.
217    [10,12]. The present calculation also suggests that the trapping rate into divacancies is proportional to
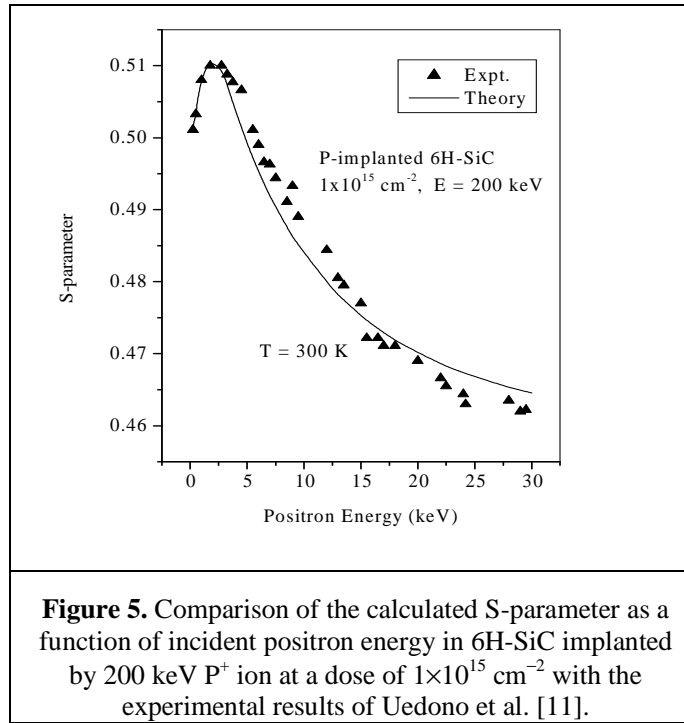218    the fluence used to irradiate the specimen (equation 27).
219

**Figure 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 $1\times10^{15}$ cm$^{-2}$ with the experimental results of Uedono et al. [25].

220
221



**Figure 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 $1\times10^{15}$ cm$^{-2}$ with the experimental results of Uedono et al. [25].

222
223

**Figure 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 $1\times10^{15}$ cm$^{-2}$ with the experimental results of Uedono et al. [11].

224

## 5. Conclusions

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 $1\times10^{15}$ cm$^{-2}$, the S-parameter initially increases up to $\approx 3$ keV and then starts decreasing. Thus, at very low positron energy (near the surface $\approx 170$ 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.

**References**
[1]    Ruff M, Mitlehner H and Helbig R 1994 *IEEE Trans. Electron Devices* **41** 1040.
[2]    Siergiej R R, Sriram S, Clarke R C, Agrawal A K, Brandt C D, Burk A A, Jr., Smith TJ, Morse A and Orphanos PA 1996 *Inst. Phys. Conf. Ser.* **142** 769.
[3]    Ohshima T, Yoshikawa M, Itoh H, Takahashi T, Okumura H, Yoshida S and Nashiyama I 1996 *Inst. Phys. Conf. Ser.* **142** 801.
[4]    Heft A, Wendler E, Heindel J, Bachmann T, Glaser E, Strunk H P and Wesch W 1996 *Nucl. Instrum. Methods Phys. Res. B* **113** 239.
[5]    Troffer T, Schadt M, Frank T, Itoh H, Pensl G, Heindl J,. Strunk H P and Maier M 1997 *Phys. Stat. Sol. A* **162** 277.
[6]    Wendler E, Heft A and Wesch W 1998 *Nucl. Instrum. Methods Phys. Res. B* **141** 105.
[7]    Rao M V, Griffiths P, Gardner J, Holland O W, Ghezzo M, Kretchmer J, Kelner G and Freitas J

250    A, Jr. 1995 *J. Appl. Phys.* **77** 2479.

251 [8] Kimto T, Inoue N and Mastunami H 1997 *Phys. Stat. Sol. A* **162** 263.

252 [9] Dannefaer S, Craigen D and Kerr D 1995 *Phys. Rev. B* **51** 1928.

253 [10] Polity A., Huth S and Lausmann M 1999 *Phys. Rev. B* **59** 10603.

254 [11] Uedono A, Tanigawa S, Ohshima T, Itoh H, Yoshikawa M, Nashiyama I, Frank T, Pensl G

255    Suzuki R, Ohdaira T and Mikado T 2000 *J. Appl. Phys.* **87** 4119.

256 [12] Brauer G, Anwand W, Coleman P G, Knights A P, Plazaola F, Pacaud Y, Skorupa W, Stormer J

257    and Willutzki P 1996 *Phys. Rev. B* **54** 3084.

258 [13] Ling C C, Weng H M, Beling C D and Fung S 2002 *J. Phys.: Condens. Matter* **14** 6373.

259 [14] Wang H Y, Weng H M and Zhou X Y 2008 *Chinese Journal of Chemical Physics* **21** 333.

260 [15] Pogrebnjak A D, Ponomarev A G, Shapak A P and Kunitskii Y A 2012 *Physics – Uspekhi* **55**

261    270.

262 [16] Triftshauser W 1998 *Proc. of the Intern. Workshop on Advanced Techniques of Positron Beam*

263    *Generation and Control,* JAERI, Japan 57.

264 [17] van Veen A, Schut H, de Vries J, Hakvoort R A and Llpma M R 1990 *Positron Beams for*

265    *Solids and Surfaces* ed P J Schultz, G Massoumi and P J Simpson (AIP, New York) p171.

266 [18] Aers G C, Jensen I C O and Walker A B 1993 *Proc. of the 5th Int. Workshop on Slow-Positron*

267    *Beam Techniques for Solids and Surfaces* ed E H Ottewitte (AIP, New York).

268 [19] Aers G C, Marshall P A, Leung T C and Goldberg R D 1995 *Appl. Surf. Sci.* **85** 196.

269 [20] Schultz P J and Lynn K G 1988 *Rev. Mod. Phy*s. **60** 701.

270 [21] Krause-Rehberg R and Leipner H S 1999 *Positron Annihilation in Semiconductors : Defect*

271    *Studies* (Berlin: Springer-Verlag).

272 [22] Kawasuso A, Itoh H, Okada S and Okumura H 1996 *J. Appl. Phys.* **80** 5639.

273 [23] Kawasuso A, Hasegawa M, Suezawa M, Yamaguchi S and Sumino K 1995 *Jpn. J. Appl. Phys.*

274    **34** 2197.

275 [24] West R N 1979 *Positrons in Solids* ed P Hautojarvi (Springer-Verlag, Berlin) p105.

276 [25] Uedono A, Itoh H, Ohshima T, Aoki Y, Yoshikawa M, Nashiyama I, Okumura H, Yoshida S,

277    Moriya T, Kawano T and Tanigawa S 1996 *Jpn. J. Appl. Phys.* **35** 5986.

278 [26] Brauer G, Anwand W, Nicht E M, Kuriplach J, Sob M, Wagner N, Coleman P G, Puska M J

279    and Korhonen T 1996 *Phys. Rev. B* **54** 2512.