# Formation and origin of the dominating electron trap in irradiated *p*-type silicon

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Deep level transient spectroscopy and minority-carrier transient spectroscopy (MCTS) have been applied to study electron-irradiated and proton-irradiated p-type Si samples with boron concentrations in the range of  $6 \times 10^{13} - 2 \times 10^{15}$  cm<sup>-3</sup>. Both impurity-lean epitaxially grown samples and Czochralski grown samples have been investigated where some of the epitaxial samples were subjected to oxygenation prior to the irradiation in order to controllably vary the oxygen concentration. The MCTS measurements reveal a dominant electron trap at  $E_c$ -0.25 eV, where  $E_c$  is the conduction-band edge, commonly ascribed to a boron-interstitial oxygen-interstitial complex ( $B_iO_i$ ). The amplitude of the level increases linearly with the irradiation dose and it anneals out at ~175 °C but shows, however, no correlation with the boron concentration. The level is dominant even at doping concentrations in the  $10^{13}$  cm<sup>-3</sup> range and, irrespective of the oxygen concentration, the generation rate decreases by almost 50% as the boron concentration increases by a factor of ~30. Comparison with numerical modeling reveals that these results are not consistent with the commonly accepted model of defect reactions in irradiated p-type Si. Different reasons for this discrepancy are discussed, such as an incomplete defect reaction model and alternative identifications of the  $E_c$ -0.25 eV level.

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#### I. INTRODUCTION

Electrically active point defects in silicon have been studied for several decades due to their fundamental importance and potential detrimental or beneficial effect on semiconductor devices. It is generally accepted that in irradiated p-type Si, the dominant hole traps are associated with the carboninterstitial carbon-substitutional pair (CiCs), a defect originally identified by photoluminescence (PL) and electronparamagnetic-resonance (EPR) studies, 1,2 the divacancy (V<sub>2</sub>), a defect originally identified by EPR,<sup>3</sup> the carbon interstitial (C<sub>i</sub>), initially identified by infrared-absorption spectroscopy studies,<sup>4</sup> and the carbon-interstitial oxygeninterstitial (C<sub>i</sub>O<sub>i</sub>) complex,<sup>5</sup> originally identified by optical and electrical techniques.<sup>6</sup> Further, the most prominent electron traps in p-type Si have been ascribed to  $C_i$ ,  $C_iC_s$ , and the boron-interstitial oxygen-interstitial pair  $(B_iO_i)$ . Specifically, the often dominating electron trap at  $E_c$  – 0.25 eV, where  $E_c$  denotes the conduction-band edge, has been attributed to B<sub>i</sub>O<sub>i</sub> primarily because of an increase in intensity with increasing boron concentration and the abundance of O<sub>i</sub>.<sup>6-8</sup> At sufficiently high boron concentrations, the intensity of the level decreases, which was attributed to the competing formation of the  $B_iB_s$  pair.<sup>8</sup> In recent theoretical work by Jones and co-workers, 9,10 and Sanati and Estreicher, 11 two forms of B<sub>i</sub>O<sub>i</sub> are predicted, indicating a more complex behavior of B-O clustering reactions than previously expected. However, the key arguments for an identification of the  $E_c$ -0.25 eV level as  $B_iO_i$  are the boron and oxygen dependen-

In the current work, we employ deep level transient spectroscopy (DLTS) and minority-carrier transient spectroscopy (MCTS) to address the boron dependence of the  $E_c$  –0.25 eV level in electron-irradiated and proton-irradiated p-type samples with a relative variation in the boron concen-

tration by a factor of 30. The samples used were mainly  $n^+pp^+$  structures, accomplished by epitaxial growth and ion implantation, in order to ensure saturation of the MCTS peak intensities, which are known to be sensitive to the injection level of minority carriers. Indeed, in layers with high doping concentration, the injection is limited by the barrier height of the pn junction while in layers with low doping concentration, the injection can be limited by the series resistance. <sup>12</sup> In this respect,  $n^+pp^+$  diodes with a thickness of the lightly doped layer, significantly smaller than the diffusion length of the minority carriers, such as in our structures, are ideal for measurements requiring a high and uniform injection level.

# II. EXPERIMENT DETAILS

Mesa structured  $n^+pp^+$  diodes were fabricated using  $pp^+$ wafers where the p layer ( $\sim$ 20  $\mu$ m in thickness) was grown by chemical vapor deposition with a uniform boron doping concentration in the range of  $6 \times 10^{13} - 2 \times 10^{15}$  cm<sup>-3</sup>, as deduced by capacitance-versus-voltage (CV) measurements. The  $p^+$  substrate was Czochralski (Cz) grown with a boron concentration of  $\sim 5 \times 10^{18}$  cm<sup>-3</sup>. The highly doped  $n^+$  region was realized by a 36 keV  $P^+$  ion implantation to a dose of  $2 \times 10^{14}$  cm<sup>-2</sup> and subsequent activation annealing at 1050 °C for 10 min. For comparison, also  $n^+p$  diodes were fabricated using p-type Cz grown wafers with a boron doping concentration of  $1.5 \times 10^{15}$  cm<sup>-3</sup>. For some selected epitaxial samples having  $2 \times 10^{15}$  B/cm<sup>3</sup>, an oxygenation process<sup>13,14</sup> involving a dry oxidation for 8 h at 1100 °C followed by a heat treatment for 24 h at 1100 °C in N atmosphere, was carried out prior to the  $n^+$ -layer formation. The SiO<sub>2</sub> layer formed during the oxidation was subsequently removed by wet etching and CV measurements revealed a uniform carrier concentration identical within less than 20% compared to that in the nonoxygenated samples. Hence, additional B doping by diffusion from the substrate is negligible as well as formation of electrically active centers by the in-diffused oxygen atoms. The latter result is consistent with that reported by other authors employing a similar oxygenation process<sup>13</sup> and suggests that the vast majority of the incorporated oxygen atoms occupy interstitial sites  $(O_i)$ , as confirmed by infrared-absorption measurements.<sup>15</sup>

The oxygen and carbon chemical concentrations in the samples were measured by secondary-ion mass spectrometry (SIMS). The oxygen concentration in the Cz material was found to be about  $1\times 10^{18}~{\rm cm}^{-3}$  while in the as-grown epitaxial layers, it increases from  $\sim 1\times 10^{16}~{\rm cm}^{-3}$  in the surface region to  $1\times 10^{17}~{\rm cm}^{-3}$  near the substrate. In the oxygenated epitaxial samples, a uniform oxygen concentration of  $4\times 10^{17}~{\rm cm}^{-3}$  was observed through the whole thickness of the epitaxial layer. The carbon concentration in the Cz material was below the detection limit of  $\sim 5\times 10^{16}~{\rm cm}^{-3}$ . This holds also for the epitaxial material, consistent with previous SIMS measurements by other authors, giving  $[C]\!\lesssim\!8\times 10^{15}~{\rm cm}^{-3}$  for the same kind of epitaxial samples  $^{16}$  (brackets denote concentration values). No variation of [O] (and [C]) with the boron concentration in the samples was found.

Ohmic contacts to front and backside surfaces were formed by applying InGa and Ag pastes, respectively. For the Cz material, a 36 keV backside boron implantation was also carried out to improve the Ohmic contact.

The samples were irradiated at room temperature (RT) by 1.8 MeV protons having a penetration depth of  $\sim$ 40  $\mu$ m, which is about twice (or more) the thickness of the epilayer. The doses used were between  $2 \times 10^{10}$  and  $4 \times 10^{12}$  cm<sup>-2</sup>. In order to extract accurate values for the defect generation rates, each kind of sample was irradiated by three different doses. The probing depth in the DLTS measurements varies from 2.5 to 15  $\mu$ m, depending on the dopant concentration, and the vacancy generation rate differs by 25% in this depth interval, as estimated by TRIM (Ref. 17) for 1.8 MeV protons. In addition, the epitaxial samples with low and high B concentrations were irradiated with 6 MeV electrons, using doses of  $6 \times 10^{13}$  and  $2 \times 10^{15}$  e<sup>-</sup>/cm<sup>2</sup>, respectively. After the RT irradiation, which lasted no more than 1 h, all the samples were stored at -20 °C until the initial DLTS/MCTS measurements were carried out followed by RT storage. Storage at -20 °C is sufficient to suppress, on the time scale of a few weeks, reactions involving migration of C<sub>i</sub>. 18

The DLTS/MCTS measurements were performed using a refined version of a setup described in detail elsewhere. Both majority (DLTS) and minority (MCTS) carrier spectra were recorded. The minority-carrier injection was carried out by applying a forward bias of 3 V during the filling pulse while the capacitance transients were acquired at a reverse bias of -10 V for both the majority and minority-carrier measurements. In addition, capture cross-section measurements were undertaken by varying the duration of the filling pulse. The forward bias of 3 V was well above the threshold sufficient for saturation of the MCTS signal of the  $E_c$ -0.25 eV level, as illustrated by the inset of Fig. 1. The concentration of injected minority carriers was estimated by TCAD simulations using the commercially available SYNOP-SYS software. As illustrated in Fig. 1, for a forward bias of

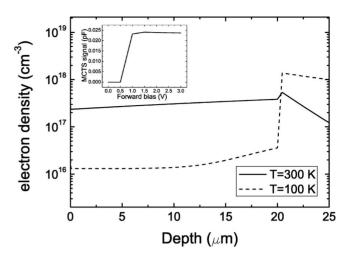


FIG. 1. Simulations of the steady-state electron density during the filling pulse in the MCTS measurements using a boron concentration of  $2 \times 10^{15}~\rm cm^{-3}$  and a forward bias of 3 V. The inset shows the measured MCTS intensity of the  $E_c$ -0.25 eV level versus forward bias pulse, illustrating the saturation of the MCTS signal.

3 V, the concentration of injected electrons in the epitaxial samples is calculated to be  $2 \times 10^{17}$  and  $1 \times 10^{16}$  cm<sup>-3</sup> at RT and 100 K, respectively, while that in the bulk Cz samples is  $2 \times 10^{16}$  and  $2 \times 10^{15}$  cm<sup>-3</sup>, respectively. Including a defect level at  $E_c$ -0.25 eV with electron and hole capture cross sections of  $2 \times 10^{-13}$  and  $1 \times 10^{-20}$  cm<sup>2</sup>, for respectively, and a concentration of 10% of the doping concentration, the simulations yield a complete occupancy of the level during 3 V forward biasing at both 100 and 300 K, irrespective of the sample used. Thus, the simulations support the assumption of complete filling of E1 during MCTS and agree with the experimentally observed saturation of the amplitude of the  $E_c$  – 0.25 eV level during MCTS. In addition, simulations of the MCTS spectra show that the influence of hole trapping by the  $V_2$  level at  $E_v + 0.20$  eV on the  $E_c - 0.25$  eV level is negligible for the experimental conditions used  $(E_n)$  denotes the valence-band edge). Thus, the concentration of the  $E_c$  -0.25 eV level can be deduced by the MCTS peak amplitude. The concentrations of the hole traps are found by the peak amplitudes in the DLTS spectra.

# III. RESULTS AND DISCUSSION

Figure 2 shows signatures of the hole traps detected by DLTS at  $E_v+0.19$  eV (H1),<sup>3</sup>  $E_v+0.30$  eV (H2)<sup>4</sup> and  $E_v+0.36$  eV (H3),<sup>5</sup> attributed in accordance with literature to  $V_2(+/0)$ ,  $C_i$ , and  $C_iO_i$ , respectively. In addition, a hole trap occurs at  $E_v+0.42$  eV (H4). The material used in Fig. 2 is the most lightly doped one,  $\sim 6 \times 10^{13}$  B/cm<sup>3</sup>, and H4 is barely present in the medium doped material and not detectable in the highly doped one, indicating that the trap is related to an impurity with low concentration such as hydrogen<sup>21,22</sup> or copper.<sup>23</sup> The H2 level, attributed to  $C_i$ , was observed during the first DLTS and MCTS scans after irradiation and -20 °C storage but then disappeared after a few days at RT in a 1:1 proportionality with the rise of the H3 level assigned to  $C_iO_i$ .

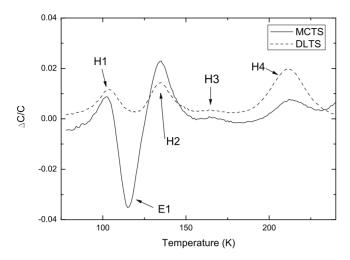


FIG. 2. Examples of normalized DLTS (dashed) and MCTS (solid) signals,  $\Delta c/c$ , taken from the proton-irradiated p-type epitaxial silicon samples having a doping concentration of  $6 \times 10^{13}$  B/cm<sup>3</sup>. The rate window used is  $(640 \text{ ms})^{-1}$ .

Further, the electron trap at  $E_c$  –0.25 eV (E1 in Fig. 2), commonly assigned to  $B_iO_i$ , dominates the MCTS spectrum. The negative charge states of the divacancy  $V_2(=/-)$  and  $V_2(-/0)$ , and the vacancy-oxygen (VO) pair are not observed due to their large hole capture cross section, promoting recombination rather than reemission of trapped electrons. <sup>24</sup> Overall, E1 is the dominating peak in Fig. 2, having a three times higher amplitude than that of  $V_2(+/0)$ . Isochronal annealing shows that E1 anneals out at ~175 °C (data not included), supporting that the E1 level is of the same origin as the  $E_c$  –0.25 eV level studied in Refs. 6–8.

Figure 3(a) reveals a linear dose dependence of the E1 intensities in the epitaxial samples. However, the generation rate, i.e., the slope of the E1 intensity versus dose, decreases with [B<sub>s</sub>]. The corresponding concentration values of E1 are given in Table I. Although the average self-interstitial and vacancy generation rates within the measurement region decrease by  $\sim 25\%$  from the low to the high doped sample, as estimated by TRIM calculations, <sup>17</sup> this difference is not sufficient to account for the observed dependence of the generation rate on [B<sub>s</sub>]. In Fig. 3(b), which summarizes the boron concentration dependence of the generation rate for the defects observed in the epitaxial and Cz samples, the production of E1 is shown to decrease by almost 50% when [B<sub>s</sub>] increases from  $6 \times 10^{13}$  to  $2 \times 10^{15}$  cm<sup>-3</sup> in the epitaxial samples. A similar trend, with a relative decrease by about 30%, is also found for the electron-irradiated samples (open symbols) where a highly uniform defect generation is expected. Figure 3(b) reveals also that (i) the generation rate of V<sub>2</sub> drops by 25% and hence stays constant with respect to the rate of vacancy generation, as estimated by the TRIM simulations, and (ii) the production of C<sub>i</sub> decreases strongly with increasing [B<sub>s</sub>] because of the competition between C<sub>s</sub> and B<sub>s</sub> for capturing Si self-interstitials.<sup>25</sup> Furthermore, in the Cz samples, the generation rate of E1 is significantly reduced while [C<sub>i</sub>] has increased due to a higher carbon content in this material. In fact, the generation rate of E1 in the low doped epitaxial samples ( $[B_s] \approx 6 \times 10^{13}$  cm<sup>-3</sup>) is more

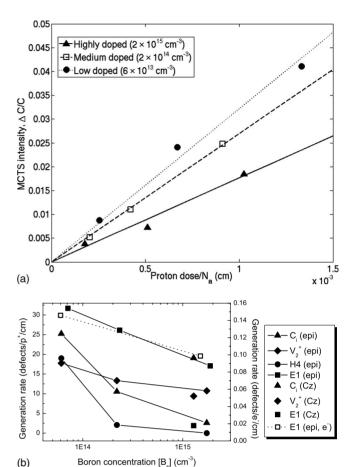


FIG. 3. (a) The dose dependence of the E1 signal as measured in the epitaxially grown samples. (b) Generation rate of the dominating point defects as a function of doping concentration for epitaxial (symbols+lines), and Cz (symbols) samples as measured after irradiation and storage at  $-20~^{\circ}$ C. In addition, open symbols connected by a dashed line refer to the right ordinate and represent the results measured for the E1 level in electron-irradiated epitaxial material.

than one order of magnitude higher than that in the Cz material ( $[B_s] \approx 1.5 \times 10^{15}$  cm<sup>-3</sup>). This is in contrast to previous reports using bulk material showing no detection of E1 in lightly boron-doped samples.<sup>6–8</sup>

These different results imply that the formation of E1 hinges closely on the purity of the samples used. E1 is com-

TABLE I. Absolute concentration values of E1 in the different epi-materials used.

| Proton dose<br>(cm <sup>-2</sup> )     | Lightly doped (cm <sup>-3</sup> ) | Medium doped (cm <sup>-3</sup> ) | Highly doped (cm <sup>-3</sup> )           |
|--|-----------------------------------|----------------------------------|--|
| $2 \times 10^{10}$                     | $6.8 \times 10^{11}$              |                                  |  |
| $5 \times 10^{10}$                     | $1.8 \times 10^{12}$              | $1.3 \times 10^{12}$             |  |
| $1 \times 10^{11}$                     | $3.1 \times 10^{12}$              | $2.6 \times 10^{12}$             |  |
| $2 \times 10^{11}$                     |                                   | $5.4 \times 10^{12}$             | T 4 × 4 0 1 2                              |
| $3.5 \times 10^{11}$                   |                                   |                                  | $7.4 \times 10^{12}$                       |
| $1 \times 10^{12} \\ 2 \times 10^{12}$ |                                   |                                  | $1.4 \times 10^{13} \\ 3.2 \times 10^{13}$ |

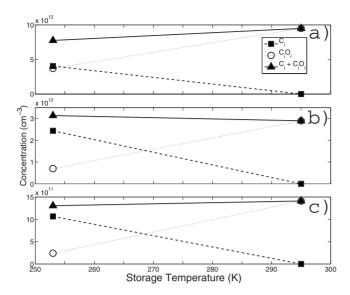


FIG. 4. Concentrations of  $C_i$  and  $C_iO_i$  (dotted lines), and their sum (solid line) measured after the -20 °C and RT storages for the highest irradiated dose in (a)  $2\times10^{15}$ , (b)  $2\times10^{14}$ , and (c)  $6\times10^{13}$  B cm<sup>-3</sup> epitaxial samples. The time elapsed from the start of the irradiations at RT to the -20 °C storage was less than 1 h.

monly assigned to  $B_iO_i$  (Refs. 6–8) and the formation is primarily controlled by the following reactions:

$$I + B_s \rightarrow B_i$$
, (1)

$$I + C_s \rightarrow C_i$$
, (2)

$$B_i + O_i \rightarrow B_i O_i,$$
 (3)

and

$$B_i + B_s \rightarrow B_i B_s$$
. (4)

In reaction (1), a Si self-interstitial (I) generated by the irradiation kicks out a B<sub>s</sub> and the resulting B<sub>i</sub> migrates until it encounters an O<sub>i</sub>, forming the stable B<sub>i</sub>O<sub>i</sub> center [reaction (3)].  $C_s$  is a main competitor to  $B_s$  for trapping of the migrating I's [reaction (2)] and the pronounced decrease in the generation rate of  $C_i$  when  $[B_s]$  increases from  $6 \times 10^{13}$  to  $2\times10^{15}$  cm<sup>-3</sup> [Fig. 3(b)], indicates that [C<sub>s</sub>] is only  $\sim 10^{14}$  cm<sup>-3</sup> in the epitaxial layers, assuming similar capture radii of I by  $B_s$  ( $R_I(B_s)$ ) and  $C_s$  ( $R_I(C_s)$ ). According to the SIMS results, the oxygen content exceeds 10<sup>16</sup> cm<sup>-3</sup> in all the samples used, which suggests that  $[O_i] \gg [B_s]$  and exhaustion of [O<sub>i</sub>] will not limit the formation of B<sub>i</sub>O<sub>i</sub> centers. However, at sufficiently high values of [B<sub>s</sub>] relative to that of  $[O_i]$ , the competing reaction (4) becomes important and enhances the generation of the B<sub>i</sub>B<sub>s</sub> pair on the expense of  $B_iO_i$ .

The  $C_i$  atoms generated by reaction (2) are known to be mobile at RT,<sup>18</sup> although slower than  $B_i$ , and can form stable centers with both  $O_i$  and  $C_s$ :

$$C_i + O_i \rightarrow C_i O_i$$
 (5)

and

$$C_i + C_s \rightarrow C_i C_s.$$
 (6)

As discussed above, it is anticipated that  $[O_i] \gg [C_s]$  in the epitaxial samples and reaction (5) will dominate. Indeed, this is supported by the results in Fig. 4, showing, within the experimental accuracy, a 1:1 correlation between the loss of  $[C_i]$  and the growth of  $[C_iO_i]$  in all the samples.

A similar set of reactions as (1)–(6) has been considered in Ref. 28. In order to elucidate if these reactions can account for the experimentally determined generation rates of E1 and  $C_iO_i$  as a function of  $[B_s]$  (Figs. 3 and 4), modeling has been performed. Applying the theory for diffusion-limited reactions, <sup>29,30</sup> the coupled differential rate equations derived from Eqs. (1)-(6) are given in Table II together with the input values used in the calculations. The differential equations are numerically solved simultaneously from time t=0, when the irradiation starts, until the defects have completed their reactions, which occurs long after the irradiation to a given fluence has finished. The ion flux used is  $2 \times 10^{10}$  H<sup>+</sup>/cm<sup>2</sup> s, which is comparable with the experimental conditions. To comply with the concentration of I-related defects observed experimentally, a net generation rate of self-interstitials of  $\sim$ 75 I/(H<sup>+</sup> cm) is deduced from the lightly doped samples. A comparison with the total generation rate of I's, as estimated by TRIM calculations 17 assuming a displacement energy threshold of 15 eV, yields that only a fraction of  $\sim 1.5\% - 2\%$  of the I's survive spontaneous (correlated) recombination with V's. Similar small fractions of surviving V's have previously been reported in low-dose ion-implanted *n*-type samples monitoring vacancy-type defects.31

The evolution in concentration of each stable defect center has been followed as a function of ion fluence in the range  $10^{11}$ – $10^{12}$  H<sup>+</sup>/cm<sup>2</sup>, and in this dilute regime, all the centers exhibit a linear dependence. From the slope of the defect concentration versus fluence, the generation rate per ion and unit length is extracted, and Fig. 5 shows a comparison between the simulated and experimental values for the different epitaxial samples studied. A close agreement is revealed for  $C_iO_i$  supporting the validity of reactions (1), (2), (5), and (6); here, it should be emphasized that the values used for  $R_I(C_s)$  and  $[C_s]_{t=0}$  are not unique but their product should remain constant relative to  $R_I(B_s)[B_s]_{t=0}$  for a given value of  $[B_s]_{t=0}$ . Also  $B_iO_i$  and E1 display good agreement at low boron concentrations ( $[B_s] \le 2 \times 10^{14} \text{ cm}^{-3}$ ) using a ratio between the capture radii  $R_{B_i}(O_i)$  and  $R_{B_i}(B_s)$  of  $\sim 0.018$ , i.e., this indicates that reaction (3) involves an energy barrier that exceeds the migration energy of  $B_i$  by  $\sim 0.1-0.2$  eV if  $R_{\rm B}$  (B<sub>s</sub>) is given by geometrical dimensions or, alternatively,  $R_{\rm B}({\rm O}_i)$  is given by the geometry while reaction (4) is enhanced because of attractive forces between B<sub>i</sub> and B<sub>s</sub>. However, for the highly doped epitaxial samples  $([B_s] \approx 2 \times 10^{15} \text{ cm}^{-3})$ , the calculated value of B<sub>i</sub>O<sub>i</sub> underestimates E1 by a factor of three and the generation of B,B, dominates strongly according to the simulations. Thus, the model exhibits a limited validity and does not fully account for the experimental data of E1. This conclusion is even more clearly illustrated by the results for the oxygenated epitaxial samples where the oxygen concentration is increased by more than one order of magnitude up to  $\sim 4 \times 10^{17}$  cm<sup>-3</sup>. As shown in Fig. 6, the generation rate of

TABLE II. Survey of the simultaneous differential rate equations for the reactions in Eqs. (1)–(6) and numerical values of the input parameters used in the computations.

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\frac{d[I]}{dt} = g_I - 4\pi D_I[I] \{ R_I(B_s)[B_s] + R_I(C_s)[C_s] \}
\frac{d[B_i]}{dt} = 4\pi D_I[I]R_I(B_s)[B_s] - 4\pi D_{B_i}[B_i]\{R_{B_i}(O_i)[O_i] + R_{B_i}(B_s)[B_s]\}
\frac{d[\mathbf{B}_i \mathbf{O}_i]}{dt} = 4\pi D_{\mathbf{B}_i} [\mathbf{B}_i] R_{\mathbf{B}_i} (\mathbf{O}_i) [\mathbf{O}_i]
\frac{d[B_i B_s]}{dt} = 4\pi D_{B_i} [B_i] R_{B_i} (B_s) [B_s]
\frac{d[B_s]}{dt} = -4\pi D_I[I]R_I(B_s)[B_s] - 4\pi [B_i]D_{B_i}R_{B_i}(B_s)[B_s]
\frac{d[C_i]}{dt} = 4\pi D_I[I]R_I(C_s)[C_s] - 4\pi D_{C_i}[C_i]\{R_{C_i}(O_i)[O_i] + R_{C_i}(C_s)[C_s]\}
\frac{d[\mathbf{C}_i \mathbf{O}_i]}{dt} = 4\pi D_{\mathbf{C}_i} [\mathbf{C}_i] R_{\mathbf{C}_i} (\mathbf{O}_i) [\mathbf{O}_i]
\frac{d[\mathbf{C}_i \mathbf{C}_s]}{dt} = 4\pi D_{\mathbf{C}_i} [\mathbf{C}_i] R_{\mathbf{C}_i} (\mathbf{C}_s) [\mathbf{C}_s]
\frac{d[C_s]}{dt} = -4\pi D_{I}[I]R_{I}(C_s)[C_s]
\frac{d[O_i]}{dI_{A_i}} = -4\pi D_{B_i}[B_i]R_{B_i}(O_i)[O_i] - 4\pi D_{C_i}[C_i]R_{C_i}(O_i)[O_i]
                                              g_1 = 1.5 \times 10^{12} cm<sup>-3</sup> s<sup>-1</sup> deduced from the experimental data with an ion flux of 2 \times 10^{10} H<sup>+</sup>/cm<sup>2</sup> s
Generation rate:
                                              D_{\rm I} = 1 \times 10^{-9} \, {\rm cm}^2/{\rm s} (rapid, see e.g. Ref. 26)
Diffusion constants:
                                              D_{\rm B} = 1 \times 10^{-12} \, {\rm cm}^2/{\rm s} (taken from Ref. 27)
(300 \text{ K})
                                              D_{\rm C} = 1 \times 10^{-15} \, {\rm cm}^2/{\rm s} (taken from Ref. 18)
                                              R_{\rm I}({\rm B}_s) = R_{\rm B}({\rm B}_s) = R_{\rm C}({\rm O}_i) = R_{\rm C}({\rm C}_i) = 5 Å (geometrical dimension)
Capture radii:
                                              R_{\rm I}(C_s) = 2.2 Å, R_{\rm B}({\rm O}_i) = 0.09 Å (fitted values)
                                              [C_s] = 1 \times 10^{14} \text{ cm}^{-3}, [O_i] = 1 \times 10^{16} \text{ cm}^{-3} (4 \times 10^{17} \text{ cm}^{-3} \text{ after oxygenation})
Initial values (t=0):
                                              [B_s] = 5 \times 10^{13} - 5 \times 10^{15} \text{ cm}^{-3}
                                              [I] = [B_i] = [B_iO_i] = [B_iB_s] = [C_i] = [C_iO_i] = [C_iC_s] = 0
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E1 after oxygenation remains essentially identical with that in the nonoxygenated samples while the simulations predict an increase of  $B_iO_i$  by a factor of  $\sim 10$ ,  $\sim 3$ , and  $\sim 1.3$  in the highly, moderately, and lightly doped samples, respectively (Fig. 5). Here, it should also be pointed out that no deep level, such as the  $E_v + 0.30$  eV level observed in highly boron-doped bulk samples<sup>6,7</sup> and tentatively associated with the  $B_iB_s$  pair, has been found to disappear or emerge on the expense of E1 in the epitaxial samples.

At least two possible reasons for the discrepancy between the commonly accepted model of defect reactions in irradiated p-type material, described by Eqs. (1)–(6), and the present experimental results for E1 can be put forward. First, E1 is correctly assigned to  $B_iO_i$  but the model of defect reactions is incomplete. The lack of oxygen dependence indicates that  $[O_i] \sim 10^{16}$  cm<sup>-3</sup> is sufficient to saturate the generation rate of E1 in the epitaxial samples but, on the other hand, a competing trap, which is boron-related and has a formation process with a stronger boron dependence than that of  $B_iO_i$ , must exist to account for the decrease in E1 with increasing  $[B_s]$ . The  $B_iB_s$  pair is one such candidate but it exhibits a too strong dependence when  $[B_s]$  is varied by a factor of 30, as shown in Fig. 5, and is not sufficient as the

only competitor. No evidence for any additional boronrelated and electrically active defect has been found in our measurements but a defect that is electrically inactive or escapes detection during the measurement conditions used cannot be excluded. Here, it may also be speculated that Fermilevel effects influence the net generation rate of surviving I's (and V's) although this appears to be inconsistent with the close agreement between the measured and simulated data for  $C_iO_i$  in Fig. 5, as well as the essentially constant generation rate of V<sub>2</sub> versus [B<sub>s</sub>] when accounting for the depth variations in elastic energy deposition. Second, a reidentification of E1 is discussed. The fact that E1 is not observed in n-type material suggest that it is either boron-related or its formation process is Fermi-level dependent. However, E1 is found in *n*-type samples counter doped with  $B_{i}^{32,33}$  indicating involvement of B and that the formation of E1 is not Fermi-level dependent. If  $B_i$  combines with an element, X, to form E1, the following considerations can be made: according to the DLTS spectrum of the sample irradiated with the highest dose [Fig. 3(a)], [E1], and thus [BX], is found to be  $\sim 3 \times 10^{13}$  cm<sup>-3</sup>. Hence, [X] must be larger than 3  $\times 10^{13}$  cm<sup>-3</sup>, assuming that [X] is the same in all the epitaxial samples. This implies that [X] is similar to or larger than

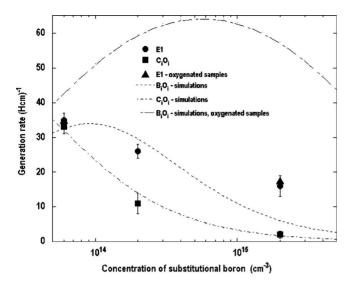


FIG. 5. Comparison between experimental values of the generation rate of  $C_iO_i$  and E1, and simulated ones for  $C_iO_i$  and  $B_iO_i$  as a function of  $[B_s]$  in the epitaxial samples. The model used is described in the text and the numerical values for the input parameters are given in Table II. Results are also included for oxygenated epitaxial samples. Error bars indicate the experimental accuracy.

 $[B_s]$  in the low doped material ( $\sim 6 \times 10^{13}$  cm<sup>-3</sup>). Possible candidates may then be boron-carbon related and boron-hydrogen related centers. Here, it should be clearly pointed out that such an assignment of E1 does not exclude the existence of  $B_iO_i$ ; there is ample evidence for  $B_iO_i$  and recent theoretical predictions for local vibrational modes of the  $B_iO_i$  pair have been confirmed by experimental data. Hence, in irradiated and oxygen-rich p-type samples,  $B_iO_i$  is, indeed, anticipated to play a major role, which favors an identification of E1 as  $B_iO_i$ . However, a reaction barrier  $B_i$  and  $O_i$  can suppress the absolute generation rate and other impurities/traps with concentrations substantially less than  $[O_i]$  may become important.

### IV. CONCLUSIONS

In conclusion, the generation rate of the dominant electron trap E1 ( $E_c$ -0.25 eV) in irradiated p-type silicon is

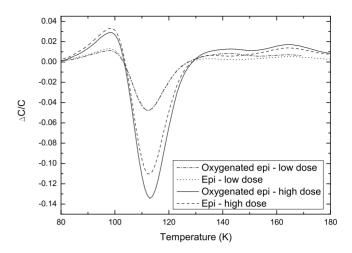


FIG. 6. MCTS spectra of oxygenated and nonoxygenated epitaxial samples ( $[B_s] \simeq 2 \times 10^{15} \text{ cm}^{-3}$ ) irradiated by protons with low ( $2 \times 10^{12} \text{ cm}^{-2}$ ) and high ( $4 \times 10^{12} \text{ cm}^{-2}$ ) doses.

found to decrease by ~50% when the boron concentration increases by a factor of ~30 from  $6\times10^{13}$  to  $2\times10^{15}$  cm<sup>-3</sup> in carbon-lean epitaxial layers. Comparison with numerical modeling shows that these results are not consistent with the commonly accepted model of defect reactions in p-type Si and this conclusion is further substantiated by the fact that oxygenation of the epitaxial layers does not influence the generation rate of E1. Hence, further studies of the defect reactions taking place in irradiated p-type Si need to be pursued, including  $in \ situ$  DLTS studies of the  $B_i$  transition to E1 in samples with controlled carbon concentrations.

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<sup>&</sup>lt;sup>1</sup>L. W. Song, X. D. Zhan, B. W. Benson, and G. D. Watkins, Phys. Rev. B **42**, 5765 (1990).

<sup>&</sup>lt;sup>2</sup>L. W. Song, X. D. Zhan, B. W. Benson, and G. D. Watkins, Phys. Rev. Lett. **60**, 460 (1988).

<sup>&</sup>lt;sup>3</sup>J. W. Corbett and G. D. Watkins, Phys. Rev. Lett. 7, 314 (1961).

<sup>&</sup>lt;sup>4</sup>A. R. Bean and R. C. Newman, Solid State Commun. **8**, 175 (1970).

<sup>&</sup>lt;sup>5</sup>L. J. Cheng and P. Vadja, J. Appl. Phys. **40**, 4679 (1969).

<sup>&</sup>lt;sup>6</sup>P. M. Mooney, L. J. Cheng, M. Süli, J. D. Gerson, and J. W. Corbett, Phys. Rev. B **15**, 3836 (1977).

 <sup>&</sup>lt;sup>7</sup>P. J. Drevinsky, C. E. Caefer, S. P. Tobin, J. C. Mikkelsen, and L. C. Kimerling, Mater. Res. Soc. Symp. Proc. **104**, 167 (1988).

<sup>&</sup>lt;sup>8</sup>L. C. Kimerling, M. T. Asom, J. L. Benton, P. J. Drevinsky, and C. E. Caefer, Mater. Sci. Forum 38-41, 141 (1989).

<sup>&</sup>lt;sup>9</sup>J. Adey, R. Jones, and P. R. Briddon, Appl. Phys. Lett. **83**, 665 (2003).

<sup>&</sup>lt;sup>10</sup> A. Carvalho, R. Jones, M. Sanati, S. K. Estreicher, J. Coutinho, and P. R. Briddon, Phys. Rev. B 73, 245210 (2006).

<sup>&</sup>lt;sup>11</sup>M. Sanati and S. K. Estreicher, Phys. Rev. B **72**, 165206 (2005).

<sup>&</sup>lt;sup>12</sup>S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley, New York, 1981), Chap. 2.4.3.

<sup>&</sup>lt;sup>13</sup>L. Fonseca, M. Lozano, F. Campabadal, C. Martinez, M. Ullán, B. S. Avset, A. Ruzin, F. Lemeilleur, and E. Nossarzewska-Orlowska, Microelectron. Reliab. 40, 791 (2000).

- <sup>14</sup>G. Casse, CERN Technical Report No. ROSE/TN/99-1, 1999 (unpublished).
- <sup>15</sup>M. Moll, E. Fretwurst, M. Kuhnke, and G. Lindström, CERN/ LEB Technical Report No. 99-8, 1999 (unpublished); ROSE/ RD48 Meeting, June 1999 (unpublished), pp. 51–80.
- <sup>16</sup>I. Pintilie, M. Buda, E. Fretwurst, G. Lindström, and J. Stahl, Nucl. Instrum. Methods Phys. Res. A 556, 197 (2006).
- <sup>17</sup>J. F. Ziegler, J. P. Biersack, and U. Littmark, *The Stopping and Range of Ions in Solids* (Pergamon, New York, 1985).
- <sup>18</sup> A. K. Tipping and R. C. Newman, Semicond. Sci. Technol. 2, 315 (1987).
- <sup>19</sup>B. G. Svensson, K.-H. Rydén, and B. M. S. Lewerentz, J. Appl. Phys. **66**, 1699 (1989).
- <sup>20</sup> Synopsys Inc., 700 East Middlefield Road, Mountain View, California 94043, USA; see also http://www.synopsys.com/
- <sup>21</sup>O. Feklisova, N. Yarykin, E. B. Yakimov, and J. Weber, Physica B (Amsterdam) 308-310, 210 (2001).
- <sup>22</sup>S. Fatima, C. Jagadish, J. Lalita, B. G. Svensson, and A. Hállen, J. Appl. Phys. **85**, 2562 (1999).
- <sup>23</sup> S. D. Brotherton, J. R. Ayres, A. Gill, H. W. van Kesteren, and F. J. A. M. Greidanus, J. Appl. Phys. **62**, 1826 (1987).

- <sup>24</sup> A. Hallén, N. Keskitalo, F. Masszi, and V. Nágl, J. Appl. Phys. 79, 3906 (1996).
- <sup>25</sup>R. D. Harris, J. L. Newton, and G. D. Watkins, Phys. Rev. B 36, 1094 (1987).
- <sup>26</sup>G. S. Oehrlein, I. Krafczik, J. L. Lindström, A. E. Jaworowski, and J. W. Corbett, J. Appl. Phys. **54**, 179 (1983).
- <sup>27</sup> A. K. Tipping and R. C. Newman, Semicond. Sci. Technol. 2, 389 (1987).
- <sup>28</sup>S. Zhao, A. M. Agarwal, J. L. Benton, G. H. Gilmer, and L. C. Kimerling, Mater. Res. Soc. Symp. Proc. 442, 231 (1997).
- <sup>29</sup>T. R. Waite, Phys. Rev. **107**, 463 (1957).
- <sup>30</sup>T. R. Waite, J. Chem. Phys. **28**, 103 (1958).
- <sup>31</sup>B. G. Svensson, C. Jagadish, A. Hallén, and J. Lalita, Phys. Rev. B 55, 10498 (1997).
- <sup>32</sup>J. R. Troxell and G. D. Watkins, Phys. Rev. B **22**, 921 (1980).
- <sup>33</sup> V. P. Markevich (private communication).
- <sup>34</sup> A. Carvalho, R. Jones, J. Coutinho, and P. R. Briddon, J. Phys.: Condens. Matter 17, L155 (2005).
- <sup>35</sup>L. I. Murin, V. P. Markevich, J. L. Lindström, and B. G. Svensson (unpublished).