The di-interstitial in silicon: Electronic properties and interactions with oxygen and carbon impurity atoms

Vasilii E. Gusakov[**,1], **Stanislau B. Lastovskii**[1], **Leonid I. Murin**[1], **Ekaterina A. Tolkacheva**[1], **Lyudmila I. Khirunenko**[2], **Mikhail G. Sosnin**[2], **Andrei V. Duvanskii**[2], **Vladimir P. Markevich**[*,3], **Matthew P. Halsall**[3], **Anthony R. Peaker**[3], **Ilia Kolevatov**[4], **Hussein M. Ayedh**[4], **Edouard V. Monakhov**[4], and **Bengt G. Svensson**[4]

[1] Scientific-Practical Materials Research Center of NAS of Belarus, 220072 Minsk, Belarus
[2] Institute of Physics of the NAS of Ukraine, 03028 Kiev, Ukraine
[3] Photon Science Institute and School of Electrical and Electronic Engineering, University of Manchester, Manchester M13 9PL, UK
[4] Department of Physics, Centre for Materials Science and Nanotechnology, Oslo University, 0318 Oslo, Norway

* Corresponding author: e-mail v.markevich@manchester.ac.uk, Phone: +441613064746
** e-mail gusakov@ifttp.bas-net.by, Phone: +375 17 284 12 90, Fax: +375 17 284 15 58

New experimental and theoretical results on the silicon di-interstitial (I_2) and its interactions with oxygen and carbon impurity atoms in Si crystals are reported. Electronic structure calculations indicate that I_2 has an acceptor and a donor level in the gap, which are close to the conduction and the valence band edges, respectively. Experimental results, which support the theoretically predicted high mobility of I_2, are discussed. It is argued that mobile I_2 can be trapped by oxygen and carbon impurities. The I_2O center has a donor level at $E_v + 0.09$ eV. Two absorption bands at 936 and 929 cm^{-1} are assigned to the local vibrational modes of the I_2O defect in the neutral and positively charged states, respectively. The binding energy of I_2O relative to the separated I_2 and O_i species is 0.22 eV. The disappearance of the I_2O complex upon thermal annealing occurs in the temperature range 50–100 °C and is accompanied by the introduction of another defect, which gives rise to two hole emission signals from energy levels at $E_v + 0.54$ and $E_v + 0.45$ eV. It is argued that these levels are related to a complex consisting of interstitial carbon and interstitial silicon atoms (C_iI). The stable configurations of the C_iI pair have been found.

© 2017 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction Self-interstitial complexes in silicon are of great importance in Si-based implanted devices as they are responsible for the diffusion enhancement and numerous defect reactions [1–3]. However, the available solid experimental data on the structure and properties of self-interstitial clusters (I_n) are very limited. The silicon di-interstitial (I_2) is the first step in the sequence of the I_n complexes. A number of theoretical studies, both *ab initio* and molecular dynamics, have been dedicated to I_2 [4–10]. It seems to be widely recognized that I_2 is a fast diffusing species, although the values of the migration energy obtained from the theoretical studies scatter widely from 0.3 up to 0.9 eV. Despite the substantial efforts, there is still some controversy with respect to the exact atomic structure of I_2 and its diffusion path (see, e.g., Refs. [6, 9] and references therein). Experimental observations of I_2 are also inconclusive. Lee et al. [11] assigned the Si-P6 signal in electron spin resonance (ESR) spectra to a positive charge state of I_2, where the two Is are located adjacent to a substitutional Si atom along the 100 axis. Some 20 years later, Lee [12] put forward a revised model where the two Is lie in the {100} plane at a position considerably off from two tetrahedral interstitial sites nearby, sharing one Si lattice atom. However, based on the results from *ab initio* density functional theory (DFT) calculations, Eberlein et al. [6] concluded that the models proposed in Refs. [11, 12] are metastable and have a magnetic field tensor at variance with that of the Si-P6 ESR signal. Londos et al. [13] have recently

assigned an absorption band at $533\,cm^{-1}$, which they have observed in the infrared absorption spectra of the neutron-irradiated Si, to a local vibrational mode due to the I_2 defect. It should be mentioned, however, that the assignment is tentative. Further, the defect, which gives rise to the $533\,cm^{-1}$ line, anneals out in the temperature range 170–200 °C [13], and this result is not consistent with the predicted high mobility of I_2.

The diffusing I_2 species are believed to interact with the interstitial oxygen (O_i) atoms and form I_2O_i complexes. Hermansson et al. [14] have argued that I_2O_i gives rise to an absorption band at $936\,cm^{-1}$. Further arguments for the assignment of the $936\,cm^{-1}$ band to the I_2O complex have been obtained from the analysis of infrared absorption spectra of Si:O crystals irradiated with high-energy protons [15]. It was found that the line at $936\,cm^{-1}$ dominated the absorption spectra of proton-irradiated Si:O crystals together with the line at $836\,cm^{-1}$ due to a vacancy-oxygen complex. This finding indicated that the I_2O defect is one of the dominant point defects in heavily irradiated oxygen-rich Si crystals. We have recently argued that the I_2O defect possesses a donor level at $E_v +0.09\,eV$ and from DFT calculations found a configuration with the electronic and dynamical properties being very close to those determined experimentally [16]. The configuration consists of the compact I_2 with a divalent O_i atom attached. The I_2O defect is not very stable and anneals out in the temperature range 50–100 °C. The value of activation energy for the I_2O thermal elimination has been found to be $1.05 \pm 0.05\,eV$ [16].

The substitutional carbon (C_s) and boron (B_s) atoms are known to be effective traps for silicon self-interstitials [17]. It can be anticipated that these impurities interact also with I_2. However, until recently neither experimental nor theoretical modeling results on such interactions and possible resulting defects have been published. It has been argued in a recent paper [18] that a radiation-induced defect, which gives rise to two DLTS signals related to hole emission from energy levels at $E_v +0.54\,eV$ and $E_v +0.45$ eV, could be associated with a complex resulting from interactions of mobile I_2s with either C_s or B_s atoms.

In the present work, we report new experimental and theoretical results on the silicon di-interstitial (I_2) and its interactions with oxygen and carbon impurity atoms in Si.

2 Experimental Experimental results have been obtained by means of Fourier-transform infrared absorption (FT-IR) spectroscopy, deep level transient spectroscopy (DLTS), and high-resolution Laplace DLTS [19]. For the DLTS measurements, a number of n^+-p and Schottky barrier diodes were prepared from p-type boron doped Si crystals, which were grown by either Czochralski (Cz), float zone, or epi techniques. So, the diodes studied have different concentrations of boron, oxygen, and carbon impurities. Some details of the diode processing can be found in Ref. [16]. Most of the diodes were irradiated with either 4–6 MeV electrons or α particles from a ^{239}Pu source at about 280 K. Thermal anneals of the irradiated samples were carried out either in a cryostat in vacuum or in a furnace in a dry N_2 ambient. It has been found that some of the interstitial-related radiation-induced defects are sensitive to injection of minority carriers. For studies of the minority-carrier injection effects we have applied forward voltage to the irradiated n^+-p diodes.

For the FT-IR measurements, the samples were cut from two Cz grown Si crystals of p- and n-type conductivity ($\rho = 0.5$ and $5\,\Omega \cdot cm$, respectively). The concentrations of O_i and C_s atoms in the crystals were determined from measurements of the intensity of the absorption bands at 1107 and $605\,cm^{-1}$ with the use of the calibration coefficients of 3.14×10^{17} and $0.94 \times 10^{17}\,cm^{-2}$, respectively. The concentrations of O_i and C_s atoms were 9.4×10^{17} and $2 \times 10^{16}\,cm^{-3}$, and 9.9×10^{17} and $7.4 \times 10^{16}\,cm^{-3}$ in n- and p-type crystals, respectively.

Irradiations with 5 MeV electrons were performed at 80 K with doses in the range $(4–5) \times 10^{17}\,cm^{-2}$. Some of the irradiated samples were subjected to 20-min isochronal annealing in the temperature range 100–400 K.

IR absorption analysis was carried out using a Bruker IFS 113v spectrometer. A spectral resolution of 0.5 or $1.0\,cm^{-1}$ was used and the samples were measured at about 10 K and at room temperature (RT).

3 Theoretical modeling details Calculations of defect configurations were carried out in the framework of density functional theory using the Quantum-ESPRESSO package along with the local spin density approximation for the exchange correlation potential [20]. Pseudopotentials were chosen in the form Si.pz-vbc.UPF and O.pz-rrkjus. UPF. The Brillouin zone was sampled with $n \times n \times n$ k-points, where $n = 3$. The plane-wave kinetic energy cut-off for valence electron wave functions was 20 Ry and the energy cut-off for the charge density was 80 Ry. The total energy was minimized until the forces acting on the atoms did not exceed $1.4 \times 10^{-4}\,eV \cdot \mathring{A}^{-1}$.

Calculations of the electronic properties of the defects were performed in the framework of the recently proposed method of calculation of the band gaps and the deep energy levels in semiconductors [21]. The advantages of this method are: it gives the calculated band gap values almost equal to the experimental values, can be used for calculations of localized states (deep energy levels of defects), and does not require the use of the so-called defects markers.

4 Results and discussion
4.1 The Si di-interstitial Figure 1a) shows the most stable configuration of the I_2 defect found in our work. The structure was obtained by minimizing the total energy of the supercell with (216 + 2) Si atoms as a function of coordinates of all atoms in the supercell. The structure shown in Fig. 1a) is similar to that reported in an earlier *ab initio* modeling study [4] but with some small differences regarding atom positions and bond lengths. It has been
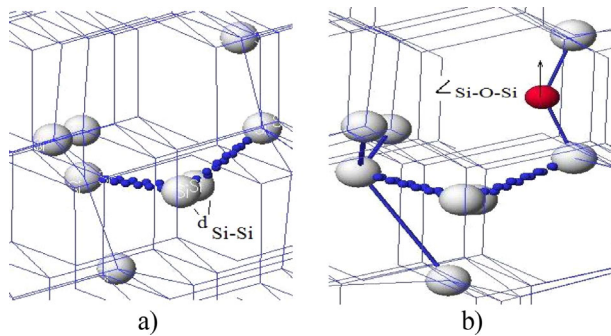
Figure 1 The most stable configurations of a) the I_2 and b) the I_2O defects. The oxygen atom is depicted in red color. $d_{Si-Si}(I_2) = 2.26$ Å; $d_{Si-Si}(I_2O) = 2.345$ Å, $\angle$Si–O–Si $= 137°$.

found from the electronic structure calculations that the I_2 defect introduces acceptor ($-/0$) and donor ($0/+$) levels into the band gap with an energy spacing between them of $E_g^{(0)} = 1.14$ eV. The calculated Si band gap for the 216 atoms supercell used was $E_g = 1.28$ eV, so, in the case of a symmetrical position of the levels with respect to the band gap, the energy levels of the I_2 defect could be located at about $E(0/-) = E_c - 0.07$ eV and $E(0/+) = E_v + 0.07$ eV.

We have compared the results of our electronic structure calculations for I_2 with the results of a combined DFT-G_0W_0 calculation for the split $\langle 110 \rangle$ Si self-interstitial (I_{Si}) [22]. In Ref. [22], the band gap value $E_g = 1.27$ eV was obtained, and the split $\langle 110 \rangle$ interstitial was found to possess energy levels at $E(0/+) \approx E_v + 0.01$ eV and $E(0/-) \approx E_c - 0.13$ eV in the band gap (see Fig. 2 in Ref. [22]). In our opinion, the similarity of the electronic properties of I_2 and the split $\langle 110 \rangle$ Si interstitial defects results from the similarity in their atomic configurations (see Fig. 1(a) above and Fig. 1(a) in Ref. [22]).
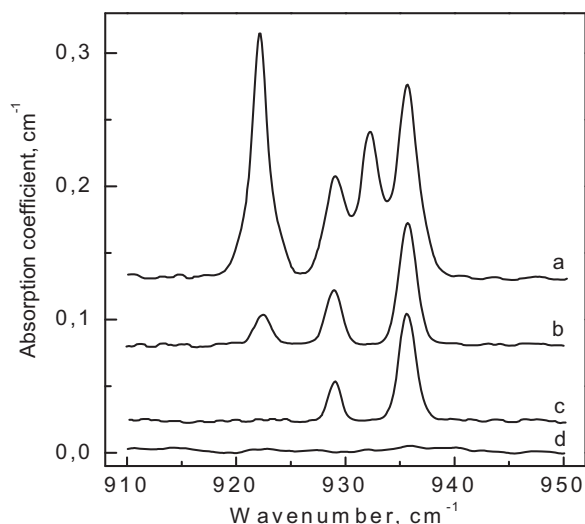

Figure 2 Infrared absorption spectra measured at 10 K for a p-type Si crystal, which was irradiated with 5 MeV electrons at 80 K ($F = 5 \times 10^{17}$ cm^{-2}) and subjected to 20-min anneals at a) 260 K, b) 301 K, c) 331 K, and d) 353 K. The spectra are baseline corrected.

The energy levels of the I_2 defect have never been detected. Among the main reasons for this failure could be i) the closeness of the energy level positions to the conduction and valence band edges as obtained in our calculations, and ii) the theoretically predicted high mobility of the center. In Ref. [16] we have presented some arguments, which confirm the hypothesis about high mobility of I_2 at room temperature. The arguments were based on the analysis of the introduction of the I_2O defect in different Si crystals upon irradiation with 4–6 MeV electrons and α particles.

4.2 Interactions of I_2 with O_i atoms – the I_2O defect It has been discussed in Ref. [16] that there are two pathways for the formation and dissociation of the I_2O defect: i) $I_2 + O_i \Leftrightarrow I_2O$ and ii) $IO + I \Leftrightarrow I_2O$. In the crystals irradiated with MeV electrons or α particles at about 280 K, the defect formation through the pathway i) is dominant and in the crystals with $[O_i] \gg [C_s]$ the concentration of the I_2O defect has been only slightly lower than that of the divacancy [16]. An assignment of the absorption band at 936 cm^{-1} to a local vibrational mode (LVM) of the I_2O defect has been confirmed in Ref. [16], and a donor level at $E_v + 0.09$ eV has been attributed to the I_2O center. The minimum energy configuration of the I_2O defect in the neutral charge state is shown in Fig. 1b). The binding energy of the I_2O complex relative to the separated I_2 and O_i species has been calculated to be 0.22 eV. A comparison of the minimum energy configurations of the I_2 and I_2O defects (Figs. 1(a) and (b)) shows that the attached oxygen atom only slightly affects the positions of Si atoms related to the di-interstitial. Furthermore, our electronic structure calculations show that the presence of the oxygen atom results in some small shifts of the energy levels of I_2. The acceptor energy level $E(0/-)$ is shifted into the conduction band and the donor level $E(0/+)$ is slightly shifted toward the middle of the band gap to about $E_v + (0.09–0.13)$ eV. The calculated position of the donor level is very close to that determined from DLTS measurements [16].

We have obtained some new information about the dynamical properties of the I_2O in the positively charged state and its annealing behavior. Figure 2 shows the infrared absorption spectra for a p-type Si crystal, which was irradiated with 5 MeV electrons at 80 K and then subjected to different heat-treatments. Strong absorption lines with their maxima at 922 and 932 cm^{-1} in the spectrum a) in Fig. 2 are related to LVMs due to the radiation-induced interstitial carbon atoms (C_i) [23]. Along with the absorption line at 936 cm^{-1} due to the I_2O defect another line with its maximum at 929 cm^{-1} is observed in the spectra a) to c) in Fig. 2. Figure 2 shows that the annealing behavior of the lines with their maxima at 936 and 929 cm^{-1} is similar. Indeed, from the analysis of changes in intensities of the lines upon 20-min isochronal annealing shown in Fig. 3 it is clear that the annealing behavior of the lines is identical. So, it is likely that both of the lines are related to the same defect, I_2O.
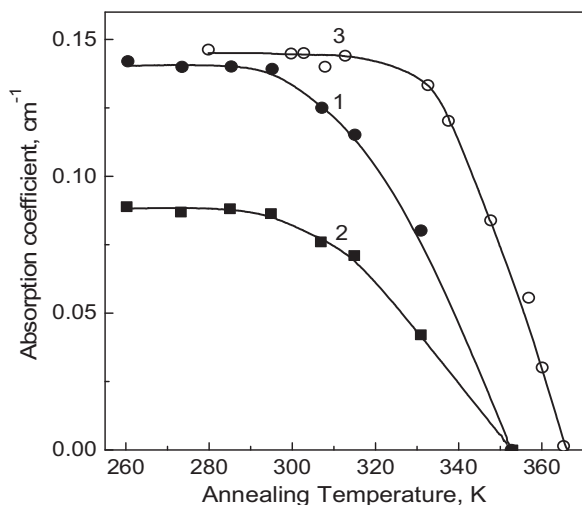
Figure 3 Changes in absorption coefficients of the absorption lines with their maxima at 1) and 3) 936 and 2) 929 cm^{-1} upon 20-min isochronal annealing of 1) and 2) a p-type Si crystal and 3) an n-type Si crystal, which were irradiated with 5 MeV electrons at 80 K. Doses of irradiation were $5 \times 10^{17} \, cm^{-2}$ for the p-type sample and $4 \times 10^{17} \, cm^{-2}$ for the n-type sample.
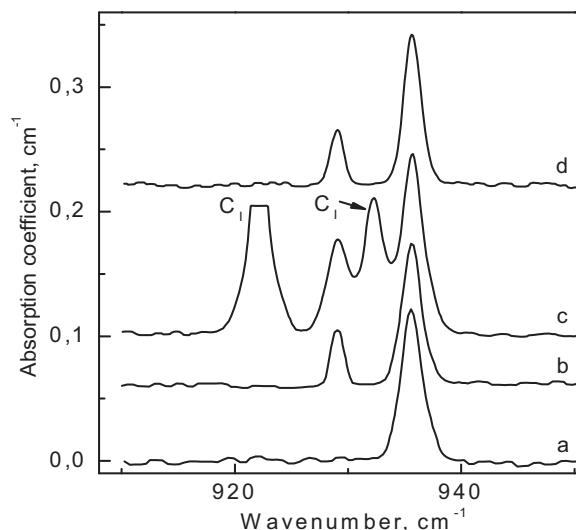

Figure 4 Infrared absorption spectra measured at 10 K for a) and b) n-type and c) and d) p-type Si crystals, which were irradiated with 5 MeV electrons at 80 K (doses of irradiation were 4×10^{17} and $5 \times 10^{17} \, cm^{-2}$ for n- and p-type crystals, respectively) and subjected to 20-min anneals at a), b), and d) 320 K, and c) 260 K. The spectrum b) has been recorded under white light illumination from an external source. The spectra are baseline corrected.

The question now is what is the exact origin of the absorption line with its maximum at 929 cm^{-1}? It has been shown in Ref. [16] that the line at 936 cm^{-1} is related to the asymmetric stretching vibration of the Si–O–Si unit of the neutral I_2O defect. Is the line at 929 cm^{-1} related to another LVM of the I_2O defect in the neutral charge state or is it a counter-part of the line at 936 cm^{-1} for the positively charged defect? It should be noted that the p-type Si crystal used for the IR absorption measurements was relatively highly doped with boron and as the dose of irradiation was not very high, it is possible that the crystal was not over-compensated by the irradiation and the Fermi level position could be close to the valence band at the temperature of the IR absorption measurements (10 K). So, part of the I_2O defects could be in the positively charged state during the measurements and give rise to different LVMs compared to those for the neutral defect.

Some answers to the questions above have been found when comparing the IR absorption spectra for the irradiated and annealed p- and n-type Si crystals shown in Fig. 4. The line at 929 cm^{-1} has not been detected in the absorption spectrum of the n-type Si crystal when the spectrum was recorded under usual measurement conditions with only optical excitation from a spectrometer light source (spectrum 4a)). However, the line at 929 cm^{-1} has appeared in the spectrum when it was recorded under illumination of the sample with white light of high intensity from an external source. The observed changes can be explained by capture of photo-generated holes by the I_2O defects in the neutral charge state and the appearance of the positively charged centers. An analysis of the changes observed shows clearly that the line at 929 cm^{-1} is a counter-part of the line at 936 cm^{-1} for the positively charged I_2O defect.

It can be seen from a comparison of isochronal annealing curves of the I_2O center in different materials (Fig. 3) that there is a significant difference in the elimination rates of the defect in n- and p-type Si crystals. It has been argued in Ref. [16] that the elimination of I_2O upon thermal annealing occurs through the reaction $I_2O \Rightarrow I_2 + O_i$. As the concentration of interstitial oxygen atoms are similar in the n- and p-type crystals studied, the enhanced elimination of the I_2O defect in the p-type crystal can be attributed to higher concentrations of sinks for the mobile I_2 species in this material. Such sinks can be associated with both substitutional carbon and boron atoms, as discussed in the introduction. Unfortunately, no significant changes have been detected in the infrared absorption spectra upon elimination of the I_2O defect in both the n- and p-type irradiated Si crystals, so the FT-IR absorption measurements have not given us new information about the possible interactions of I_2 with either C_s or B_s.

4.3 Interactions of I_2 with C_s atoms – the IC_i defect However, it has been found that the elimination of a level at $E_v + 0.09$ eV, due to I_2O, in the DLTS spectra is accompanied by the introduction of two hole traps at $E_v + 0.45$ eV and $E_v + 0.54$ eV. Figure 5 shows the elimination of the I_2O defect detected as changes in the concentration of the $E_v + 0.09$ eV level and changes in the concentrations of the $E_v + 0.45$ eV and $E_v + 0.54$ eV traps.

The observation and characterization of these traps have been reported by us recently in Ref. [18]. It was found that the $E_v + 0.45$ eV and $E_v + 0.54$ eV traps are related to two energy levels of a bistable defect. In the lowest energy
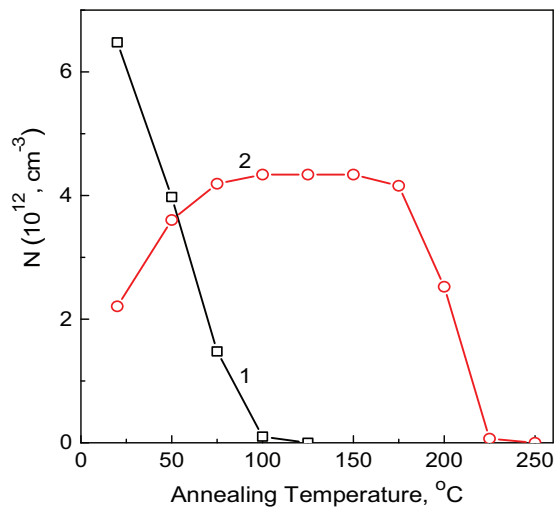
Figure 5 Changes in concentrations of 1) the hole trap with the energy level at $E_v +0.09$ eV and 2) the hole traps with the energy levels at $E_v +0.45$ eV and $E_v +0.54$ eV upon 30-min isochronal annealing in an n$^+$-p diode from epi Si, which was irradiated with 6 MeV electrons at about 280 K to a dose of 8×10^{14} cm^{-2}.

configuration, this defect is electrically inactive in p-type Si. We have not detected any energy levels related to this configuration in the irradiated Si diodes with p-type base. However, an injection of minority carriers (electrons) upon the application of a forward voltage to the irradiated n$^+$-p junctions resulted in transformation of the defect to a configuration which has two energy levels at $E_v +0.45$ eV and $E_v +0.54$ eV [18]. The reverse transition to the lowest energy configuration occurs in the temperature range 50–100 °C, and is characterized by the activation energy of 1.25 eV and a frequency factor of 5×10^{15} s^{-1}. The transformations are fully reversible and can be repeated many times without any concentration losses. It was suggested in Ref. [18] that the bistable defect could be due to a complex of a self-interstitial silicon atom with an interstitial carbon (C_iI) or a complex consisting of I and an interstitial boron atom (B_iI). Similar to the case of the I_2O defect, there are two pathways for the formation and dissociation of the C_iI and B_iI defects: i) $I_2 + C_s(B_s) \Leftrightarrow C_iI(B_iI)$ and ii) $C_i(B_i) + I \Leftrightarrow C_iI(B_iI)$.

The available information about the C_iI defect is limited. Strong arguments were presented that LVM absorption lines at 960 and 966 cm^{-1} are related to this defect [24]. The lines were observed in heavily irradiated carbon rich Si crystals and it was suggested that the C_iI defect is formed through the pathway ii). The defect responsible for the 960 and 966 cm^{-1} lines was found to anneal out in the temperature range 200–250 °C [24, 25]. The interaction of Si self-interstitials with interstitial carbon atoms have also been considered in combined model-potential molecular-dynamic simulations and *ab initio* calculations [26]. The C_iI complex was found to have two stable configurations. In the lowest energy configuration the binding energy of the

defect was calculated to be about 2.0 eV, so, confirming that the complex is a very stable one.

Regarding the B_iI defect, neither experimental nor theoretical modeling results on the $B_i + I$ and $I_2 + B_s$ interactions and the possible resulting defects have been published.

An analysis of our experimental data on the formation and annihilation of the defect responsible for the energy levels at $E_v +0.45$ eV and $E_v +0.54$ eV, provides some arguments in favor of its identification as the C_iI complex rather than the B_iI one. First, the effective introduction of the traps with the levels at $E_v +0.45$ eV and $E_v +0.54$ eV upon the disappearance of the I_2O defect have been observed in the diodes with the base from silicon having C_s concentration much higher than B_s concentration $\{[C_s] = (2–3) \times 10^{16}$ cm^{-3} and $[B_s] = (3–4) \times 10^{14}$ cm$^{-3}\}$. Taking into account that the I_2 defect is in the neutral charge state upon annealing, and therefore there are no Coulomb attraction effects, C_s is expected to be much more effective in capturing mobile I_2 than B_s just because of its much higher concentration. Secondly, the traps with the levels at $E_v +0.45$ eV and $E_v +0.54$ eV anneal out in the temperature range 200–250 °C upon 30-min isochronal annealing (Fig. 5). So, the annealing behavior of the traps is similar to that for the C_iI defect with its LVMs at 960 and 966 cm^{-1}.

In a DFT study we have placed the I_2 defect in the vicinity of a C_s atom in the $(215Si + 1C_s + 2Si)$ supercell and have minimized the total energy of the supercell allowing all the atoms to relax. Two stable configurations of the neutral C_iI defect have been found, which are shown in Fig. 6. It should be mentioned that the opposite to the case of the I_2O defect very significant changes in the positions and bonds of some Si atoms and the carbon atom occurred upon relaxation. The binding energy of the C_iI center in the minimum energy configuration shown in Fig. 6a has been calculated to be 1.65 eV relative to the separated C_i and I defects. This value is close to that found in a previous ab initio modeling study of the C_iI defect [26] and is consistent with the experimental results on the thermal stability of the
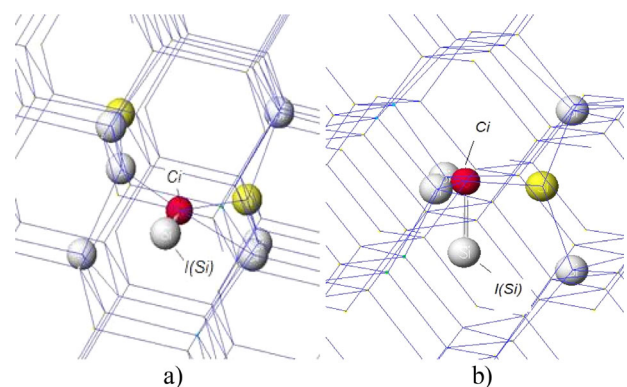

Figure 6 Stable configurations of the C_iI defect. a) Shows the minimum energy configuration, and b) the configuration which is higher in energy by 0.27 eV compared to the most stable one. The carbon atom is depicted in red color.

C_iI complex. The metastable configuration shown in Fig. 6b) is higher in energy by 0.27 eV compared to the most stable one.

5 Conclusions Our experimental results confirm the predicted high mobility of the Si di-interstitial defect at room temperature. Our *ab initio* modeling results suggest that the I_2 defect has an acceptor and a donor gap level close to the conduction and valence band edges, respectively, however, we were not able to detect these levels in our experiments.

Further, we have presented evidence that the mobile I_2 defects can interact with interstitial oxygen and substitutional carbon atoms. We have found minimum energy configurations of the resulting I_2O and C_iI complexes and determined their binding energies, and the positions of energy levels of these defects. Two absorption bands at 936 and $929 \, cm^{-1}$ have been assigned to the local vibrational modes of the I_2O defect in neutral and positively charged states, respectively. It should be mentioned that we have observed some enhancements of the I_2 related defect reactions upon the injection of minority carriers (electrons) into the irradiated n^+-p diodes. These enhancement effects are likely to be similar to those for the Si self-interstitials [17] and are currently under investigation.

References

[1] N. E. B. Cowern, G. Mannino, P. A. Stolk, F. Roozeboom, H. G. A. Huizing, J. G. M. van Berkum, F. Cristiano, A. Claverie, and M. Jaraíz, Phys. Rev. Lett. **82**, 4460 (1999).

[2] S. Libertino, S. Coffa, and J. L. Benton, Phys. Rev. B **63**, 195206 (2001).

[3] D. Stiebel, P. Pichler, and N. E. B. Cowern, Appl. Phys. Lett. **79**, 2654 (2001).

[4] J. Kim, F. Kirchhoff, W. G. Aulbur, J. W. Wilkins, F. S. Khan, and G. Kresse, Phys. Rev. Lett. **83**, 1990 (1999).

[5] S. K. Estreicher, M. Gharaibeh, P. A. Fedders, and P. Ordejón, Phys. Rev. Lett. **86**, 1247 (2001).

[6] T. A. G. Eberlein, N. Pinho, R. Jones, B. J. Coomer, J. P. Goss, P. R. Briddon, and S. Öberg, Physica B **308–310**, 454 (2001).

[7] M. Cogoni, B. P. Uberuaga, A. F. Voter, and L. Colombo, Phys. Rev. B **71**, 121203(R) (2005).

[8] M. Posselt, F. Gao, and D. Zwicker, Phys. Rev. B **71**, 245202 (2005).

[9] Y. A. Du, R. G. Hennig, and J. W. Wilkins, Phys. Rev. B **73**, 245203 (2006).

[10] S. Lee and G. S. Hwang, Phys. Rev. B **78**, 045204 (2008).

[11] Y. H. Lee, N. N. Gerasimenko, and J. W. Corbett, Phys. Rev. B **14**, 4506 (1976).

[12] Y. H. Lee, Appl. Phys. Lett. **73**, 1119 (1998).

[13] C. A. Londos, G. Antonaras, and A. Chroneos, J. Appl. Phys. **114**, 193513 (2013).

[14] J. Hermansson, L. I. Murin, T Hallberg, V. P. Markevich, J. L. Lindström, M. Kleverman, and B. G. Svensson, Physica B **302–303**, 188 (2001).

[15] G. Davies, S. Hayama, L. Murin, R. Krause-Rehberg, A. Sengupta, C. Davia, and A. Karpenko, Phys. Rev. B **73**, 165202 (2006).

[16] V. P. Markevich, A. R. Peaker, B. Hamilton, V. E. Gusakov, S. B. Lastovskii, L. I. Murin, N. Ganagona, E. V. Monakhov, and B. G. Svensson, Solid State Phenomena **242**, 290 (2016).

[17] G. D. Watkins, Phys. Status Solidi A **186**, 167 (2001).

[18] S. B. Lastovskii, V. P. Markevich, H. S. Yakushevich, L. I. Murin, and V. P. Krylov, Semiconductors **50**, 751 (2016).

[19] L. Dobaczewski, A. R. Peaker, and K. Bonde Nielsen, J. Appl. Phys. **96**, 4689 (2004).

[20] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gertsmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, J. Phys.: Condensed Matter. **21**, 395502 (2009).

[21] J. Gusakova, B. K. Tay, and V. Gusakov, Phys. Status Solidi A **213**, 2834 (2016).

[22] P. Rinke, A. Janotti, M. Scheffler, and C. G. Van de Walle, Phys. Rev. Lett. **102**, 026402 (2009).

[23] A. R. Bean and R. C. Newman, Solid State Commun. **8**, 175 (1970).

[24] S. P. Chapell and R. C. Newman, Semicond. Sci. Technol. **2**, 691 (1987).

[25] L. I. Murin, J. L. Lindström, G. Davies, and V. P. Markevich, Nucl. Instr. Methods Phys. Res. B **253**, 210 (2006).

[26] A. Mattoni, F. Bernardini, and L. Colombo, Phys. Rev. B **66**, 195214 (2002).