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

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New experimental and theoretical results on the silicon di-interstitial (I2) and its interactions with oxygen and carbon impurity atoms in Si crystals are reported. Electronic structure calculations indicate that I2 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 I2, are discussed. It is argued that mobile I2 can be trapped by oxygen and carbon impurities. The I2O center has a donor level at \( E_v + 0.09 \text{ eV} \). Two absorption bands at 936 and 929 cm\(^{-1}\) are assigned to the local vibrational modes of the I2O defect in the neutral and positively charged states, respectively. The binding energy of I2O relative to the separated I2 and Oi species is 0.22 eV. The disappearance of the I2O complex upon thermal annealing occurs in the temperature range 50–100 \( ^\circ \text{C} \) 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 \( E_v + 0.45 \text{ eV} \). It is argued that these levels are related to a complex consisting of interstitial carbon and interstitial silicon atoms (CiI). The stable configurations of the CiI pair have been found.

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 (I2) is the first step in the sequence of the I\(_n\) complexes. A number of theoretical studies, both \( \textit{ab initio} \) and molecular dynamics, have been dedicated to I2 [4–10]. It seems to be widely recognized that I2 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 I2 and its diffusion path (see, e.g., Refs. [6, 9] and references therein). Experimental observations of I2 are also inconclusive. Lee et al. [11] assigned the Si-P6 signal in electron spin resonance (ESR) spectra to a positive charge state of I2, 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 \( \textit{ab initio} \) density

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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\(_2\)O\(_i\) complexes. Hermansson et al. [14] have argued that I\(_2\)O\(_i\) gives rise to an absorption band at 936 cm\(^{-1}\). Further arguments for the assignment of the 936 cm\(^{-1}\) band to the I\(_2\)O 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\(_2\)O defect is one of the dominant point defects in heavily irradiated oxygen-rich Si crystals. We have recently argued that the I\(_2\)O 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\(_2\)O defect is not very stable and anneals out in the temperature range 50–100 °C. The value of activation energy for the I\(_2\)O thermal elimination has been found to be 1.05 ± 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\(_2\)S 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\(^{-1}\)-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 \(\alpha\) 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\(^{-1}\)-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 Ω·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 × 10\(^{17}\) cm\(^{-2}\), respectively. The concentrations of O\(_i\) and C\(_s\) atoms were 9.4 × 10\(^{17}\) and 2 × 10\(^{16}\) cm\(^{-3}\), and 9.9 × 10\(^{17}\) and 7.4 × 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) × 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 × 10\(^{-4}\) eV·Å\(^{-1}\).

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
The band gap value $\text{Si}(\text{I}_2)$ gap, the energy levels of the I$_2$ defect could be located at symmetrical position of the levels with respect to the band $E_{\text{g}}$. Calculations for I$_2$ with the results of a combined DFT-G0W0 modeling study [4] but with some small differences regarding atom positions and bond lengths. It has been shown from the electronic structure calculations that the I$_2$ defect introduces acceptor ($\text{I}_2$) and donor ($\text{I}_2^-$) levels into the band gap with an energy spacing between them of $E_{\text{g}}^{\text{I}_2} = 1.14$ eV. The calculated Si band gap for the 216 atoms supercell used was $E_{\text{g}} = 1.28$ 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 $E(0^-) = E_{\text{c}} - 0.07$ eV and $E(0^+) = E_{\text{v}} + 0.07$ eV.

We have compared the results of our electronic structure calculations for I$_2$ with the results of a combined DFT-G0W0 calculation for the split (110) Si self-interstitial (I$_5$I) [22]. In Ref. [22], the band gap value $E_{\text{g}} = 1.27$ eV was obtained, and the split (110) interstitial was found to possess energy levels at $E(0^+) \approx E_{\text{c}} + 0.01$ eV and $E(0^-) \approx E_{\text{v}} - 0.13$ 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 (110) Si interstitial defects results from the similarity in their atomic configurations (see Fig. 1(a) above and Fig. 1(a) in Ref. [22]).

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$_2$O defect in different Si crystals upon irradiation with 4–6 MeV electrons and $\alpha$ particles.

### 4.2 Interactions of I$_2$ with O$_i$ atoms — the I$_2$O defect

It has been discussed in Ref. [16] that there are two pathways for the formation and dissociation of the I$_2$O defect: i) I$_2$ + O$_i$ $\leftrightarrow$ I$_2$O and ii) I$^+$ + I $\leftrightarrow$ I$_2$O. In the crystals irradiated with MeV electrons or $\alpha$ particles at about 280 K, the defect formation through the pathway i) is dominant and in the crystals with [O$_i$] $\ll$ [C$_\text{s}$] the concentration of the I$_2$O defect has been only slightly lower than that of the vacancy [16]. An assignment of the absorption band at 936 cm$^{-1}$ to a local vibrational mode (LVM) of the I$_2$O defect has been confirmed in Ref. [16], and a donor level at $E_{\text{v}} + 0.09$ eV has been attributed to the I$_2$O center. The minimum energy configuration of the I$_2$O defect in the neutral charge state is shown in Fig. 1b). The binding energy of the I$_2$O 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$_2$O defects (Figs. 1a) 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 $E_{\text{v}} + (0.09–0.13)$ 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$_2$O 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$_\text{s}$) [23]. Along with the absorption line at 936 cm$^{-1}$ due to the I$_2$O 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$_2$O.

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$_2$O defect. Is the line at 929 cm$^{-1}$ related to another LVM of the I$_2$O defect in the neutral charge state or is it a counterpart 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 overcompensated by the irradiation and the Fermi level position was not very high, it is possible that the crystal was not overcompensated 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$_2$O 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 white light illumination from an external source. The observed changes can be explained by capture of photo-generated holes by the I$_2$O 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 counterpart of the line at 936 cm$^{-1}$ for the positively charged I$_2$O defect.

It can be seen from a comparison of isochronal annealing curves of the I$_2$O 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$_2$O upon thermal annealing occurs through the reaction I$_2$O $\rightarrow$ I$_2$ + O. As the concentration of interstitial oxygen atoms are similar in the n- and p-type crystals studied, the enhanced elimination of the I$_2$O 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$_2$O 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$_2$O, 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$_2$O 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 $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$ traps are related to two energy levels of a bistable defect. In the lowest energy 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 $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$ [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 $5 \times 10^{15} \, \text{s}^{-1}$. 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 (CiI) or a complex consisting of I and an interstitial boron atom (BiI). Similar to the case of the I$_2$O defect, there are two pathways for the formation and dissociation of the CiI and BiI defects: i) I$_2 + C_s (B_s) \Leftrightarrow C_i (B_i)$ and ii) $C_i (B_i) + I \Leftrightarrow C_i (B_i)$. The available information about the CiI 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 CiI 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 CiI 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 BiI 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 $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$, provides some arguments in favor of its identification as the CiI complex rather than the BiI one. First, the effective introduction of the traps with the levels at $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$ upon the disappearance of the I$_2$O defect have been observed in the diodes with the base from silicon having Cs concentration much higher than Bs concentration $[\{C_s\} = (2-3) \times 10^{16} \, \text{cm}^{-3}$ and $[B_s] = (3-4) \times 10^{14} \, \text{cm}^{-3}]$. Taking into account that the I$_2$ defect is in the neutral charge state upon annealing, and therefore there are no Coulomb attraction effects, Cs is expected to be much more effective in capturing mobile I$_2$ than Bs just because of its much higher concentration. Secondly, the traps with the levels at $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$ 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 CiI 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 Cs atom in the (215Si + 1Cs + 2Si) supercell and have minimized the total energy of the supercell allowing all the atoms to relax. Two stable configurations of the neutral CiI defect have been found, which are shown in Fig. 6. It should be mentioned that the opposite to the case of the I$_2$O 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 CiI center in the minimum energy configuration shown in Fig. 6a has been

![Figure 5](image1.png) Changes in concentrations of 1) the hole trap with the energy level at $E_v +0.09 \, \text{eV}$ and 2) the hole traps with the energy levels at $E_v +0.45 \, \text{eV}$ and $E_v +0.54 \, \text{eV}$ 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 $8 \times 10^{14} \, \text{cm}^{-2}$.

![Figure 6](image2.png) Stable configurations of the CiI 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.
calculated to be 1.65 eV relative to the separated C\textsubscript{1} and I defects. This value is close to that found in a previous ab initio modeling study of the C\textsubscript{1}I defect [26] and is consistent with the experimental results on the thermal stability of the C\textsubscript{1}I 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\textsubscript{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\textsubscript{2} defects can interact with interstitial oxygen and substitutional carbon atoms. We have found minimum energy configurations of the resulting I\textsubscript{2}O and C\textsubscript{1}I complexes and determined their binding energies, and the positions of energy levels of these defects. Two absorption bands at 936 and 929 cm\textsuperscript{-1} have been assigned to the local vibrational modes of the I\textsubscript{2}O defect in neutral and positively charged states, respectively. It should be mentioned that we have observed some enhancements of the I\textsubscript{2} related defect states, respectively. It should be mentioned that we have observed some enhancements of the I\textsubscript{2} related defect reactions upon the injection of minority carriers (electrons) into the irradiated n\textsuperscript{-}p diodes. These enhancement effects are likely to be similar to those for the Si self-interstitials [17] and are currently under investigation.

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