Carbon, oxygen and intrinsic defect interactions in germanium-doped silicon

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Abstract

Production and annealing of oxygen-vacancy (VO) and oxygen-carbon (C_iO_i, C_iO_iI) defects in germanium-doped Czochralski-grown silicon (Cz-Si) containing carbon are investigated. All the samples were irradiated with 2 MeV fast electrons. Radiation-produced defects are studied using infrared spectroscopy by monitoring the relevant bands in optical spectra. For the VO defects, it is established that the doping with Ge affects the thermal stability of VO (830 cm^{-1}) defects as well as their fraction converted to VO_2 (888 cm^{-1}) defects. In Ge-free samples containing carbon, it was found that carbon impurity atoms do not affect the thermal stability of VO defects, although they affect the fraction of VO defects that is converted to VO_2 complexes. Considering the oxygen–carbon complexes, it is established that the annealing of the 862 cm^{-1} band associated with the C_iO_i defects is accompanied with the emergence of the 1048 cm^{-1} band, which has earlier been assigned to the C_sO_{2i} center. The evolution of the C_iO_iI bands is also traced. Ge doping does not seem to affect the thermal stability of the C_iO_i and C_iO_iI defects. Density functional theory (DFT) calculations provide insights into the stability of the defect clusters (VO, C_iO_i, C_iO_iI) at an atomic level. Both experimental and theoretical results are consistent with the viewpoint that Ge affects the stability of the VO but does not influence the stability of the oxygen–carbon clusters. DFT calculations demonstrate that C attracts both O_i and VO pairs predominately forming next nearest neighbor clusters in contrast to Ge where the interactions with O_i and VO are more energetically favorable at nearest neighbor configurations.

1. Introduction

Si-based devices can be influenced by impurities such as interstitial oxygen O_i and substitutional carbon C_s, which are usually present in crystals grown by the Czochralski technique. Oxygen and carbon impurity atoms can, in turn, be effective traps for vacancies V and self-interstitials I, respectively. Irradiation of Si with MeV electrons gives rise to pairing of oxygen atoms with mobile vacancies to form VO centers [1, 2]. These have extensively been studied by various experimental techniques [1–5]. Substitutional carbon atoms in irradiated Si are converted to carbon interstitials C_i which are mobile at room temperature, and they can interact with O_i and C_s atoms

to form C_iO_i and C_iC_s complexes, respectively [6]. With increasing irradiation dose, the C_iO_i, C_iC_s and C_i defects act as traps for self-interstitials resulting in the formation of larger clusters, e.g. C_iO_iI, C_iC_sI and C_iI defects. Defect processes leading to the appearance of carbon-related complexes have extensively been studied so far [6–15]. However, there are still important issues that need to be further investigated. For example, the identification of defects formed during the annealing of carbon-related complexes is not well established yet.

Doping of Si crystals with isovalent impurities such as C, Ge and Sn is a convenient way to affect its physical properties. In this respect, Ge impurity atoms are widely used for defect

Table 1. Details of the samples E4, E3 and Ge8.

Samples	d (mm)	[Ge] (cm^{-3})	$[C_s]_o$ 10^{16} (cm^{-3})	$[C_s]_{a.i.}$ 10^{16} (cm^{-3})	$[O_i]_o$ 10^{17} (cm^{-3})	$[O_i]_{a.i.}$ 10^{17} (cm^{-3})	Fluence 10^{17} (cm^{-2})	a_{VO} (cm^{-1})	Fraction a_{VO_2}/a_{VO}
E4	1.88	–	<1	–	9.6	9.2	5	0.37	0.83
E3	1.91	–	16	9.6	10.2	9.8	5	0.62	0.56
Ge8	1.78	2×10^{20}	9	<2	7.7	6.9	5	0.66	0.33

engineering in Cz-Si [16]. The tetrahedral covalent radius of Ge atoms in the Si lattice is larger than that of the Si host atoms. Thus, the substitutional Ge atoms give rise to compressive elastic strains in the Si lattice, which can affect quasi-stationary concentrations of vacancies, self-interstitials and, hence, secondary defect reactions running in the course of irradiation and annealing. On the other hand, carbon, another isovalent impurity in Si, having a smaller tetrahedral radius than that of host atoms induces tensile strains that also affect the concentrations of intrinsic defects. Therefore, it is important to investigate the impact of Ge and C doping on the behavior and properties of oxygen-vacancy and oxygen–carbon defects in Si.

When annealed at about 300 °C, mobile VO defects (830 cm^{-1}) can be transformed into VO_2 complexes (888 cm^{-1}) by trapping oxygen atoms. At about the same temperature, C_iO_i defects are also annealed out [6]. In actual fact, VO and C_iO_i centers are the main radiation defects in irradiated Cz-Si. Regarding the impact of Ge doping on the behavior and properties of radiation-produced defects in Cz-Si, there is a need to broaden investigations carried out in recent years [17–20], especially those concerning oxygen and carbon, the two main impurities in Si.

The aim of the present study is to investigate both experimentally and theoretically (i) the effect of the isovalent impurities Ge and C on the stability of the VO defects and their conversion to VO_2 defects, and (ii) the effect of Ge doping on the stability of C_iO_i and C_iO_iI complexes in Cz-Si.

2. Methodology

2.1. Experimental methods

Three groups of Cz-Si samples were studied. The first group of samples with low carbon concentration, labeled E4, was Ge free. The second group of samples with high carbon concentration, labeled E3, was also Ge free, whereas the third group of carbon-rich samples, labeled Ge-8, was Ge doped. The samples were irradiated with 2 MeV electrons at ∼80 °C, using the Dynamitron accelerator at Takasaki-JAERI (Japan). The irradiation fluence was 5×10^{17} cm^{-2} for all the irradiated samples. The initial concentrations of the carbon and oxygen impurities $[C_s]_o$ and $[O_i]_o$, as well as their concentrations after irradiation $[C_s]_{a.i}$ and $[O_i]_{a.i}$ are cited in table 1. Following the irradiation, they were subjected to isochronal annealing in 20 min steps. After each annealing step, IR spectra were recorded at room temperature by means of a Fourier transform infrared (FTIR) spectrometer of type JASCO-470 plus, operated with a resolution of 1 cm^{-1}. The intrinsic

two-phonon absorption was subtracted by using a float-zone sample of equal thickness.

2.2. Theoretical methods

The experimental results reported here provide information on the thermal stability and formation of the clusters. They can be associated with the density functional theory (DFT) results, which provide information on the binding energies, E_b, defined by

$$E_b = E_{\text{defect cluster}} - \Sigma E_{\text{isolated defects}}.$$

In this definition, negative binding energies imply that a cluster is energetically favorable with respect to its constituent isolated components.

To investigate the C, Ge, O and intrinsic defect interactions in Si, we used the DFT code CASTEP [21]. The Perdew–Burke–Ernzerhof generalized gradient approximation functional, ultrasoft pseudopotentials [22, 23] and a 64-atom Si supercell were applied in all the calculations. The plane wave basis energy cutoff was 350 eV and the Monkhorst-Pack $(2 \times 2 \times 2)$ k-point sampling was used [24]. The unit-cell parameters and atomic coordinates were allowed to relax by the application of energy minimization. The criteria are that the largest forces were less than 0.05 eV Å^{-1} and a total energy convergence tolerance not exceeding 10^{-5} eV/atom. The method used efficiently describes the structure and defect chemistry of Si and other related materials [25–28]. For isovalent-doped Si, there are a number of recent DFTs using this methodology [29, 30].

3. Results and discussion

Figures 1(a)–(c) represent the fragments of IR spectra recorded on the E4, E3 and Ge8 samples, respectively, just after the irradiation as well as at characteristic temperatures in the course of the isochronal anneal sequence: (i) at ∼350 °C where the VO signal is about to disappear from the spectra and (ii) above ∼400 °C where the VO_2 signal attains its maximum intensity. The bands associated with VO, VO_2, C_iO_i and C_iO_iI complexes are clearly seen. Figures 2(a)–(c) demonstrate the evolution of the VO and VO_2 bands for the E4, E3 and Ge8 samples, respectively. It is well known that upon annealing, the VO defect is converted to the VO_2 complex at $T \approx 300$ °C. It was found that some features of these complexes are influenced by the presence of Ge. Notably, it has been established that the annealing temperature of VO defects in the Ge-doped samples shifts to lower temperatures, $T \approx 220$ °C, compared to that observed in the Ge-free samples, $T \approx 290$ °C; cf figures 2(a)
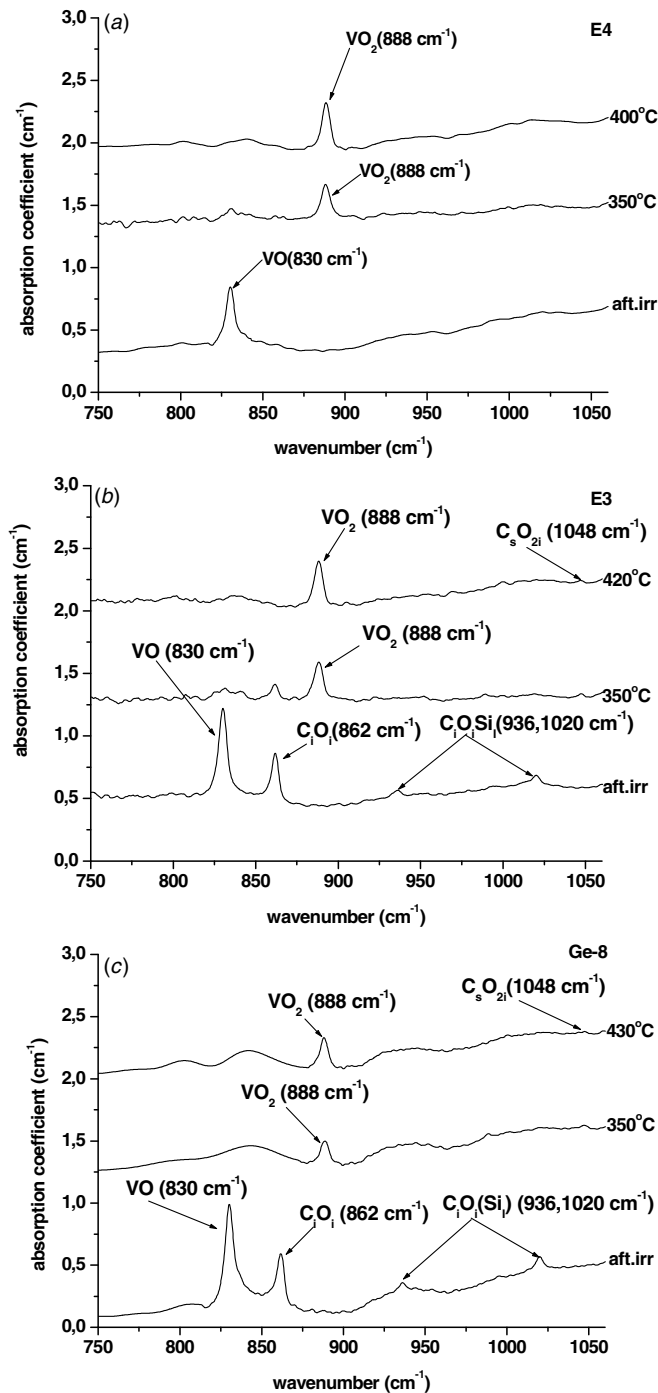
Figure 1. IR spectra of the E4 (*a*), E3 (*b*) and Ge8 (*c*) samples after irradiation and at characteristic temperatures in the course of the isochronal anneal sequence.

Figure 2. Thermal evolution of the VO (830 cm^{-1}) and VO$_2$ (888 cm^{-1}) bands for the E4 (*a*), E3 (*b*) and Ge8 (*c*) samples.

and (*c*). Together with this, it is noticed that the fraction of VO defects converted to VO$_2$ complexes is greatly reduced in Ge-doped Cz-Si. There is a correlation with elastic strains induced by Ge impurity atoms in the Si lattice [19, 20, 31]. Consequently, the fraction of self-interstitials participating in the annealing of VO defects is influenced by the presence of Ge. This annealing behavior can be explained by considering the following reactions: VO + O$_i$ → VO$_2$ and VO + I → O$_i$. In irradiated materials, large-scale defect clusters, which are
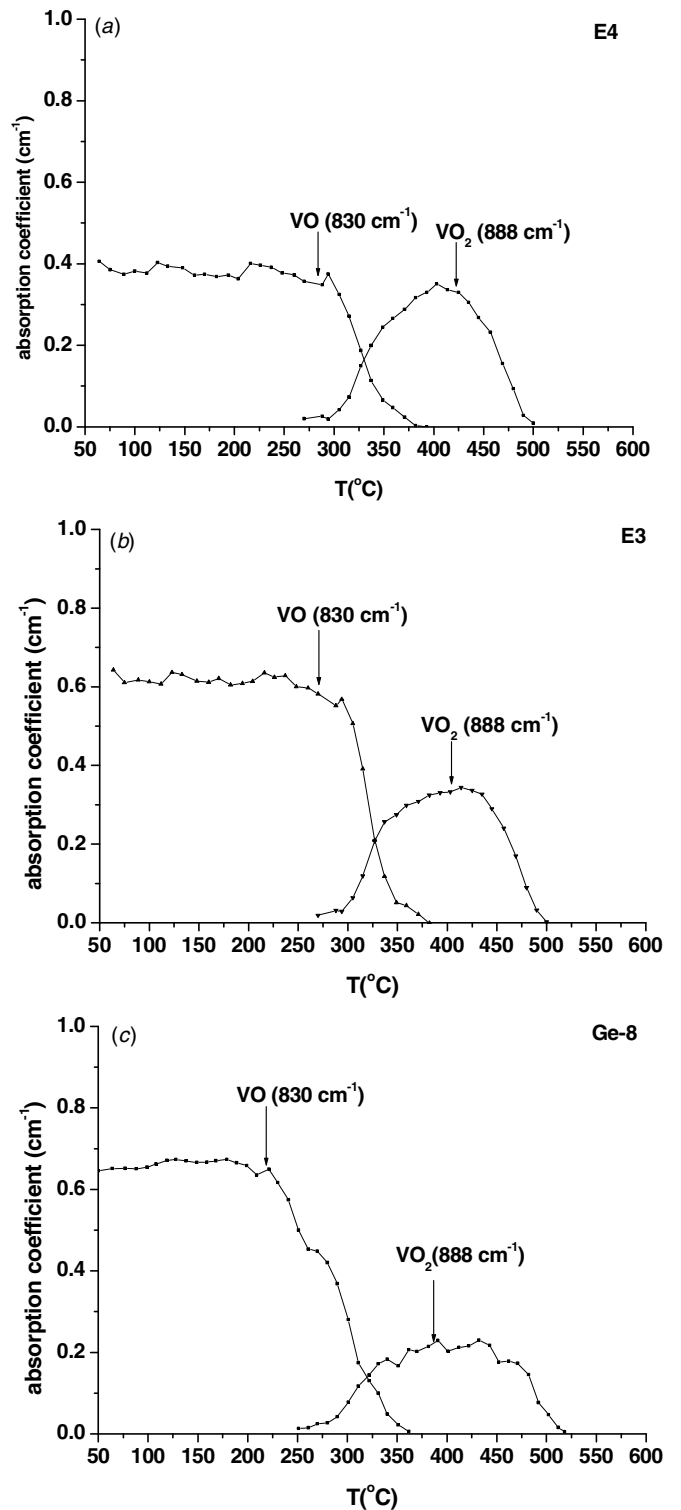
formed in the course of irradiation [32], serve as a source of self-interstitials. It can be argued that the doping of Si with Ge atoms of larger atomic size induces elastic strains in the crystal lattice, which, in turn, enhance the release of self-interstitials from these clusters [20, 31]. As a result, the reaction VO + I → O$_i$ can run at lower temperatures, and this is in line

with our observation. Actuallly, the onset of the annealing of VO defects occurs at a lower T. Similarly, the enhancement of the VO + I $\rightarrow$ O$_i$ reaction, in reference to the reaction VO + O$_i$ $\rightarrow$ VO$_2$, should lead to a reduced concentration of VO defects available for the transformation into VO$_2$ complexes, as the Ge concentration increases. This is also in agreement with the present experimental data (table 1). Actually, the ratio a_{vo2}/a_{vo}, where a denotes the absorption coefficient, is substantially reduced in Ge-doped Si. Finally, it is worth noting that the VO$_2$ defect (figures 1, 2) achieves its maximum intensity at higher temperatures than that where VO disappears completely from the spectra. This is an interesting point indicating that complementary mechanisms and other reaction channels participate in the formation of the VO$_2$ defect. Their appearance becomes pronounced after the disappearance of the VO defect from the spectra. The phenomenon is complicated and merits further investigation.

From an atomistic point of view, an interstitial oxygen atom O$_i$ is strongly bonded to two neighboring Si atoms. In Ge-doped Si, it was previously concluded, using DFT calculations, that the O$_i$ atoms do not form bonds to substitutional Ge atoms, because they repel each other [33]. This conclusion appears to be reasonable, as a larger Ge atom further restricts the available space for an O$_i$ atom in the lattice. As a result, the O$_i$ atoms preferentially form bonds to Si host atoms. From the other side, a vacancy V, another constituent of VO$_n$ complexes, should preferentially be located closely to a Ge atom [34]. This has also been established by earlier experiments and computational work on Si$_{1-x}$Ge$_x$ alloys over a range of compositions [35, 36]. It is a consequence of the less rigid Ge–Si and Ge–Ge bonds compared to the Si–Si bonds. Finally, DFT calculations revealed that the VO pair (schematic in figure 3(a)) associated with a Ge atom is more stable if the Ge atom assumes a site close to the vacancy forming a GeVO cluster (refer to figure 3(b)), and it is less stable if the Ge atom is closer to the oxygen atom in the VO pair forming a GeOV cluster [33]. It can be suggested that it is more difficult for the reaction VO + O$_i$ $\rightarrow$ VO$_2$ to run in Ge-doped Si, since Ge atoms located in the neighborhood of VO complexes can repel diffusing O$_i$ atoms. This in turn entails a reduced formation of VO$_2$ clusters. The phenomenon should be related to the Ge–O$_i$ interaction, which was calculated to be repulsive by 0.85 eV at nearest neighbor (NN) configuration [33]. Obviously, the kinetics of these processes need further investigations to separate the contributions of the competing defects.

Figure 2(b) gives evidence that, contrary to the case of Ge doping, the thermal stability of VO defects is not affected by the presence of carbon, since in both cases VO complexes are annealed at about 290 °C; cf figures 2(a) and (b). However, the fraction of VO defects converted to VO$_2$ complexes is lower in Cz-Si containing carbon (table 1). We note that a Ge atom has a covalent radius larger than the radius of a Si atom, r_{Ge} = 1.22 Å and r_{Si} = 1.17 Å, correspondingly. This gives rise to compressive stress in the lattice, in contrast to carbon atoms with a smaller covalent radius, r_c = 0.77 Å, leading to tensile stress. It appears that the tensile stresses induced in the Si lattice in the case of the smaller carbon atoms cannot affect
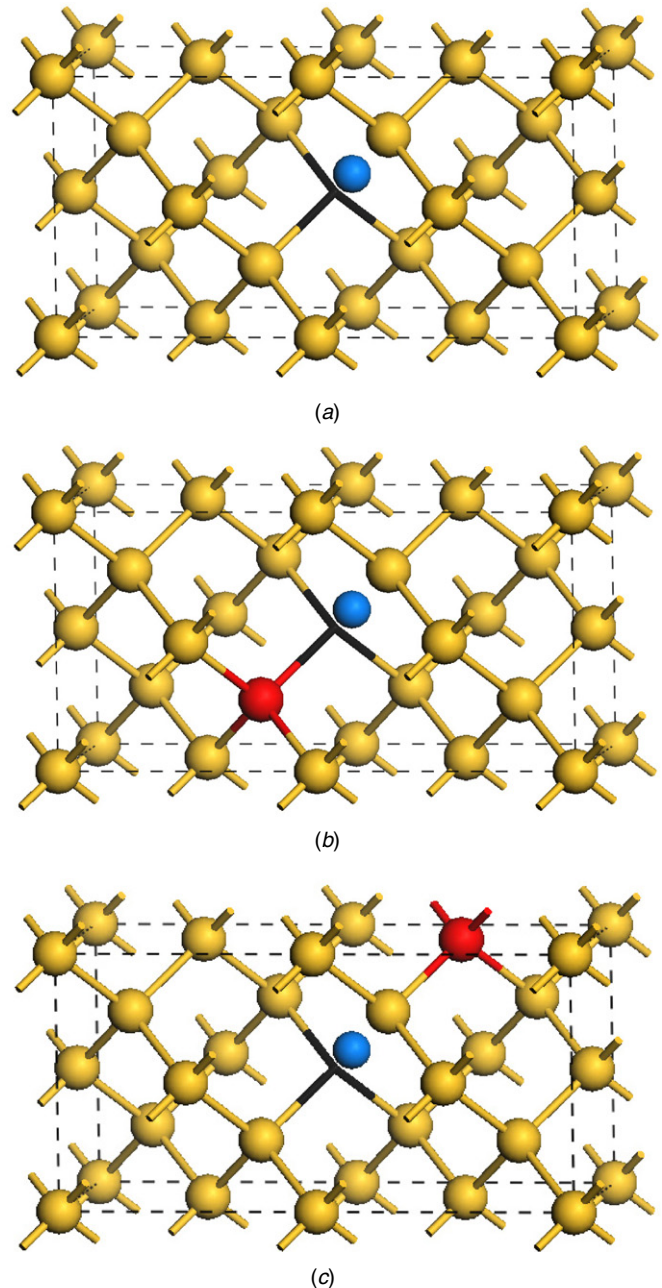

(a)

(b)

(c)

Figure 3. A representation of (a) the A-center, (b) the nearest neighbor GeVO cluster and (c) the next nearest neighbor COV cluster in Si. Yellow and red spheres represent the Si and Ge (or C) atoms respectively. O$_i$ are represented by blue spheres and V by the black sticks.

(This figure is in colour only in the electronic version)

the binding energy of the Si interstitial clusters, and therefore, the reaction VO + I $\rightarrow$ O$_i$ cannot start at lower temperatures. This is in contrast to the case of compressive stresses induced by the larger Ge atoms, which affect the binding energy of the Si interstitial clusters leading to the onset of the above reaction at lower temperatures. Along with this, when silicon interstitials begin to liberate from clusters in the presence of carbon, some of the free self-interstitials are temporarily trapped by C$_s$, forming interstitial carbon C$_i$. At temperatures around 300 °C, the interstitial carbon atoms are very mobile
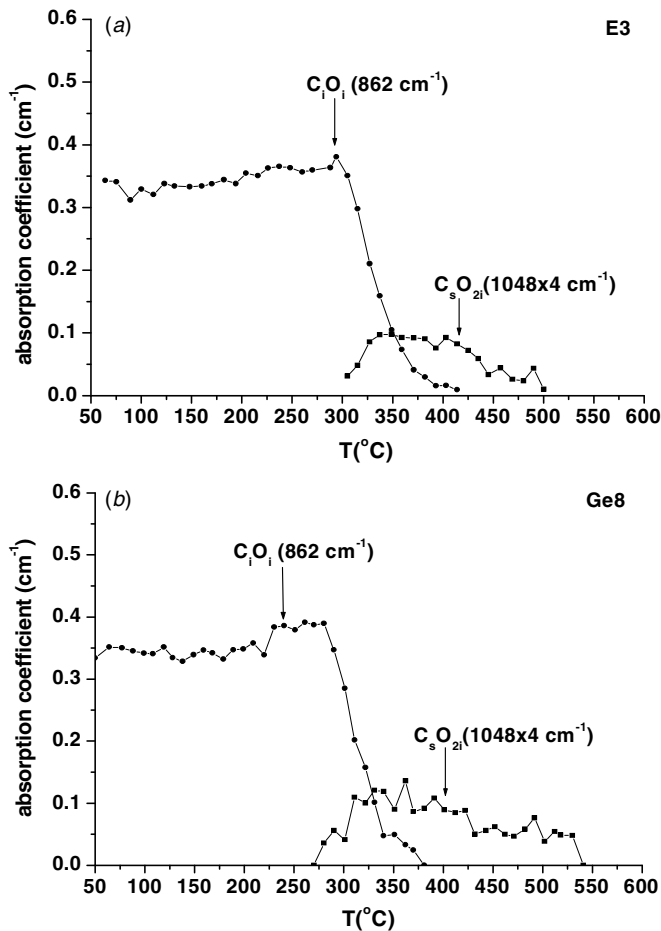
Figure 4. Thermal evolution of the C_iO_i (862 cm^{-1}) band together with the C_sO_{2i} (1048 cm^{-1}) band for the E3 (*a*) and Ge8 (*b*) samples.

and either they convert again to substitutional carbon, $C_s + I \leftrightarrow C_i$, or/and they are captured by other impurity atoms, for instance by O_i, forming C_iO_i defects. Because of the first process, the quasi-stationary concentration of Si interstitials upon annealing around 300 °C is increased leading to the enhanced reaction $VO + I \rightarrow O_i$. Thus, fewer VO defects are available to participate in the reaction $VO + O_i \rightarrow VO_2$, and therefore fewer VO_2 defects form. Actually, the reduced formation of VO_2 defects is clearly seen in the IR spectra. Because of the second process, an enhancement of the C_iO_i formation process is expected at around 300 °C, which is really present in the evolution curve of C_iO_i complexes; cf figures 4(*a*) and (*b*).

The interaction of C_s with O_i is markedly different compared to the interaction of Ge with O_i, as C_s attracts O_i when they are at next nearest neighbor (NNN) [33, 37, 38]. These differences will impact the trapping of VO pairs by C and Ge. In previous DFT calculations [33], it was calculated that the VO pairs are attracted by C to form CVO clusters. Again the NNN configurations (refer to figure 3(*c*)) are prevalent indicating that the interaction of C with VO will be more effective at larger distances. These interactions can in turn retard the diffusion of the VO pairs leading to the formation of fewer VO_2 clusters. Therefore, it is important to investigate in

future work the impact of the isovalent dopants on the kinetics of the VO pairs.

Regarding the oxygen–carbon defects, it was established that the annealing of C_iO_i (862 cm^{-1}) defects is accompanied with the emergence of a weak band at 1048 cm^{-1} in IR spectra; cf figures 4(*a*) and (*b*). Importantly, this band was earlier assigned by Inoue *et al* [39] to C_sO_{2i} defects formed via the reaction path $C_iO_i + VO \rightarrow C_sO_{2i}$. Additionally, two bands at 1052 and 1099 cm^{-1}, detected with IR measurements taken at cryogenic temperatures, are reportedly associated with C_sO_{2i} defects [40]. These bands were observed after irradiation at temperatures over a range of 400–600 °C. For the formation of these complexes, the following reaction was suggested: $VO_2 + C_i \rightarrow C_sO_{2i}$. It is proposed that the 1052 cm^{-1} band observed in optical measurements at cryogenic temperatures corresponds to the 1048 cm^{-1} band recorded at room temperature in this study. Here, we could not detect the 1099 cm^{-1} band. It is possible, however, that this weak band is overlapped with a strong O_i band at 1106 cm^{-1} in the spectral range considered.

Figure 5 represents the evolution of the 1020 and 936 cm^{-1} bands that were previously assigned to the C_iO_iI complex [6, 11, 41]. In the annealing experiments, the bands begin to decay at ∼120 °C, disappearing almost completely in IR spectra at ∼180 °C. It is notable that the thermal stability of oxygen–carbon defects C_iO_i and C_iC_s is practically unaffected by the Ge presence, at least at the Ge concentrations discussed, up to [Ge] $= 2 \times 10^{20}$ cm^{-3} [20]. The present results extend this conclusion for the C_iO_iI defects as well.

From a theoretical point of view, the interactions of C with the defects in Si have extensively been studied [42, 43]. Here, the picture emerging from our experimental data is that the thermal stability of C_iO_i and C_iO_iI complexes is not significantly influenced by the presence of Ge. In a previous DFT work [33], it was concluded that Ge impurity atoms repel O_i atoms in the Si lattice. To investigate further the association of Ge with C in Si, we performed DFT calculations using the methodology and parameters reported in earlier work [33, 44–46]. These calculations revealed that the C_s atoms do not bind with Ge atoms at the NN positions, being repelled by an energy of 0.14 eV. It is, therefore, unlikely that a Ge atom assumes a site in the close vicinity of an oxygen–carbon defect because of energetically unfavorable relations. Consequently, it is expected that the Ge atoms in Si do not influence the thermal stability of oxygen–carbon complexes, and therefore there is good agreement between experiment and theory. Again, the kinetics of these processes need further systematic investigations using a Monte Carlo approach, similarly to the study of Pinacho *et al* [40]. In their study, Pinacho *et al* [42] used the Monte Carlo approach in synergy with input from DFT to develop a comprehensive model for C diffusion and clustering in Si but at high temperatures, i.e. 850 and 900 °C. It will be necessary to extend these approaches to lower temperatures in order to directly compare with experimental results.

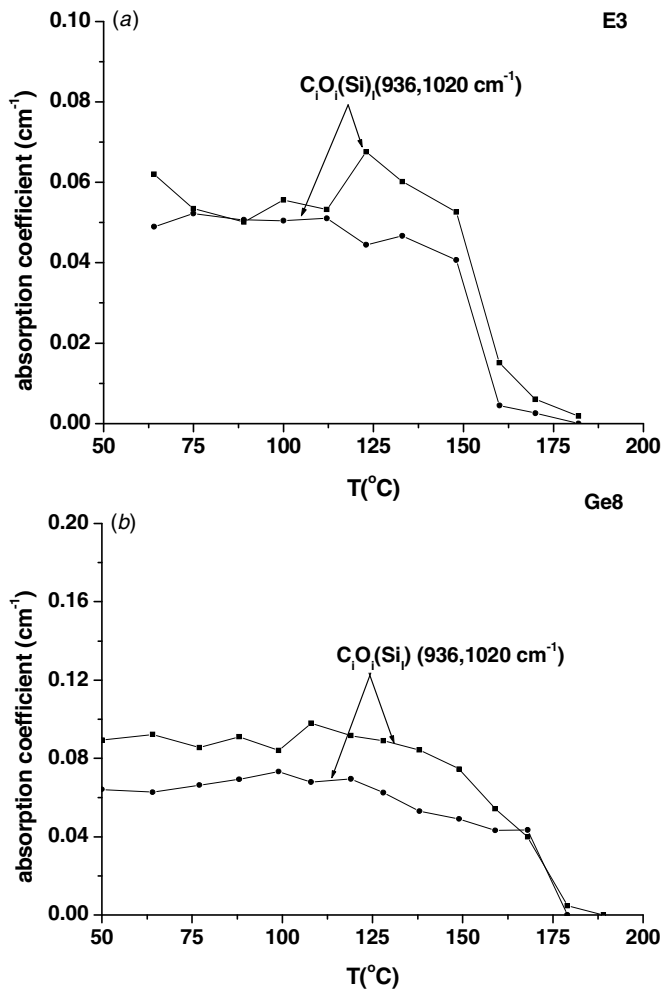**Figure 5.** Thermal evolution of the C_iO_iI (936 cm^{-1}, 1020 cm^{-1}) bands for the E3 (*a*) and Ge8 (*b*) samples.

4. Conclusions

In this study, we investigate the C, Ge, O and intrinsic defect interactions in Ge-doped Si from a FTIR and DFT point of view. The experimental results determine the thermal stability and evolution of the clusters, and therefore they can be linked to the DFT results, which are used to calculate the binding energies (i.e. how stable these clusters are).

The impact of Ge and C doping on the evolution of VO complexes in Cz-Si was studied. It was established that the conversion of VO defects to VO$_2$ complexes is sensitive to the Ge presence, both in lowering the temperature of the VO annealing and decreasing the [VO$_2$]/[VO] ratio. These results can be explained by an enhanced release of self-interstitials from defect clusters, affecting the balance between the reactions VO + O$_i$ → VO$_2$ and VO + I → O$_i$. Additionally, regarding C-doping, it was found that in Ge-free Cz-Si containing carbon, the [VO$_2$]/[VO] ratio is affected as well, actually it is reduced. This effect is explained in the framework of a model where carbon impurity atoms in Si may increase the quasi-stationary concentration of self-interstitials upon annealing, thus enhancing the reaction VO + I → O$_i$, or equivalently suppressing the reaction VO + O$_i$ → VO$_2$.

Finally, the effect of Ge doping on the thermal stability of the oxygen–carbon (C$_i$O$_i$, C$_i$O$_i$I) defects was found negligible in our investigations.

From an atomistic simulation perspective, Ge will bind with V and VO pairs; however, it will repel O$_i$ and C$_s$ atoms. Therefore, in Ge-doped samples, the stability of VO pairs will be affected, but Ge will not impact the stability of C$_i$O$_i$ and C$_i$O$_i$I clusters significantly. Carbon impurities in Si behave differently as they strongly associate with both VO and O$_i$.

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