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The self-interstitial in silicon and germanium

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ABSTRACT

Low temperature irradiation experiments show a remarkable contrast between Si and Ge, suggesting that the behavior of self-interstitials and vacancies is very different in the two materials. The present paper reviews theoretical and experimental investigations of the defects in an attempt to understand these differences.

1. Introduction

Detailed studies of radiation defects in Ge started more than 50 years ago mainly using electrical techniques, and a review can be found in Ref. [1]. Progress in the identification of these defects was interrupted by investigations into radiation defects in Si, but has now become topical again owing to the higher carrier mobilities realized in Ge devices. The availability of electron paramagnetic resonance (EPR) spectroscopy for Si, but not Ge, has greatly contributed to the understanding of vacancy and related defects in that material. However, the properties of the isolated interstitial remain elusive [2,3]. In Ge, recent deep level transient spectroscopy (DLTS) [4–6] and infra-red absorption spectroscopy [7,8] studies have succeeded in identifying new radiation defects paired with impurities; perturbed angular correlation spectroscopy (PACs) studies [9] have led to important findings on the mobility and electrical activity of *V* and *I*; and lately, these two defects, created following low temperature radiation, have been investigated by *in situ* DLTS by Mesli et al. [6]. There is also an increasing number of theoretical investigations which have attempted to explain the experimental data [10–31]. It can however, be said that there is little overlap in the effects of *e*-irradiation of Si and Ge. This paper will concentrate on the discussion of these differences.

2. Low-temperature electron-irradiation experiments

Low temperature 1–3 MeV *e*-irradiation has strikingly different effects on n-type and p-type Si, as well as on n-type and p-type Ge [32,33]. During irradiation, the self-interstitial in p-Si seems to be mobile at temperatures as low as 4 K, readily forming complexes with B, Al, C, O and other impurities [3]. In contrast, Hall effect measurements show that *e*-irradiation of p-Ge at 4 K produces hardly any changes in the conductivity [34], and a decrease of the carrier concentration is observed only under optical excitation or after annealing above 100 K [35–38].

In n-type material, the situation is inverted. Frenkel pairs introduced in Ge at 4 K are believed to anneal out in a prominent annealing stage at $\simeq$ 65 K and can be responsible for more than 80% of the conductivity drop in $\sim$ 1 MeV irradiated samples [39,40]. In contrast, 1 MeV *e*-irradiation of n-Si at the same temperature produces electron removal rates of less than 0.02 cm^{-2}, but these show an abrupt increase of orders of magnitude if the radiation is performed above 60 K [33]. In parallel, EPR reveals the trapping of V^{2-} by oxygen in low-resistivity material after annealing at 100 K [2], but self-interstitials remain undetected at least below 140–175 K [3]. This is presumably due to their high mobility and reactivity which makes it very difficult to observe and characterize in an isolated state.

However, there are suggestions that different radiation treatments might lead to single interstitials. The AA12 EPR and the E1 DLTS centers, observed in intrinsic or p-Si following heavy irradiation with protons or alpha-particles [41], have been assigned to an isolated self-interstitial at the caged tetrahedral interstitial site [41,19]. It might be that in this case for example, di-interstitals are

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created which are able to trap an immobile vacancy at the end of the irradiation process. The AA12 is an isotropic center showing a resolved hyperfine interaction with a single Si atom, as expected from an interstitial at a T_d site. This center was correlated with the DLTS E1 center, with a (0/+) level at $E_c - 0.39$ eV, which is observed between 77 and 270 K. E1 anneals readily under minority carrier injection, or otherwise at 270–350 K, when well known interstitial-impurity complexes start to form [41]. In Cz–Si, the AA12 is not observed immediately after irradiation, but it appears at 200 K following the annealing of the AA13 center, which has been attributed to a metastable self-interstitial-oxygen complex [42].

Remarkably, in contrast with Si, information about the properties of isolated *I* and *V* in Ge has first been obtained by PACs trapping experiments [9]. In these experiments, vacancies and interstitials were introduced by 1.2 MeV *e*-irradiation at 77 K, and their interaction with radioactive probes monitored as a function of the temperature and Fermi level position. The presence of *V* and *I* trapped at In probes was revealed by the observation of two quadrupole interactions labeled Q1 and Q2, respectively [9]. The vacancies, responsible for Q1, were only trapped at the negatively charged In probes when neutral, that is for a Fermi level below $E_v + 0.2$ eV. This indicates a (−/0) or (2−/0) acceptor level of *V* at that position, and this has been supported theoretically [43,30]. The Q2 signal resulting from the trapping of I^+ or I^{2+} by In was not observed in heavily n-doped Ge. This can be readily understood if the (0/+) level of *I* lies approximately at $E_c - 0.04$ eV. However subsequently, in an effort to reconcile a theoretical prediction for an acceptor level for the self-interstitial close to E_c [22], it was suggested that Q2 arises from a neutral interstitial migrating to In^-. It seems unlikely to us that the over-sized In^-probe would be an effective trap for I^0; given the high density of chemical donors present, we believe that is I^+ which is mobile at 200 K and complexes with In. Estimates of the diffusion barriers of V^0 and I^+ support this interpretation [24].

Very recently, *in situ* DLTS characterization of Ge with ≤ 3 MeV electrons starting at the irradiation temperature (22 K) opened up the possibility of monitoring the primary irradiation products and their dynamics before they interacted with each other or with impurities [6]. In n-type Ge, Frenkel pairs and liberated interstitials were observed, along with the double acceptor state of the E-center (*V*–Sb). The former was found to have a level of about 0.14 eV below the conduction band. It is known that Frenkel pairs are double acceptors [39] and presumably this level is the deeper one. Since the pairs exist with a range of sizes, it must represent an average value. The separated constituents, *I* and *V*, remained stable up to about 160 K—similar to that found by the PACs study. The presence of the self-interstitial was signaled by two coupled electron traps, the (0/+) and (+/2+) levels, placed at 0.08 and 0.24 eV below the conduction band (respectively), in excellent agreement with the theoretical predictions [24], and close to the M2 and M3 levels found by an early study [44]. In p-type Ge, despite the difficulty caused by the drift of the vacancy toward the junction, it was possible to one of its levels at about $E_v + 0.14$ eV. This is assigned to a $(2-/-)$ level of the vacancy and it was suggested that *V* does not possess any other levels. Such an assignment leads to conflict with the PACs and early Hall effect studies.

3. First-principles calculations

Several theoretical calculations have considered the properties of the self-interstitial in Si [10–21] and in Ge [22–24]. The equilibrium structures for *I* were found to be similar in both materials: a split-interstitial structure [Fig. 1(a)] or an interstitial near the *H* site [Fig. 1(b)] in the neutral charge state, and a caged interstitial (near the interstitial *H* and *T* sites) in the single or double positive charge state. This raises the question as to why such dissimilar effects are observed in the two materials.

In order to address this issue, we present here a comparative study of the relative energies, electric levels and transformation barriers for the most relevant structures of the self-interstitial. The calculations were performed using the density functional Aimpro code [45], as outlined in Ref. [24]. Contracted (C44G*) basis sets of Cartesian Gaussian orbitals (CGOs)[46] were optimized for bulk germanium and bulk Si. Test calculations were performed in order to confirm that the final results are converged with respect to the real space basis set used. The crystals were modeled by large clusters, generated using the experimental lattice constant of Ge ($a_{0,Ge}$ =5.657 Å) or Si ($a_{0,Si}$ = 5.431 Å) [47]. The values given in the present paper were calculated in the $Ge_{329}H_{172}$(Si_{329} H_{172}) clusters. Donor and acceptor levels were calculated using the semi-empirical marker method [46], adopting substitutional Au and S as markers [48–52].

It is important to note, that because of the tiny band gap found in local density calculations in Ge, clusters provide the only reliable way of treating the electrical activity of defects in contrast with supercell techniques. However, we shall show that the levels found for defects in Si are insensitive to the use of cluster or supercell methods.

3.1. Structure and energetics

In Ge, the most stable configuration of I^0 is a ⟨1 1 0⟩-split interstitial (D) [Fig. 1(a)] [22,23,24]. We found this to be about 0.50 eV lower in energy than the neutral I_H (Table 1). When positively charged, I_D does not remain aligned along the ⟨1 1 0⟩, but relaxes to a C_{1h} configuration labeled I_{D_d} [represented in white in Fig. 1(a)]. The distortion energy is 0.16 eV.

In contrast, in Si neutral I_D is practically degenerate in energy with the caged configuration, close to the *H* site. Moreover, in the positive charge state, the barrier between I_D^+ and $I_{H_d}^+$ is absent.

The caged self-interstitial behaves similarly in both materials. Its energy minimum depends on the charge state: in Ge, it is at the *H* interstitial site when the caged interstitial is neutral (I_H^0), at the *T* interstitial site when double positive (I_T^{2+}), and in a C_{3v} configuration, where the interstitial atom is between *H* and *T*, when single positively charged ($I_{H_d}^+$) [Fig. 2]; the same happens in Si, with the only difference that the caged self-interstitial is slightly displaced from the *H* site also in the neutral charge state [21,23,53]. The displacement from the center of the hexagonal ring is 0.32 Å, and the distortion energy is about 0.05 eV only. In the positive charge state the distortion is larger (0.73 Å). This affects a comparison of its energy levels with those of Refs. [19,17] who apparently considered only the D_{3d}- I_H and C_{2v}- I_D structures. In both materials, the *T* site was the only energy minimum found for I^{2+}.

We also investigated the possibility of existence of negative charge states (I^- and I^{2-}). However, both in Si and Ge, we did not

Table 1
Calculated energies (eV) of the self-interstitials in Si and Ge, in the ⟨1 1 0⟩-split interstitial (*D*), hexagonal (*H*) and tetrahedral (*T*) configurations, relative to the most stable species in each charge state (0 to 2+). Letters indicate an unstable initial configuration.

Configuration	Ge			Si		
	0	+	+2	0	+	+2
D/D_d	0.00	0.08	*T*	0.00	H_d	*T*
H/H_d	0.50	0.00	*T*	0.06	*T*	*T*
T	*H*	H_d	0.00	H_d	H_d	0.00

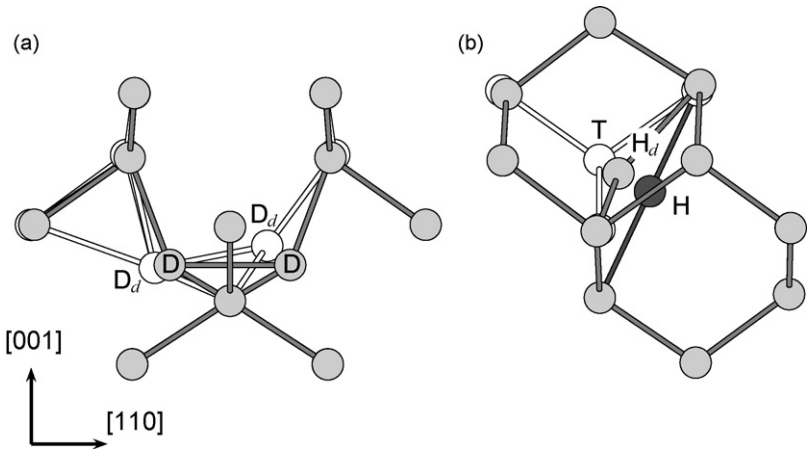

Fig. 1. Charge-dependent structures of the self-interstitial: (a) split-interstitial, with grey and white spheres representing the undistorted, ⟨1 1 0⟩ aligned (D) and distorted (D_d) defect structures, respectively, and (b) caged interstitial, with the positions of the interstitial atom at the H, H_d and T caged sites represented in dark grey, light grey and white, respectively.

Table 2
Comparison between the calculated vertical electrical levels (eV) of the self-interstitial in Si and Ge, in the ⟨1 1 0⟩-split and caged configurations. Rows marked Au_s and S_s indicate the marker used to calculate the level. The gaps are taken to be, respectively 0.74 and 1.17 eV.

Configuration		Ge		Si	
	Marker	(0/+)	(+/2+)	(0/+)	(+/2+)
D/D_d	Au_s	$E_v - 0.11$			
	S_s	$E_v - 0.10$			
$H/H_d/T$	Au_s	$E_c - 0.25$		$E_c - 0.23$	
	S_s	$E_c - 0.26$	$E_c - 0.08$	$E_c - 0.43$	$E_c - 0.26$

find I to be negatively charged for any Fermi energy, since the (−/0) level is outside the band gap.

3.2. Electrical levels

We consider first Ge. Cluster calculations suggest that the ⟨1 1 0⟩-split interstitial is electrically inactive (Table 2) [24]. Previous supercell calculations also placed its (0/+) level below the valence band maximum, although it is not clear whether a distortion was considered [23]. The same (supercell) study found an acceptor level close to the conduction band edge, in disagreement with the cluster results [22,23]. However, this discrepancy can be understood as arising from the band gap problem which places the conduction band very close to E_v [46].

In Si, the picture changes with regard to the donor level. The capture of a hole leaves the I_D defect unstable by removing the energy barrier separating $I^+_{D_d}$ and $I^+_{H_d}$; thus, the transformation to be considered is $I_D + h^+ \rightarrow I^+_{H_d}$ with the corresponding donor level at $E_c - 0.49$ eV. As in Ge, it is difficult in this case to establish a comparison with previous studies, which apparently did not consider the distorted structures found by us [19,17].

The caged interstitial is a double donor in both materials. The calculated vertical levels are shown in Table 2. We note that the difference between the $E(+/2+)$ and $E(0/+)$ associated with the caged interstitial, either in Si or Ge, is within the calculational error (estimated to be about 0.1–0.2 eV), and therefore the I_H/I_T system is not necessarily negative-U.

If enough thermal energy is provided, we expect the self-interstitial to assume the lowest energy structure in each charge state, which is I^0_D, $I^+_{H_d}$ or I^{2+}_T, and in such circumstances, the (0/+) and (+/2+) levels, associated with the $I^0_D \rightarrow I^+_H + e^-$ and $I^+_{H_d} \rightarrow I^{2+}_T + e^-$ transitions, are in negative-U order. In Ge, the (0/+) level, associated with $I^0_D \rightarrow I^+_H + e^-$ is found to be close below the valence band maximum, at $E_v - 0.03$ eV, using substitutional Au_s as marker, and well below the $I_{H\rightarrow T}{}^{(+/+2)}$ level at $E_c - 0.2$ eV. Hence, the defect will be

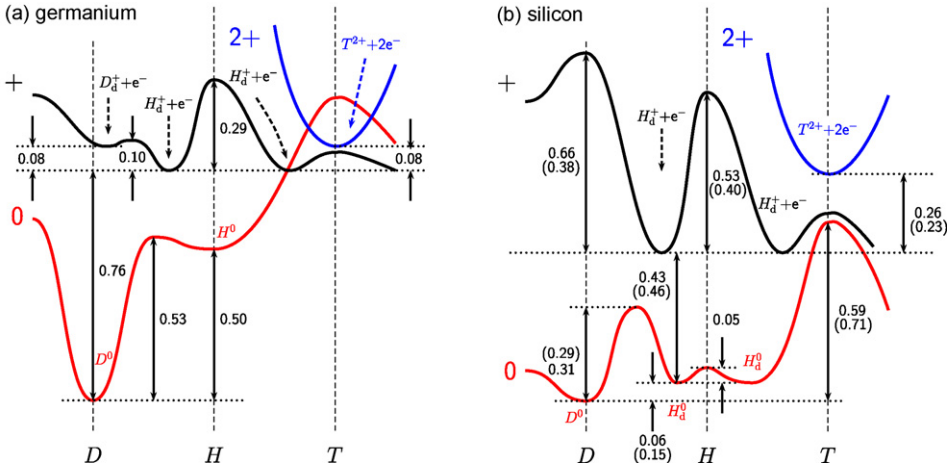

Fig. 2. Proposed configuration-coordinate diagrams for the self-interstitial in n-type Ge [24](a) and Si (b). Values in brackets are obtained in Si_{216}supercells.

thermodynamically stable only in the neutral and double positive charge states, with $E(0/+2)$ at about mid-gap. In Si, the situation is similar, but the $E(0/+2)$ level is now at about $E_c - 0.4$ eV. If the atomic rearrangement takes place in the neutral charge state, the energy required is about 0.53 eV in Ge and 0.31 in Si.

Energy levels close to the conduction band have been assigned to I by low temperatures studies in both Ge and Si. The calculations indicate that these are related to the first or second donor levels of the caged self-interstitial. In Ge, the (0/+) and (+/2+) levels were placed, respectively at $E_c - 0.08$ eV and $E_c - 0.24$ eV by DLTS [6]. PACs experiments have also placed a donor level at about $E_c - 0.040$ eV. Both are consistent with the theoretical results for the I_T/I_H system, given a 0.2 eV uncertainty. The interpretation of conductivity experiments is more controversial. However, the theoretical results also suggest an explanation for the observation of the two-state defect in p-Ge, with a level at about $E_c - 0.2$ eV [37,36,24].

In Si, it has been proposed that the E1 DLTS center and the AA12 EPR center are related to I_T [41,19]. The donor level of E1 (at $E_c - 0.39$ eV) is consistent with our calculations [$E(2+/+) = E_c - 0.3$ eV and $E(0/+) = E_c - 0.4$ eV]. E1 is correlated with the AA12 EPR center, which has T_d symmetry, with a ^{29}Si hyperfine interaction on one atom, and compatible with an assignment to I^+at a T site. It is difficult to conceive a model of a larger defect which would give rise to such hyperfine interactions.

4. Diffusion

Another remarkable difference between the self-interstitial in Si and Ge is found in the charge dependence of the migration energies. While in the former the migration energy increases monotonically with the removal of electrons from the defect, in the latter the most mobile species is the thermodynamically unstable positive charge state. This is readily seen as a consequence of the configuration-coordinate diagrams in Fig. 2.

The neutral self-interstitial has energy minima at D and H in Ge, or D and H_d in Si (Section 3.1), and migrates via a succession of transformations between the two structures (see Fig. 1 in Ref. [55]). In Ge, a diffusion step $I_D \rightarrow I_H \rightarrow I'_D$ requires a single activation energy of 0.53 eV (Fig. 2). In Si, the minimum energy path involves a low-energy (0.05 eV) reorientation of H_d by passing through the undistorted H site ($I_D \rightarrow I_{H_d} \rightarrow I'_{H_d} \rightarrow I'_D$) but the dominant energy barrier is also that of the transformation from the split-interstitial to the caged site, which is 0.31 eV. This is not the same path considered by Needs [16] where the interstitial atom does not leave the $(\bar{1}\,1\,0)$ plane and which we found to be higher in energy.

The migration of the positive self-interstitial requires a succession of jumps between H_d sites with an activation energy of 0.29 eV in Ge and 0.53 eV in Si.

The double positive charge state is the less mobile, requiring an activation energy of 1.23 eV in Ge, or 1.46 eV in Si, to move between T sites, zig-zagging along the $\langle 1\,1\,1\rangle$. The calculated migration barriers for the neutral and positive charge states are in good agreement with a recent NEB calculation.[17]

5. Relation between *I* and *V* and the effects of radiation in Si and Ge

The key question now is whether the comparative study between the self-interstitial in Si and Ge helps to explain the asymmetries between the observed effects of radiation in the two materials. Before analyzing this, it is useful to summarize the basic properties of V and I in Si and Ge.

The vacancy in both materials has different charge states. In Si, it can exist in five charge states from $V^=$ to V^{2+}[2]. In Ge, we believe it is stable in at least two: V^{2-}, and V^0; V^-may be just stable or the defect is a negative-U center [43]. In contrast, the interstitials on Si and Ge have similar configurations in their three charge states: in the neutral charge state, at a $\langle 1\,1\,0\rangle$ split-interstitial configuration and between the H and T sites in the positive and double positive charge states. They have similar (+/2+) levels, at about $E_c - 0.3$ eV in Si and $E_c - 0.1$ eV in Ge. When reconfiguration between different defect structures is allowed, both defects are negative-U with the donor level lying below the (+/2+) level. No acceptor level was found for any configuration studied in both Si and Ge.

The major differences arise from the relative stability of the split and caged configurations. The vertical (0/+) level of the split-interstitial is below the valence band for Ge (calculated $\sim E_c - 0.8$ eV), whereas in Si the same structure becomes unstable in the positive charge state. It spontaneously relaxes to the neighborhood of the H site, and the resulting (0/+) level is deep in the gap, at $E_c - 0.5$ eV. In Ge, it seems that there are two completely different interstitial forms. I_D is electrically inactive and therefore always remains neutral.

Thus, in p-Si, unstable I^{2+}– V^{2+} pairs are expected to form during or following low temperature irradiation [31]. Since I is very mobile, it will preferentially be trapped at B^-or Al^-, or possibly O and C. This interpretation assumes that during 1 MeV electron irradiation, long range diffusion of I is possible due to an athermal Bourgoin mechanism [3,13]. In fact, the configuration-coordinate diagram allows this possibility, provided that the concentration of minority carriers is enough large: the trapping of two electrons by I_T^{2+} leaves the I_T interstitial unstable, and it tends to relax to the $I_{H_d}^+$ configuration where a barrier of 0.25 eV exists to the I_D site, or is possibly carried to a I_D site. The I_D^0 configuration has a gap donor level at $E_v + 0.49$ eV, and in principle can trap a hole leading to I_H^+. Following this, a second hole trapping can switch the defect to a T site which can be different from the starting point. This draws a possible process for long range migration.

Clearly, the situation had to be different in p-Ge as the vacancy is neutral and I_T^{2+}- V^0 pairs are attractive, likely recombining during irradiation if one of the partners is mobile. Surviving self-interstitials are presumably I_D, which are electrically inactive and cannot migrate athermally during irradiation. This makes p-Ge very resistant to damage, in comparison with p-Si which is easily damaged by near-threshold, low dose electron-irradiation.

In n-Si, the defect introduction rates below 60 K are also low [33,2]. During irradiation below 60 K, the self-interstitial seems able to move rapidly by switching between I^0 and I^{2+}, ultimately recombining with near-by V^{2-} rather than with the positively charged dopants. This suggests an explanation for the recombination of the majority of I–V pairs below 60 K during the irradiation process. The expected radiation products, V^{2-} and I^0, apparently only form above ~60–70 K when V^{2-} can become mobile and is able to escape from the correlated self-interstitial [3]. However, the details of the process are unclear: for example, why does not V^{2-} combine with I^0 above 65 K?

Although the charge states of the defects – V^{2-} and I^0 – are the same in Si and Ge, their evolution is very different n-doped material. In Ge, the carrier removal rates at 4 K are very large showing that long range motion of interstitials does not occur as readily as in Si. However, V^{2-} also migrates at about 60 K in Ge and leads to recovery at this temperature.

6. Summary

Density functional calculations show that the self-interstitial in germanium is a bistable defect, preferring a split-interstitial configuration when neutral, but a caged interstitial position when

positive or double positively charged. Although these two defect forms also exist in Si, an important difference is that in this material, I_D is electrically active and can act as a hole trap, spontaneously switching to the $I^+_{H_d}$ site. Thus a long-range migration path is established. Using these results it is possible to explain some of the striking effects seen in low temperature irradiation of Ge, as well as some important differences between the materials.

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