Short communication

A-centers and isovalent impurities in germanium: Density functional theory calculations

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ABSTRACT

In the present study density functional theory calculations have been used to calculate the binding energies of clusters formed between lattice vacancies, oxygen and isovalent atoms in germanium. In particular we concentrated on the prediction of binding energies of A-centers or oxygen interstitials that are at nearest and next nearest neighbor sites to isovalent impurities (carbon, silicon and tin) in germanium. The A-center is an oxygen interstitial atom near a lattice vacancy and is an important impurity-defect pair in germanium. In germanium doped with carbon or silicon, we calculated that most of the binding energy of the cluster formed between A-centers and the carbon or silicon atoms is due to the interaction between the oxygen interstitial atom and the carbon or silicon atoms. For tin-doped germanium most of the binding energy is due to the interaction of the oversized tin atom and the lattice vacancy, which essentially provide space for tin to relax. The nearest neighbor carbon–oxygen interstitial and the silicon–oxygen interstitial pairs are significantly bound, whereas the tin–oxygen interstitial pairs are not. The results are discussed in view of analogous investigations in isovalently doped silicon.

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1. Introduction

The technological requirement to replace silicon (Si) with higher mobility substrates has regenerated interest in the use of alternative substrates such as silicon germanium ($Si_{1−x}Ge_x$) alloys and germanium (Ge) in advanced nanoelectronic and photovoltaic applications [1–15]. The advantages of these substrates include their relative compatibility with Si manufacturing processes, their smaller band gap and increased dopant solubility compared to Si [1–3]. Additionally, developments in high-dielectric constant (high-k) dielectrics allow their incorporation [15]. The aggressive scaling of modern devices leads to devices with characteristic dimensions of nanometers and therefore the understanding of defect processes and the stability of related complexes is increasingly important in group IV semiconductors [13,14,16–18].

Vacancies (V) in Ge are the dominant point defects controlling processes such as self-diffusion, dopant diffusion and cluster formation [1,4,9,19–21]. The pressure and doping dependence of self-diffusion investigated by Werner et al. [20] clearly demonstrates the importance of the vacancy in Ge. However, the doping dependence was assigned to neutral and singly negatively charged vacancies [20]. More recent results clearly reveal that the vacancy in Ge is doubly negatively charged even under intrinsic conditions [8]. Moreover, the diffusion behavior of copper in Ge provides additional evidence of the dominance of vacancies in Ge [21].

In Czochralski-grown Ge the concentration of oxygen (O) is not as significant as is in Si [1]. The experimental solubility of O in Ge is of the order 10^{18} cm^{-3} (Ref. [22]). Nevertheless, O can be incorporated into Ge when H_2O vapour or oxygen gas is present in the growth atmosphere [1]. Importantly, O interstitials (O_i) are electrically inactive in Ge and consequently O is not a problematic impurity [1]. The interaction of vacancies with oxygen in Ge to form A-centers has been experimentally identified in Ge [23–27]. In previous density functional theory (DFT) investigations Coutinho et al. [28] have studied O in Ge and predicted that VO and VO_2 clusters are stable.

Carbon (C), Si and tin (Sn) are important isovalent impurities in Ge. In recent experimental and theoretical work it was demonstrated that donor atom diffusion in Ge can be retarded in the presence of C [8,29,30]. The solubility of C in Ge is limited (about 2×10^{14} cm^{-3} (Ref. [31]). There is complete solubility of Si in Ge (and vice versa) with the properties of the resultant alloy being strongly influenced by the composition [12]. Finally, Sn is stable in the diamond structure (grey tin) at low temperatures [32]. The solution of Sn in Ge can influence its defect properties as previ-

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ous DFT work predicts the formation of Sn–V complexes [33,34]. In previous, experimental work Chizmeshya et al. [35] synthesized $Sn_{1-x}Ge_x$ alloys with a high Sn content.

The main aim of the present study is to contribute towards a better understanding of the role and association of isovalent impurities with O_i and A-centers in Ge. The results are compared with experimental and theoretical studies in Si.

2. Methodology

2.1. Details of calculations

Calculations were performed using the plane wave DFT code CASTEP [36,37]. Exchange and correlation interactions are described using the generalized gradient approximation (GGA) corrected density functional of Perdew, Burke and Ernzerhof (PBE) [38] in conjunction with ultrasoft pseudopotentials [39]. The plane wave basis set was expanded to a cut-off of 350 eV. A $2 \times 2 \times 2$ Monkhorst-Pack (MP) [40] k-point grid is adopted with a supercell consisting of 64 atomic sites. In all the calculations the unit cell parameters and atomic fractional coordinates were allowed to relax (constant pressure conditions).

2.2. Approximations

The efficacy, limitations and convergence of the computational methodology used was discussed in recent studies [41,42]. DFT calculations based upon the GGA (or the local density approximation) underestimate the formation energies of defects in Ge (or Si or SiGe), mainly because of the lack of exact exchange in these functionals [43,44]. For this reason the present paper is focused on binding energies (differences in energy) and clusters in their neutral charge state as these are expected to be less sensitive to systematic errors in the exchange-correlation energy (as would be the formation energies of charged defects). The calculation of formation energies will be addressed in future work using more advanced computational techniques. The 64 atomic site supercell is sufficient as discussed in recent work in Si, SiGe and Ge [17,19,30,45]. In the 64 supercell the oxygen atoms (or dopant atoms) are separated from their periodic images by six nearest neighbor sites. At these distances the dopant–dopant interactions are practically zero, and hence the dopant and its periodic image interactions will not affect the results. Larger MP k-point grids and supercell sizes lead to small differences in the defect energies, consistently with previous work in Si [46]. An example, is the formation energy of the neutral Si vacancy (predicted to be 3.23 eV), which is only 0.06 eV higher compared to the 256 supercell calculation of Probert and Payne [46].

3. Results and discussion

The association of isovalent impurities with oxygen and/or point defects such as V in Ge is not investigated in such detail as in Si. Device properties can be influenced by the distribution of impurities, dopants and defects. Therefore, processes such as cluster formation can be technologically important.

A way to examine cluster formation is by quantifying the attraction or repulsion between the dopants and/or defects, which form a defect cluster. The binding energy of m substitutional D atoms to an O_i atom and n V to form a $D_m V_n O_i$ cluster in Ge is:

$$E_b(D_m V_n O_i Ge_{N-m-n}) = E(D_m V_n O_i Ge_{N-m-n}) - mE(DGe_{N-1})$$

$$-E(O_i Ge_N) - nE(VGe_{N-1}) + (m+n)E(Ge_N) \quad (1)$$

where $E(D_m V_n O_i Ge_{N-m-n})$ is the energy of a N lattice site supercell (here $N=64$) containing N-m-n Ge atoms, mD atoms, one O_i atom

Table 1
Predicted binding energies (eV) for the nearest neighbor (NN) DO_i pairs [refer to Fig. 1(b)] and the next nearest neighbor (NNN) DO_i pairs [refer to Fig. 1(c)].

Defect pair	NN	NNN
CO_i	−0.40	−0.35
SiO_i	−0.92	−0.01
SnO_i	0.45	0.07

and nV; $E(DGe_{N-1})$ is the energy of a supercell containing one D atom and $N-1$ Ge atoms; $E(O_iGe_N)$ is the energy of a supercell containing one O_i atom and N Ge atoms; $E(VGe_{N-1})$ is the energy of a supercell containing a V and $N-1$ Ge atoms; and $E(Ge_N)$ is the energy of the N Ge atom supercell. A negative binding energy implies that the defect cluster is stable with respect to its constituent point defect components.
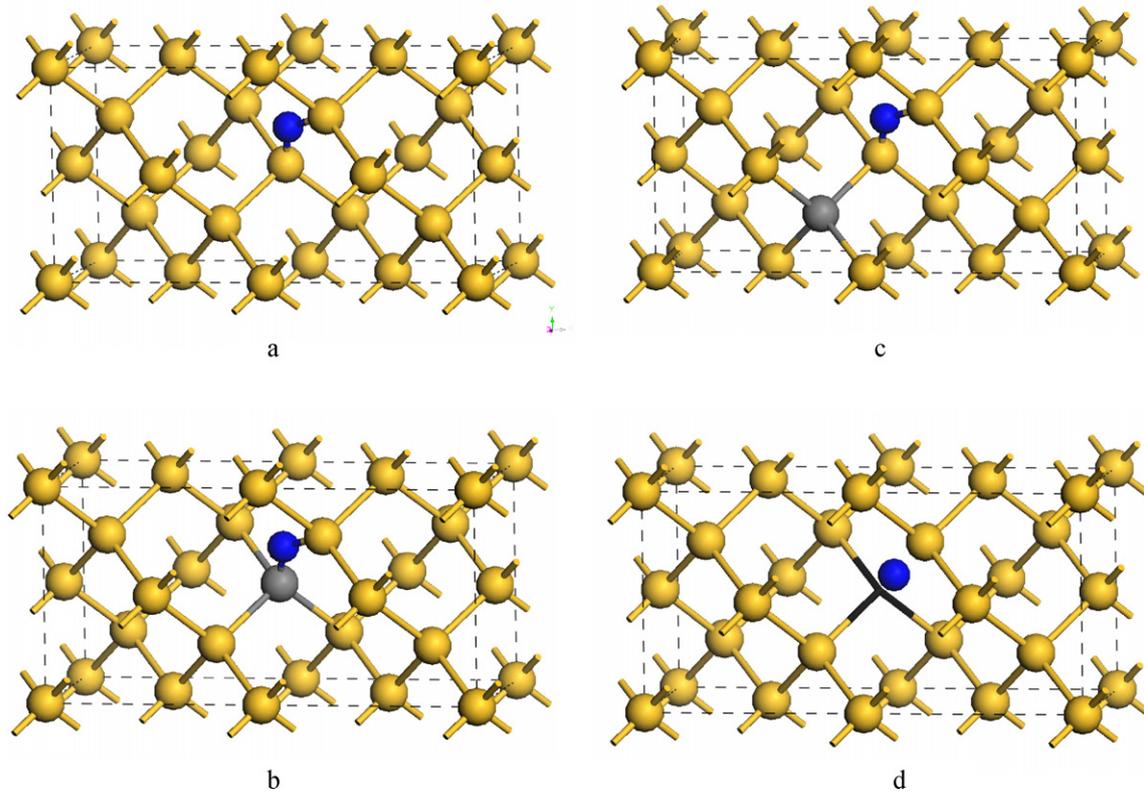
In Fig. 1(a) we represent how an oxygen interstitial atom bonds to two neighbouring Ge-atoms. Table 1 lists the predicted binding energies required to associate the O_i with an isovalent impurity to form nearest neighbor (NN) and next nearest neighbor (NNN) CO_i, SiO_i and SnO_i pairs [refer to Fig. 1(b) and (c), respectively]. The binding energy of these pairs can be calculated using Eq. (1) with $m=1$ and $n=0$. The most bound pair is the NN SiO_i pair (−0.92 eV, see Table 1), however, when the Si atom is placed at a NNN with respect to the O_i the binding energy is reduced to −0.01 eV. Therefore, a migrating O_i can only be associated to a Si atom if it forms a bond with it. Considering C containing pairs they are less bound than the NN SiO_i pair but retain most of their binding energy at the NNN configuration (Table 1). Consequently, C atoms will behave differently than Si in Ge as they can attract O_i from further away. The positive SnO_i interaction both at NN and NNN configurations (see Table 1), indicates that the Sn and O_i interaction is repulsive. This will mean that these two species will not be in the vicinity of each other. This is not surprising as the Sn is the largest isovalent atom considered (and larger compared to Ge) therefore the introduction of the O_i will limit the available space for its introduction in the lattice.

The A-center in Ge (Fig. 1(d)) was predicted to be bound with −0.45 eV (using Eq. (1) with $m=0$ and $n=1$). This is comparable to the −0.36 eV value of Coutinho et al. [28] (using local-density functional theory) as the 0.09 eV difference can be attributed to the differences in the computational methodologies. When an A-center approaches an isovalent impurity in Ge the binding energy of the resultant clusters (see Table 2) differs from the binding energy of the A-center in undoped Ge. For most clusters considered, the NN configurations are more bound compared to the NNN configurations (see Fig. 2 and Table 2). The NN $SiVO$ is less bound than the NNN $SiVO$ cluster as the Si–V interaction is not energetically favorable. In previous DFT work [17] it was calculated that both the NN and NNN SiV pairs in Ge are not stable but of the two configurations the NNN is more favorable (positive binding energies

Table 2
Predicted binding energies (eV) of the neutral VO [refer to Fig. 1(d)], VO pairs in the presence of nearest neighbor (NN) isovalent impurities to the V [DVO refer to Fig. 2(a)], VO pairs in the presence of NN isovalent impurities to the O_i [DOV refer to Fig. 2(c)], VO pairs in the presence of next nearest neighbor (NNN) isovalent impurities to the V [DVO refer to Fig. 2(b)], VO pairs in the presence of NNN isovalent impurities to the O_i [DOV refer to Fig. 2(d)].

Defect cluster	NN	NNN
VO	−0.45	–
CVO	−0.94	−0.86
$SiVO$	−0.26	−0.55
$SnVO$	−1.09	−0.64
COV	−0.94	−0.92
$SiOV$	−1.22	−0.55
$SnOV$	−0.89	−0.65

Fig. 1. A representation of (a) oxygen interstitial, (b) the nearest neighbor DO_i pairs, (c) the next nearest neighbor DO_i pairs, and (d) the A-center in Ge. Yellow and grey spheres represent the Si and D atoms, respectively and O_i are represented by blue spheres. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)
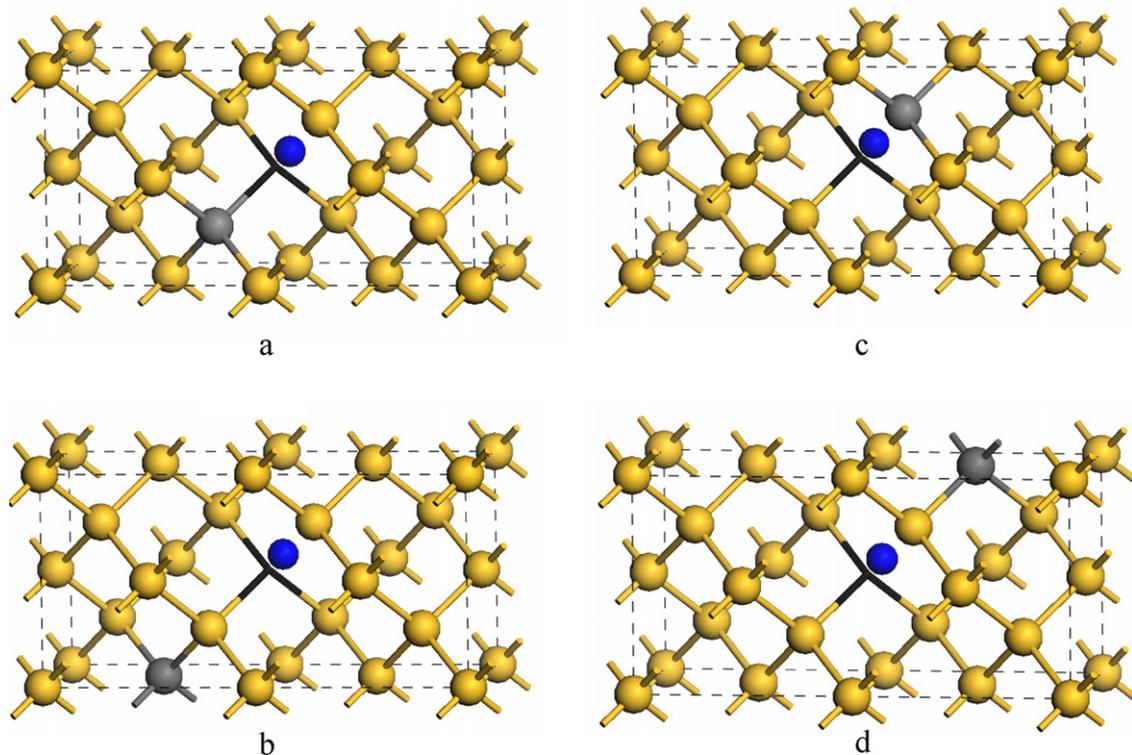
Fig. 2. A representation of (a) the nearest neighbor (NN) DVO cluster, (b) the next nearest neighbor (NNN) DVO cluster, (c) the NN DOV cluster and (d) the NNN DOV cluster in Ge. Yellow and grey spheres represent the Si and D atoms, respectively. O_i are represented by blue spheres and V by the black sticks. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

of 0.24 eV and 0.03 eV, respectively). In the diamond lattice there are two possible NN configurations of an isovalent substitutional impurity with respect to the A-center. At the first configuration the isovalent atom is at a NN site to the vacancy forming a DVO cluster [see Fig. 2(a)], whereas in the second configuration it is closer to the O$_i$ atom [see Fig. 2(c)]. For C both configurations are equally bound, for Sn and Si the first and second configurations are more bound, respectively (see Table 2). These differences illustrate the complex changes of the binding energies that can exist when an A-center associates with an isovalent atom in Ge. Additionally, it is possible to form Si$_x$O$_y$V$_z$ clusters in which the oxygen atoms populate substitutional sites in the lattice as discussed in a recent study [47].

It is of interest that although the Sn atom repels the O$_i$ it is strongly bound (by −1.09 eV, see Table 2) when part of the SnVO cluster. This is because in the SnVO cluster the large Sn atom relaxes in the vacant space provided by the V. Note that the binding energy of the SnV pair is −0.61 eV [33], implying that the relaxation of the oversized Sn atom in the vacant site reduced the energy of the system (compared to the situation where Sn and V were isolated). Conversely, for the CVO (or SiVO) clusters most of their binding energy is due to the interaction between the C and O$_i$ (or between the Si and O$_i$, respectively) (see Table 1). The binding energies for the CV and SiV pairs are −0.07 eV and 0.25 eV, respectively [33]. Finally, for C the NNN cluster configurations are within 0.08 eV from the NN configurations, whereas for Si and Sn clusters the differences are more pronounced.

Experimental results on the interaction of A-centers with isovalent impurities in Ge are not existent to our knowledge. Conversely, these issues have been examined in more detail in Si [48–53]. Comparing with previous studies concerning the association of isovalent impurities with oxygen in Si a number of differences can be traced. Fig. 3 compares the binding energies with respect to the sum of covalent radii for the most bound DO$_i$ pairs and DVO (or DOV) clusters in Ge and Si. For DO$_i$ pairs, the SiO$_i$ pair in Ge is far more bound than the GeO$_i$ pair in Si (see Table 1). Therefore, under equilibrium conditions it would be expected that the concentration of SiO$_i$ in Ge will be higher than the concentration of GeO$_i$ in Si (only of course in the case that the initial concentration of O$_i$ and isovalent impurities is equal in both host materials). The CO$_i$ and SnO$_i$ pairs have similar energies in Si and Ge, however, only the CO$_i$ pairs are bound (see Fig. 3(a)). The DVO or DOV clusters in Si are more bound compared to the analogous clusters in Ge (refer to Fig. 3(b)). The differences in cluster binding energies in Si and Ge are more significant for the smaller (i.e. C) and larger (i.e. Sn) isovalent dopants. Consequently, A-centers in isovalent-doped Ge will behave differently compared to A-centers in isovalent-doped Si.

The binding energy of the A-center in Ge and its association with isovalent impurities on NN and NNN sites can affect the interdiffusion of group IV semiconductor heterostructures. In that respect intentionally doping with oxygen may be effective to retard the interdiffusion of such heterostructures containing C or Si. This is consistent with the previous experimental study of Silvestri et al. [54], which determined that Si diffusion in Ge is retarded by the presence of oxygen. The situation for Sn is more complicated as Sn repels O$_i$ but clusters with A-centers. The present paper is a continuation of efforts to understand the interaction of isovalent impurities with oxygen and vacancies in group IV semiconductors. These can be important for the thermal stability of group-IV semiconductor heterostructures. To clarify further these issues it will be necessary to perform further diffusion experiments with oxygen and isovalent impurities as a range of concentrations as these will illuminate their effect.

Depending upon the experimental conditions (i.e. annealing temperature, damage in the lattice by implantation, etc.) there is the possibility for the formation of more geometrically complicated
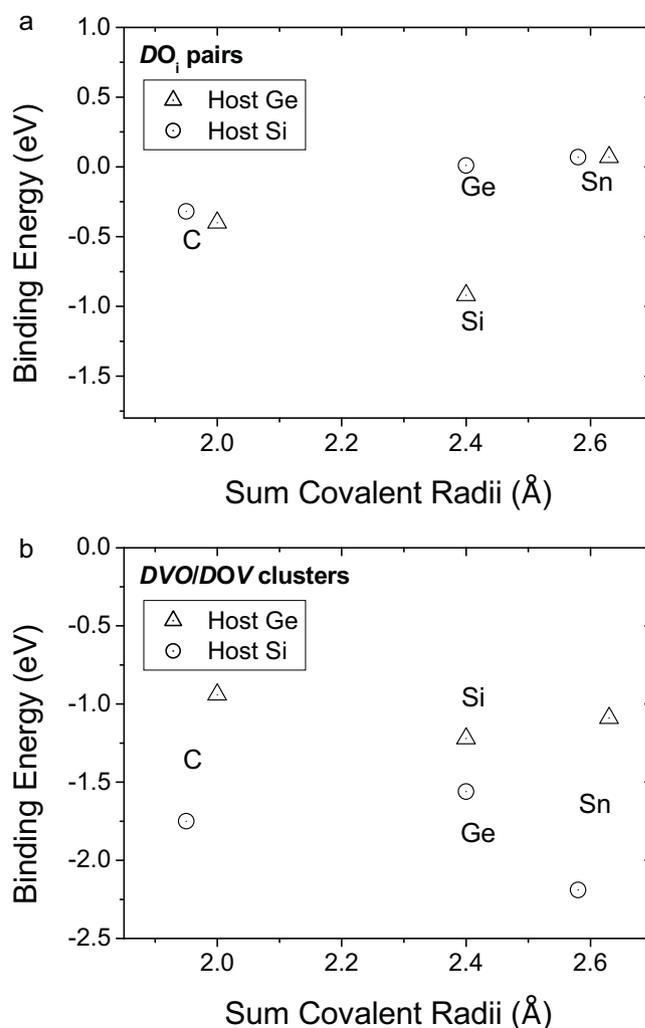

Fig. 3. Binding energies (eV) with respect to the sum of covalent radii (isovalent impurity and host atom) for the most bound (a) DO$_i$ pairs and (b) DVO or DOV clusters considered in Ge (present study) and in Si (refer to Ref. [53]).

defect clusters. These may prove to be important when assessing the effect of isovalent impurities in the stability of A-centers in Ge. For example, the solubility of carbon in Ge is very low but it is possible to grow Ge–C layers with carbon concentrations of a few percent or to implant C into Ge [31,55]. In the latter case only a fraction of the carbon is on substitutional site whereas carbon contents of about 1% can be obtained on substitutional sites in Ge epitaxial layers grown by means of molecular beam epitaxy. In turn, the diffusion properties of C may be affected by the built-in strain [55].

4. Conclusions

Electronic structure calculations were applied to investigate the interaction of isovalent impurities with O$_i$ and A-centers in Ge. We predicted that O$_i$ binds with C and Si impurities in Ge but not with Sn. The binding energies of A-centers in the vicinity of isovalent atoms in Ge are higher compared to the binding energies of A-centers in undoped Ge. Clusters formed between isovalent atoms, O$_i$, and vacancies in Si are more bound compared to Ge. This will imply that these clusters will behave differently in Si and Ge and also in Ge-rich or Si-rich regions of Si$_{1−x}$Ge$_x$ alloys. It should be expected that under conditions were the concentration of the impurities, oxygen and vacancies in Si is equal to Ge, the

concentration of D*V*O/DO*V* clusters will be more significant in Si. These clusters will also be more thermally stable in Si than in Ge but their kinetics will need to be studied in detail with diffusion experiments.

Acknowledgements

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