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Fluorine codoping in germanium to suppress donor diffusion and deactivation

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Electronic structure calculations are used to investigate the stability of fluorine-vacancy (F_nV_m) clusters in germanium (Ge). Using mass action analysis, it is predicted that the F_nV_m clusters can remediate the concentration of free V considerably. Importantly, we find that F and P codoping leads to a reduction in the concentration of donor-vacancy (DV) pairs. These pairs are responsible for the atomic transport and the formation of D_nV clusters that lead to a deactivation of donor atoms. The predictions are technologically significant as they point toward an approach by which V-mediated donor diffusion and the formation of inactive D_nV clusters can be suppressed. This would result in shallow and fully electrically active n-type doped regions in Ge-based electronic devices. © *2009 American Institute of Physics*. [doi:10.1063/1.3224900]

I. INTRODUCTION

Since boron (B) has a very low diffusivity in Ge, it will form well defined p-type regions.[1] Conversely, n-type dopants such as phosphorus (P), arsenic (As), and antimony (Sb) exhibit an enhanced diffusion behavior under extrinsic doping conditions,[2–4] which hinders the formation of shallow doped regions. It has been determined that donor diffusion in Ge is mediated by V.[4] Moreover, the formation of D_nV clusters containing n donor atoms around a V leads to a deactivation of a significant proportion of the donor profile, especially under high concentration conditions.[5] This is consistent with the recent experimental study of Brunco *et al.*,[6] where the peak concentration of P was attributed to the formation of P clusters. To address the issues of enhanced donor diffusion and deactivation of donor species, codoping with carbon (C) has been considered.[7,8] It was found that even though codoping with C leads to a retardation of donor atom transport via the formation of less mobile $C(VD)_n$ clusters, such clusters trap additional donor atoms.[7,8] Accordingly, the deactivation problem remains unsolved by carbon codoping. To effectively retard both the diffusion and the deactivation of donor atoms, the concentration of free vacancies must be effectively reduced or kept apart from the donor species. In this way, the formation of DV pairs can be hampered. Thereby not only the diffusion of the donor atoms via DV pairs but also the formation of D_nV clusters via the interaction of DV pairs with substitutional donors[7] can be suppressed.

A number of experimental[9–11] and theoretical[12–17] studies address the issue of doping Si with F. These provide evidence that F_nV_m clusters are stable in Si. In particular, simulation studies suggested that the most abundant F_nV_m clusters are those in which all the V dangling bonds are saturated by F.[16] Interestingly, recent experimental work[10] on F-implanted preamorphized Si determined that the predicted F_nV_m clusters do not exist in detectable concentrations. Nevertheless, that study[10] is consistent with theoretical work[14] as F implantation can effectively suppress the transient-enhanced self-interstitial mediated diffusion of acceptor atoms such as B.

In the present study, we propose doping with F to affect the concentration of free V in Ge, thereby suppressing D diffusion. We apply electronic structure calculations to identify the most stable F_nV_m clusters in Ge (for $\{m=1, n=1-4\}$ and $\{m=2, n=1-6\}$). With the use of mass action analysis, we report the relative concentration of these clusters in Ge over a wide temperature range. Additionally, we investigate F and P codoping and its effect on P diffusion and deactivation.

II. THEORETICAL METHODOLOGY

The calculations were performed with the density functional theory (DFT) code CASTEP (Ref. 18) using the Perdew–Burke–Ernzerhof generalized gradient approximation functional[19] and ultrasoft pseudopotentials.[20] A 64 site tetragonal diamond structure Ge supercell was repeated in space using periodic boundary conditions. A plane wave basis with an energy cutoff of 350 eV and a $2\times2\times2$ Monkhorst–Pack[21] **k**-point sampling was employed. In all the calculations, the unit-cell parameters and the atomic coordinates were relaxed using energy minimization until the largest forces were less than 0.05 eV/Å with a total energy convergence tolerance not exceeding 10^{-5} eV/atom. The efficacy of this approach to adequately describe the defect chemistry of Ge and related materials has been demonstrated by comparing predictions with experimental results.[22–24] We also carried out some calculations for F_nV_m clusters in Si and found binding energy values that were very similar to those reported previously.[13,14] For example, our predicted binding energy of the FV pair in Si is −2.23 eV, which is in excellent agreement with the DFT study of Lopez *et al.*[14] (−2.0 eV) and the experimental value of Pi *et al.*[9] (−2.2 eV).

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It has been previously established that the bandgap of Ge is underestimated due to the inappropriate description of exchange.[25] For this reason, the present study focuses on uncharged supercell calculations and binding energies (differences in energies, see definition below), which are expected to be less affected by the systematic errors in the exchange-correlation energy.

The attraction between F interstitial atoms, D substitutional atoms, and V can be quantified by calculating the binding energies. For example, the binding energy of n F interstitial atoms to m V and x D atoms to form a $D_xV_mF_n$ cluster in Ge is given by

$$E_b(D_xV_mF_nGe_{N-x-m}) = E(D_xV_mF_nGe_{N-x-m}) - xE(D_xGe_{N-1}) - mE(VGe_{N-1}) - nE(FGe_N) + (x+m+n-1)E(Ge_N), \quad (1)$$

where $E(D_xV_mF_nGe_{N-x-m})$ is the energy of an N lattice site supercell (here, N=64) containing $N-x-m$ Ge atoms, x D atoms, n F atoms, and m V; $E(DGe_{N-1})$ is the energy of a supercell containing one D and $N-1$ Ge atoms; $E(FGe_N)$ is the energy of a supercell containing one F and N Ge atoms; $E(VGe_{N-1})$ is the energy of a supercell containing one V and $N-1$ Ge atoms; and $E(Ge_N)$ is the energy of the N Ge atom supercell. A negative binding energy indicates that the $D_xV_mF_n$ cluster is more stable with respect to x isolated D, n isolated F, and m isolated V.

III. RESULTS AND DISCUSSION

When the F interstitial is in-between two Ge atoms in a bond-center position, it forms two covalent σ bonds, releasing one electron to the crystal, and effectively becomes positively charged for most conditions (see Lopez *et al.*[14] for a more detailed discussion of F interstitials in Si). We have also considered, in Ge, the tetrahedral position for the F interstitial. In this position, the F interstitial must capture an electron to complete its outer shell, and as such it is expected to be negatively charged. We find the bond-center position for the Ge interstitial to be favored by 0.38 eV compared to the tetrahedral position. These predictions agree with previous results for F interstitials in Si.[13,14]

As the bond-center F interstitials are positively charged, they should repel each other, whereas the tetrahedral F interstitials should repel each other because they are negatively charged. Conversely, F interstitial pairs consisting of a bond-center and a tetrahedral interstitial should be bound (F_2). The predicted binding energy for this F_2 pair is −0.97 eV.

In Ge, V dominate most defect processes due to their lower formation energies and consequently their higher concentrations compared to self-interstitials.[26] For this reason, the interaction between F interstitials and Ge self-interstitials was not considered in the present study. Doubly negatively charged V have been identified to be dominant in Ge under intrinsic and n-type doping conditions.[2,7] Here, F_nV_m clusters were considered to be formed from isolated F interstitials, corresponding to the low energy bond-center configuration and isolated V, whose energy was calculated in a charge neutral cell in which the charge was allowed to redistribute to the lowest energy configuration (binding energies are reported in Table I).

TABLE I. Binding energies E_b (eV) for F_nV_m clusters in Ge.

Defect cluster	E_b
F_2	−0.97
V_2	−0.48
V_3	−1.25
V_4	−2.14
FV	−1.19
F_2V	−2.22
F_3V	−3.27
F_4V	−5.00
FV_2	−1.94
F_2V_2	−3.53
F_3V_2	−4.87
F_4V_2	−5.90
F_5V_2	−7.23
F_6V_2	−8.56

For every V in the Ge lattice, there exist four dangling bonds. When a F interstitial encounters a dangling bond, the bond is saturated by forming an FV pair. The predicted binding energy of the FV pair is −1.19 eV (see Table I), and the F–Ge bond distance is 1.8 Å. F interstitials are attracted to the V forming stable F_nV clusters until all four dangling bonds are saturated. The most stable F_nV cluster configurations are those where the F atoms are displaced from inline V–F–Ge dangling bond directions so that the F atoms are more greatly separated, and Ge–F bond distances are also increased. Consider, for example, the F_4V cluster. In the cluster with inline Ge–F bonds [see configuration in Fig. 1(b) of Ref. 15], the F–F distance is 2.30 Å. The cluster assumes the lower energy configuration [see configuration in Fig. 1(a) of Ref. 15], which is more favorable by −2.20 eV (the F–F distance is 2.64 Å). An analogous behavior has been recently observed for F_nV clusters in Si.[14,15]

For F_nV_m clusters containing two lattice V, the situation is similar with F atoms saturating the dangling bonds and displaced from direct V–F–Ge configurations (see Table I). The energy gain for every F interstitial added is more than 1 eV for all F_nV_m clusters considered. Generally, clusters in which all dangling bonds are saturated exhibit the highest binding energies.

To quantify the relative concentrations of F_nV_m clusters, we applied mass action analysis,[27] so that the concentration of an F_nV_m cluster (i.e., $[F_nV_m]$), relative to the concentration of unbound F atoms (i.e., [F]), and the concentration of unbound V (i.e., $[V]$) is given by

$$\frac{[F_nV_m]}{[F]^n[V]^m} = \exp\left(\frac{-E_b(F_nV_m)}{k_BT}\right), \quad (2)$$

where k_B is Boltzmann's constant and T is the absolute temperature. The binding energies of clusters are reported in Table I.

From Eq. (2), it can be concluded that the formation of the larger clusters is not only dependent on the temperature and the binding energy differences between the clusters but

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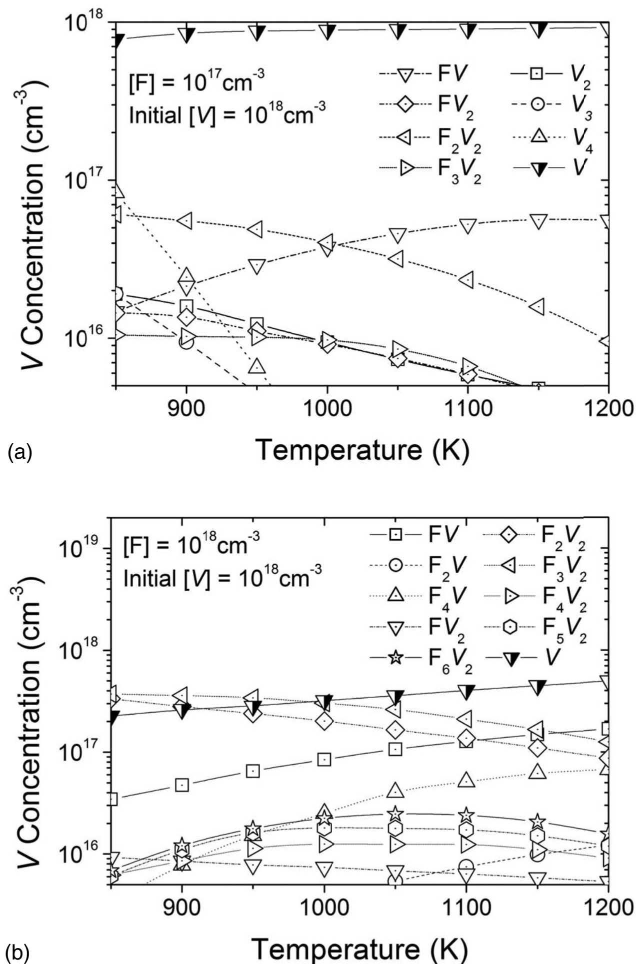

FIG. 1. The temperature dependence of the concentration of F_nV_m clusters for an initial V concentration of 10^{18} cm^{-3} and F concentrations of (a) 10^{17} cm^{-3} and (b) 10^{18} cm^{-3}.

also on [F] and [V]. Here, we assume that the implanted F concentration is either 10^{17} cm^{-3} [see Fig. 1(a)] or 10^{18} cm^{-3} [see Fig. 1(b)] and that the concentration of V is 10^{18} cm^{-3}. The value assumed for the V concentration simulates conditions that exist after dopant implantation.[5] Ion implantation is mainly used to introduce the dopant of interest into the semiconductor. This V concentration, which is significantly higher compared to the equilibrium concentration of V in Ge, will depend on the experimental conditions (e.g., implantation energy and dose). Changes to the vibrational entropy of the system are assumed to be small and are not included.[27] Mass action analysis has been previously applied to address cluster formation in semiconductors.[5,8,28–30] Using Eq. (2), two sets of simultaneous equations for F_nV_m clusters were considered. The first for an initial V concentration of 10^{18} cm^{-3} and F concentration of 10^{17} cm^{-3} and the second for an initial V concentration of 10^{18} cm^{-3} and F concentration of 10^{18} cm^{-3}. These were solved separately using an iterative minimization approach.

Figure 1 represents the temperature dependence of the V concentration of F_nV_m clusters in Ge. In Fig. 1(a), the implanted F concentration is an order of magnitude lower compared to the V concentration (i.e., $[F]=10^{17}$ cm^{-3} and $[V]=10^{18}$ cm^{-3}). Below 865 K, if local equilibrium could be reached, most of the V that are clustered form V_4 clusters, but the concentration of this cluster falls rapidly as temperature rises. In the temperature range of 865–1005 K, F_2V_2 is the dominant cluster, although most V still remains as isolated species. With increasing temperature, the F_2V_2 clusters gradually dissolve and the mobile FV clusters become dominant. At this low F concentration, all other clusters considered, such as F_3V_2 and FV_2, are insignificant (i.e., they never trap more than ~2% of V in the temperature range considered), but the vast majority of the V remain isolated.

In Fig. 1(b), the implanted F concentration is equal to the V concentration (that is, $[F]=[V]=10^{18}$ cm^{-3}). Up to 1165 K (i.e., over most of the temperature range considered), the F_3V_2 cluster (which traps 37% of V at 850 K) and the F_2V_2 (which traps 33% of V at 850 K) dominate the trapped V concentration. Only above 1165 K, significantly higher than the Ge processing temperature [which is about 865 K (Ref. 6)] does the concentration of FV pairs increase so that they trap more V than any other cluster. For this higher implanted F concentration, the larger electrically inactive clusters (i.e., all dangling bonds are saturated) such as F_4V and F_2V_6 appear, but they are of limited importance. Finally, all other clusters such as the F_5V_2, F_4V_2, and FV_2 clusters only trap a few percent of V. Overall, at this level of F doping, essentially all the V are trapped. It should be noted that a F doping level equal or even higher than the V concentration is favorable for trapping. The relative fraction of trapped vacancies will increase when the vacancy concentration decreases and the fluorine doping level is kept constant at, e.g., 10^{18} cm^{-3}. In this respect, the trapping efficiency of fluorine is not limited to ion-implanted Ge but also to Ge samples whose vacancy concentrations are close to the thermal equilibrium value.

Recently, it has been demonstrated that the diffusion of the n-type dopants P, As, and Sb is strongly enhanced under extrinsic doping conditions. This observation has been rationalized on the basis of a V mechanism operating where the mobile species is a singly negatively charged DV pair.[4] The enhanced diffusion originates from the electric field associated with the incorporation of substitutional donors at concentrations exceeding the intrinsic carrier concentration.[4] It is this enhanced diffusion of the charged DV pairs that hampers the formation of shallow donor profiles. Additionally, n-type doping also increases the concentration of doubly negatively charged V, which gives rise to an enhanced Ge self-diffusion.

One way to overcome the technological problem caused by the mobile DV pairs (which lead to less sharp doped regions) would be to introduce F so that F_nV_m clusters are formed in preference to DV pairs. The formation of F_nV_m clusters will reduce the concentration of free V and critically, through defect equilibria, also the concentration of DV pairs, leading to reduced D atom diffusion. A reduction in D diffusion could also result from the interaction between substitutional D and F and between the DV pairs with F. As donor atoms are positively charged, they will repel bond-center configuration F interstitials; however, tetrahedral F interstitials will be attracted. Indeed, it is found that both PF and AsF pairs are bound with energy of about −0.5 eV (see

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TABLE II. Binding energies E_b (eV) for clusters formed between F interstitials, V, and donor atoms in Ge.

Defect cluster	E_b
PV	−0.52[a]
PF	−0.55
PVF	−1.72
PVF$_2$	−2.80
PVF$_3$	−3.90
AsV	−0.60[a]
AsF	−0.52
AsVF	−1.76
AsVF$_2$	−2.87
AsVF$_3$	−4.00

[a]Reference 12.

Table II). Additionally, PV or AsV pairs have been determined to be singly negatively charged,[4] and they could therefore attract bond-center configuration F interstitials that saturate the dangling bonds of the V. The predicted binding energies of these clusters are given in Table II.

It is also technologically important to access the impact that F doping has on the activation of the donor atoms. Recent experiments on the diffusion of P, As, and Sb in Ge provide clear evidence that under extrinsic doping conditions neutral dopant-defect clusters are formed, which strongly reduce the concentration of electrically active donors.[7] In the present study, we have considered both P-doped and P and F codoped Ge. Figure 2(a) represents the temperature dependence of the concentration of P related clusters, unbound P atoms, and unbound V, assuming an initial V concentration of 10^{18} cm^{-3} and P concentration of 10^{19} cm^{-3}. For this figure, we have used the binding energies for P$_n V_m$ clusters that were predicted using the same methodology of the present study.[8,31,32] At lower temperatures, the P$_4V$ clusters are the dominant clusters in concentration; however, as the temperature increases, they break up into smaller P$_nV$ clusters and isolated defects. At around 850 K:, the PV pairs become the dominant clusters [Fig. 2(a)]. Notably, at this temperature most of the P atoms are isolated with P$_nV$ clusters accounting for only a few percent of the total P concentration [Fig. 2(a)]. As the temperature increases further, P$_nV$ clusters decrease further in significance. Nevertheless, P$_nV$ clusters may form during cooling from high temperatures and in nonequilibrium conditions such as implantation. These are the clusters that are predicted to be potentially important for the deactivation of donor atoms in Ge. Figure 2(b) represents the temperature dependence of the concentration of P related clusters, unbound P atoms, and unbound V,for P and F codoping assuming an initial V concentration of 10^{18} cm^{-3}, F concentration of 10^{18} cm^{-3}, and P concentration of 10^{19} cm^{-3}. It is clear that P and F codoping leads to the reduction in the deactivating P$_nV$ clusters and the mobile PV pairs [compare Fig. 2(a) with Fig. 2(b)]. Importantly, the formation of PF or PVF$_n$ clusters is never of significance [see Fig. 2(b)], whereas a significant proportion of V is trapped in F$_nV_m$ (mainly F$_2V_2$ and F$_3V_2$) clusters. An analogous behavior is also predicted for As and F codoping.

For the temperature range considered, less than 0.1% of

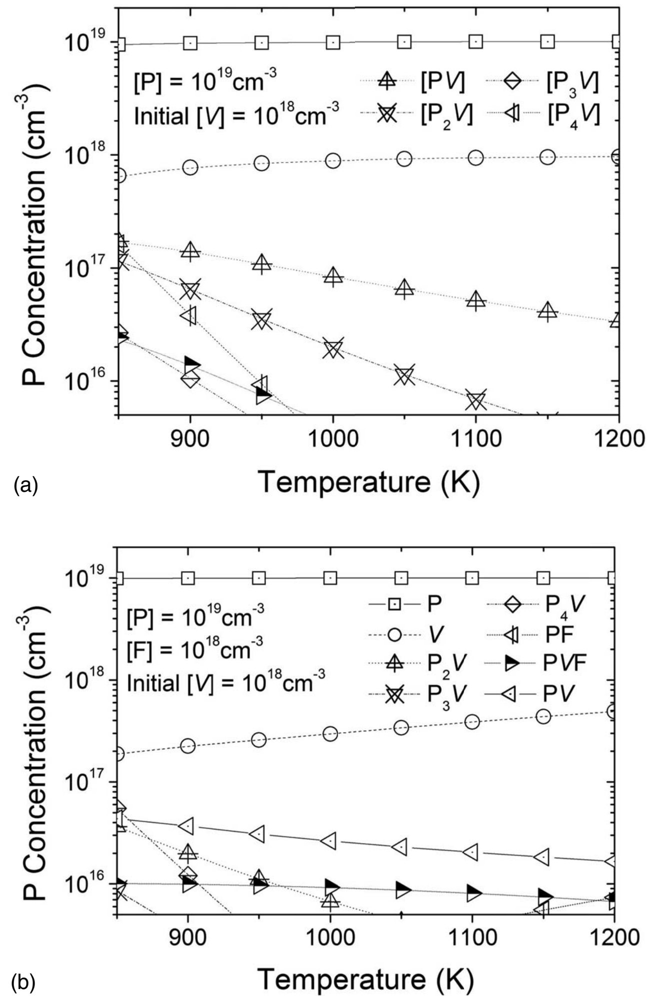

FIG. 2. The temperature dependence of the concentration of P related clusters, unbound P atoms, and unbound V for (a) P-doped Ge with an initial V concentration of 10^{18} cm^{-3} and P concentration of 10^{19} cm^{-3} and (b) P and F codoped Ge with an initial V concentration of 10^{18} cm^{-3}, F concentration of 10^{18} cm^{-3}, and P concentration of 10^{19} cm^{-3}.

P atoms are bound in PVF$_n$ (n=1–3) clusters [see Fig. 2(b)]. These are formed by F atoms saturating the dangling bonds of PV pairs (see Table II for binding energies of PVF$_n$ and AsVF$_n$ clusters). Additionally, their formation will affect the diffusion of the P (or As) atoms via a ring mechanism of diffusion.[33] In particular, for the V of the PV (or AsV) pair to move to the second nearest neighbor site with respect to the P (or As) atom, the F interstitials also have to be displaced in a concerted manner. This concerted mechanism of diffusion is presently under investigation.

IV. CONCLUSION

In summary, F doping in Ge will lead to the formation of stable F$_nV_m$ clusters. Codoping with F and donors such as P and As is expected to hinder the formation of DV pairs and therewith the formation of donor-vacancy complexes such as D$_2V$ that are favored by the Coulomb interaction between the negatively charged DV pairs and the positively charged donors. In this way, not only the diffusion of donor atoms should be retarded; the deactivation should also be reduced. With the proposed approach of codoping with F, the require-

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ments for the formation of shallow and heavily doped *n*-type regions in Ge-based devices could be fulfilled. Kinetics could prove to be important in the formation of the clusters as the local equilibrium between clusters may be kinetically hindered. Therefore, it is necessary to calculate the diffusion barriers of the different dopants, vacancies, and their clusters. Cluster formation under different conditions must be investigated to verify the present predictions.

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