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LETTER TO THE EDITOR

Electronic structure and Jahn–Teller instabilities in a single vacancy in Ge

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Abstract

Density functional modelling studies of the single vacancy in large Ge clusters are presented. We take a careful look at the origin of Jahn–Teller instabilities as a function of the vacancy net charge, resulting in a variety of structural relaxations. By comparing electron affinities of the vacancy with those from defects with well established gap states, we were able to estimate three acceptor states for the vacancy at $E(-/0) = E_v + 0.2$ eV, $E(=/-) = E_c - 0.5$ eV and $E(\equiv/=) = E_c - 0.3$ eV. As opposed to the Si vacancy, the defect in Ge is not a donor. We also show that these dissimilarities have fundamental consequences for the electronic/atomic picture of other centres, such as transition metals in germanium crystals.

Understanding the most elemental defects in semiconductors, vacancies (V) and self-interstitials (I), is a fundamental step in grasping the countless solid-state reactions that may occur during crystal growth, device processing and operation stages. Thanks to powerful spectroscopic techniques such as the electron paramagnetic resonance (EPR) approach, a detailed picture of the single vacancy in silicon has early emerged [1, 2], with important consequences for the understanding of many other fundamental and technological problems related to this material, such as self-diffusion, impurity diffusion, and the electronic structure of many centres such as transition metals.

Carrier mobility limitations in Si associated with a mostly probable replacement of SiO_2 as a gate dielectric with new high κ materials have led to serious consideration being given to the use of novel semiconductor materials for mainstream chip technology [3]. The main contenders are germanium and germanium rich silicon–germanium alloys.

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In contrast to that for Si, the short spin–lattice relaxation time in Ge, together with the abundance of spin-9/2 ^{73}Ge species with large nuclear momentum, has hampered the detection of clear EPR defect signals. Consequently, a detailed picture of many elemental centres in Ge is still missing, and the single Ge vacancy is perhaps the most embarrassing case. Despite these difficulties, significant progress has been made by recent perturbed angular correlation spectroscopy (PACS) studies for Ge crystals, where, on the basis of the formation kinetics of ^{111}In–V pairs as a function of the Fermi level location, an $E(-/0) - E_v \sim 0.2$ eV acceptor state has been linked with the single vacancy [4]. The annealing temperature for V has also been estimated at ∼200 K, and this was later confirmed by positron lifetime spectroscopy and x-ray diffraction [5, 6].

The success in modelling a Ge vacancy is also far from that attained in Si. Firstly, density functional theory, together with the local density approximation, predicts a nearly vanishing band gap for Ge when employing the invariably used supercell approach. This poses serious problems when modelling gap levels, as the calculated nearly metallic density of states of Ge overlaps all defect states. For instance, the vacancy–oxygen complex (VO) in Ge has an acceptor state at $E_v + 0.27$ eV [7], and local vibrational mode frequencies at 620 and 669 cm^{-1} were assigned to Ge–O–Ge units in VO^0 and VO^- [8, 9], respectively. Recent density functional supercell calculations [10] on the other hand give an acceptor state resonant with the conduction band, and the additional electron in VO^- actually falls in a conduction band state, resulting in a negligible difference between the vibrational frequencies of neutral and negatively charged centres. Secondly, its has been shown that Jahn–Teller driven reconstructions between vacancy *dangling bonds* produce long ranged strain fields which can only be accommodated by several hundreds of ligand atoms surrounding the defect [11, 12]. These strains span the characteristic length of computationally affordable supercells, resulting in spurious defect–defect interactions and, consequently, the predicted structures depend on the supercell size and shape, as well as on the scheme adopted for sampling the Brillouin zone [13]. These are among the reasons that make theoretical modelling reports on defects in Ge scarce. Early density functional modelling studies employing the Green's function method [14] proposed five gap levels for the defect, corresponding to six stable charge states, from double positive (++) up to triple negative (≡). Unfortunately, these dealt with perfect unrelaxed vacancies only, and we know that a proper description of the Jahn–Teller distortions could well alter this picture. These distortions were recently investigated by means of density functional cluster calculations [15], but no electrical levels were reported. The fully relaxed supercell calculations by Fazzio *et al* [16] predict (++/+), (+/0), (−/0) and (=/−) gap levels, and in line with the cluster calculations from [15], the resulting Jahn–Teller distortions were quantitatively smaller and qualitatively similar to those in the Si vacancy.

In this letter we present a close look at the atomic and electronic structure of the Ge vacancy by means of a spin density functional study using the AIMPRO code [17]. The pseudopotentials of Hartwigsen *et al* account for core electrons [18], and the local spin density approximation uses the Padé parametrization [19]. Valence states and the electron density are represented with the help of s, p, d-like Cartesian–Gaussian functions. We employ large hydrogen-terminated $Ge_{376}H_{196}$ spherical clusters with a vacant site at each centre, corresponding to a total of 28 shells of Ge ligand atoms. This approach has been successful in reproducing the measured electronic and structural details of the single-vacancy [11] and double-vacancy [12] centres in Si. Prior to defect studies, perfect clusters ($Ge_{377}H_{196}$) were fully relaxed, and under these conditions the lowest unoccupied Kohn–Sham state lies 2.17 eV above the highest occupied one. The large gap width is a consequence of surface confinement of the cluster states. All Ge–H surface units were then locked to their sites, a Ge atom was removed from the centre of the cluster and all remaining ligand atoms where freely allowed

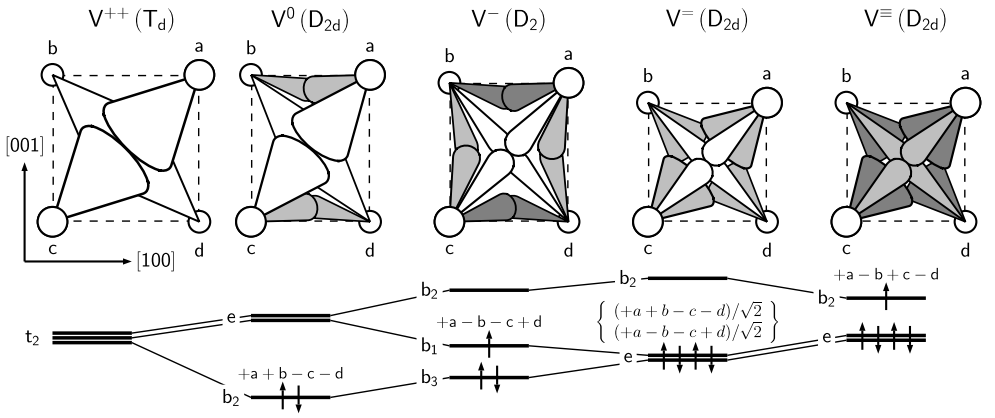

Figure 1. Scheme of the structural distortions in a Ge vacancy for several charge states of interest (up). Only low spin paramagnetic states are represented. The symmetry of each structure is shown within parentheses. Unoccupied, highest occupied and lower (fully occupied) levels are represented in white, light grey and dark grey bonds, respectively. The Jahn–Teller splitting pattern of the triplet (t_2) gap level is also shown (down), along with the symmetry representation of each level and the LCAO description of the highest occupied level.

to attain their equilibrium locations. Alternatively, the relaxation was constrained to a certain point group symmetry.

We are particularly interested in locating electrical levels. To do so, we adopt the *marker method* [20], were donor and acceptor states are calculated with respect to analogous levels from well established centres (marker defects). Hence, ionization energies (electron affinities) of the vacancy are compared to a similar calculation for the marker, and the difference is offset by the experimental donor (acceptor) level location of the latter. This method was shown to predict levels with an error bar of ∼0.2 eV, but when the marker and the defect under scrutiny possess electron states which are similar in symmetry and extent, deviations from the measurements fall below 0.1 eV [21]. For donor markers, we have chosen substitutional sulfur ($E_c - E(0/+) = 0.28$ eV and $E_c - E(+/++) = 0.59$ eV) [22], selenium ($E_c - E(0/+) = 0.27$ eV and $E_c - E(+/++) = 0.51$ eV) [22], silver and gold ($E(0/+) - E_v = 0.035$ eV and $E(0/+) - E_v = 0.044$ eV, respectively) [23, 24]. For acceptor markers, substitutional silver ($E(-/0) - E_v = 0.116$ eV, $E_c - E(=/-) = 0.261$ eV and $E_c - E(\equiv/=) = 0.113$ eV) [23], and substitutional gold ($E(-/0) - E_v = 0.135$ eV, $E_c - E(=/-) = 0.215$ eV and $E_c - E(\equiv/=) = 0.056$ eV) [24], were adopted. The 4d and 5d shells on Au and Ag, respectively, were explicitly treated as valence states.

The removal of a Ge atom from the lattice produces four radicals located at the vertices of a perfect tetrahedron, labelled a, b, c and d in figure 1. Each radical may couple to their three neighbours, and within T_d symmetry they hybridize as a_1 and t_2 states. The singlet is resonant within the valence band, whereas the triplet is located within the gap. Analogously to the Si vacancy [1], the doubly positive vacancy in Ge (V^{++}) has an empty t_2 gap state, and is perfectly tetrahedral. Let us consider a simple linear combination of atomic orbitals (LCAO) arising from a, b, c and d dangling bonds (see V^{++} in figure 1). The triplet state components are $t_{2x} = +a - b - c + d$, $t_{2y} = +a - b + c - d$, and $t_{2z} = +a + b - c - d$ [1]. When this is partially occupied, electron–phonon coupling drives an Jahn–Teller distortion when the relaxation energy exceeds the exchange–coupling energy, in which case the occupancy follows Hund's rule. Jahn–Teller distortions were investigated for charge states between

Table 1. Symmetry (Symm.), spin state (S), ab, ac atomic distances (according to figure 1), relative volume change ($100 \times \Delta v/v_0$) with respect to the volume of a perfect vacancy ($v_0 = 7.3662$ Å^3 with $ab = ac = 3.9686$ Å), and Jahn–Teller relaxation energies (E_{JT}) for the Ge vacancy in several charge states. All distances and energies are given in Å and eV, respectively. The lattice constant for all calculations, $a_0 = 5.6125$ Å, was obtained from a volumetric relaxation of a Ge unit cell using periodic boundary conditions.

	V^{++}	V^{+}	V^{0}	V^{-}	$V^{=}$	$V^{\equiv}$
Symm.	T_d	D_{2d}	D_{2d}	D_2	D_{2d}	D_{2d}
S	0	1/2	0	1/2	0	1/2
ab	4.0056	3.7107	3.3008	3.2684	3.2596	3.2083
ac	4.0056	3.8519	3.7038	3.6189	3.5401	3.3789
ac/ab	1.0000	1.0381	1.1221	1.1072	1.0860	1.0532
$100 \times \Delta v/v_0$	2.82	−12.1	−29.1	−34.4	−40.8	−44.7
E_{JT}	—	0.06	0.10	0.00	0.11	0.04

++ (double positive) and ≡ (triple negative), by comparing the energy of atom- and spin-relaxed tetrahedral vacancies with similar calculations after trigonal (D_{3d}, C_{3v}, C_3), tetragonal (D_{2d} and S_4), orthorhombic (D_2, C_{2v}), monoclinic (C_2, C_{1h}) and triclinic (C_1) distortions. The D_{3d} structure is made up of two semi-vacancies that result on placing a Ge at the inversion centre of a perfect divacancy [13]. It is noteworthy that the local density approximation (LDA) treatment for the exchange–correlation energy tends to favour high spin states, and hence to underestimate Jahn–Teller distortion energies. However, in the limit of strong distortions (like for vacancy centres in Si) we expect to obtain the right symmetry and distortion directions, as well as the right order of magnitude for the energies. For example, local density cluster calculations of the Si divacancy give $E_{JT} = 0.10$ and 0.15 eV for V_2^+ and V_2^-, respectively [15]. These are far away from the early results 1.3 and 2.4 eV from EPR data [25], but are close to the most recent estimates of 0.16 and 0.54 eV, respectively [26].

Structural details of fully relaxed vacancies in several charge states are shown in table 1. Charge states ++, +, 0, −, = and ≡ occur with T_d, D_{2d}, D_{2d}, D_2 (or T_d), D_{2d} and D_{2d} point group symmetries, respectively. These results are at variance with previous calculations [15, 16], which proposed C_{2v} symmetry for the negatively charged states. Our disagreement with [15, 16] is justified after looking more closely at each individual state. The V^{++} (t_2 state is empty) has tetrahedral symmetry, showing a minute ($\Delta v/v_0 \sim 0.03$) volume increase with respect to the unrelaxed vacancy volume v_0 (table 1). When one or two electrons are added (+ and 0 charge states), the t_2 state splits through D_{2d} distortion into a half-occupied or fully occupied b_2 state, respectively, lying below an empty doublet state. Figure 1 shows that for the neutral vacancy $b_2 = +a + b - c - d$, which is a bounding state between ab and cd atom pairs. Its single and double occupancies lead to a structure with [001] axial symmetry, corresponding to Jahn–Teller relaxation energies (E_{JT}) of 0.06 and 0.10 eV when compared to tetrahedral relaxed V^+ and V^0 with $S = 1/2$ and 1 states, respectively. These are in line with previous calculations (0.02 and 0.12 eV for V^+ and V^0 [15]), and of the same order of magnitude as those estimated for the Si vacancy (0.05 and 0.32 eV for V^+ and V^0 [11]). Table 1 shows that each electron on the b_2 state produces a ∼16% volume shrinkage, and the bond length anisotropy fraction (ac/ab) tells us that V^+ and V^0 are compressive along [001] and tensile along [100] and [010], respectively.

For the negative charge state we investigated several atomic/electronic configurations, of which we emphasize (i) C_{2v} and (ii) D_2 low spin states ($S = 1/2$) resulting from further Jahn–Teller splitting of the e state in V^0, as well as (iii) a high spin state ($t_2^{\uparrow\uparrow\uparrow}$) with T_d symmetry and $S = 3/2$. Other structures were tested, and they turned out to be unstable or energetically

depreciated. Unlike in Si, a low spin C_{2v} symmetric V^- is not stable and relaxes to the D_2 structure. The electronic structure of the latter is $b_3^{\uparrow\downarrow}b_1^{\uparrow}b_2^0$, and its D_2 deformation follows from the occupancy of one of the e components, say, $+a-b-c+d$. This is a bonding state between ad and bc radicals, and therefore they are pulled towards each other (see the light grey orbital in figure 1). We also found that the D_2 ($S=1/2$) and tetrahedral ($S=3/2$) structures are essentially degenerate, with a slight preference ($\sim$3 meV) for the latter. Considering the fact that the local spin density approximation may be overestimating the exchange term by up to a few tenths of an electronvolt in favour of the high spin state, it is not clear which state is the most stable. We note that an $S=3/2$ state has been obtained by Lento *et al* [27] for a Si vacancy in a perfectly ordered SiGe zinc-blende supercell calculation. However, they favoured high spin T_d symmetric structures for the other charge states as well.

In the double-minus charge state ($V^=$), the vacancy suffers a tetragonal Jahn–Teller distortion, ending with D_{2d} symmetry. However, its electronic and atomic structures differ from that of V^0. $V^=$ has four available electrons to be accommodated in the t_2 state, and here we found a splitting order corresponding to a $e^{\uparrow\downarrow\uparrow\downarrow}b_2^0$ ground state. The T_d relaxed high spin state $t_2^{\uparrow\uparrow\uparrow\downarrow}$ ($S=1$) is unstable and lies $E_{JT}=0.11$ eV above the D_{2d} distorted structure. The defect, as represented in figure 1, is tensile along its [010] principal symmetry axis, whereas it is compressive along [100] and [001] directions, i.e., $ac/ab>1$ (see table 1). Its volume is about 60% of the original perfect vacancy. We also looked at a D_{2d} symmetric $V^=$ defect with $b_2^{\uparrow\downarrow}e^{\uparrow\uparrow}$ occupancy ($S=1$) by starting with a structure similar to that of V^0. This turned out to be metastable by about 0.4 eV above the $e^{\uparrow\downarrow\uparrow\downarrow}b_2^0$ ground state. Finally, the triple-minus charge state also shows a Jahn–Teller effect, although weaker than in V^0 and $V^=$. Like $V^=$, the defect has a tensile D_{2d} distortion with its principal axis along [010], $E_{JT}=0.04$ eV, and its volume is close to that of $V^=$.

As mentioned earlier, we use the marker method to locate the electric (occupancy) levels for the Ge vacancy. Let us first look at the donor states using S and Se markers. These are substitutional group VI centres with T_d symmetry. Four of its valence electrons resonate with the vacancy triplet state, shifting the fully occupied t_2^6 orbital below the valence band top. We are then left with a fully occupied $a_1^{\uparrow\downarrow}$ gap state that is responsible for their double-donor activity. Accordingly, we find that the first ionization energy for the vacancy is $I_V(0/+)=E(V^+)-E(V^0)=4.70$ eV, whereas for sulfur $I_S(0/+)=4.03$ eV only. Knowing that the $S_s(0/+)$ state has been measured at $E_c-0.28$ eV [22], we then place the V(0/+) state at $E_c-0.28$ eV $-[I_V(0/+)-I_S(0/+)]$ which is $E_c-0.95$ eV, and below the valence band top. This means that, unlike in Si, the vacancy in Ge does not have a (0/+) state in the gap. However, if, like in Si, the defect has a sufficiently large negative energy of correlation (U) between first and second donor states, it could produce a (0/++) level above the valence band top. Hence we looked at its second ionization energy, where $I_V(+/++)-I_S(+/++)=0.38$ eV, and from the measured (+/++) level for sulfur at $E_c-0.59$ eV [22], we place the V(+/++) level at $E_c-0.97$ eV. We must stress the fact that up to now, there is only experimental evidence for an acceptor state in the lower half of the Ge band gap ($\approx E_v+0.2$ eV) [4], and therefore our results are consistent with the available measurements. Similar results are obtained by using Se_s as a marker, and they are reported in table 2. Note that the agreement between (0/+) and (+/++) calculated levels using these two markers shows that the method accounts well for the relative S_s and Se_s donor levels energies.

Before making use of gold and silver (0/+) marker levels, let us briefly describe the atomic and electronic structure of these centres. We found that the so-called *Watkins vacancy model* (which has been widely applied to these centres in Si) [28], also applies to Ge, provided that we use the Ge vacancy model described above. Atomic Ag:[Kr].$4d^{10}.5s^1$ and

Table 2. Donor and acceptor levels (eV) for the Ge vacancy. Calculations employ S, Se, Ag and Au marker impurities (see the text).

Marker	S_s	Se_s	Ag_s	Au_s
V(+/++)	$E_c - 0.97$	$E_c - 0.91$		
V(0/+)	$E_c - 0.95$	$E_c - 0.98$	$E_v - 0.11$	$E_v - 0.12$
V(−/0)			$E_v + 0.20$	$E_v + 0.17$
V(=/−)			$E_c - 0.50$	$E_c - 0.54$
V(≡/=)			$E_c - 0.25$	$E_c - 0.27$

Au:[Xe].$4f^{14}.5d^{10}.6s^1$ have their d states lying within the valence density of states, leaving their 5s and 6s electrons resonating with the vacancy triplet state. This means that substitutional Au_s^q and Ag_s^q defects, where $q = 1, 0, -1, \ldots$ stands for their charge states +, 0, −, . . ., show similar Jahn–Teller distortions to those found for $V^{(q-1)}$. Curiously, ground states of Au_s^0 and Ag_s^0 are spin-1/2 with D_2 symmetry, and hence they adopt the configuration of V^- with low spin. The spin-3/2 Au_s^0 and Ag_s^0 centres are metastable by 0.05 eV. We also note that $Au_s^{\equiv}$ and $Ag_s^{\equiv}$ have perfect tetrahedral symmetry as their t_2^6 states are fully occupied. Applying the above-mentioned procedure, we found that $I_V(0/+)$ exceeds $I_{Ag}(0/+)$ and $I_{Au}(0/+)$ by 0.14 and 0.16 eV, placing the V(0/+) at $E_v - 0.11$ eV and $E_v - 0.12$ eV, respectively, and again ruling out any donor state for the vacancy.

Acceptor states were looked at by using Ag_s and Au_s acceptor markers. Now we use electron affinities A, i.e., for the vacancy we have $A_V(-/0) = E(V^-) - E(V^0) = -3.29$ eV, while for Ag_s and Au_s we obtain $A_{Ag}(-/0) = -3.37$ eV and $A_{Au}(-/0) = -3.32$ eV, respectively. This places the V(−/0) state 0.08 and 0.03 eV above $Ag_s(-/0)$ and $Au_s(-/0)$ acceptor levels, or at $E_v + 0.20$ eV and $E_v + 0.17$ eV, respectively, matching the location that has been estimated from the PACS measurements [4]. A similar procedure has been applied for second and third acceptor states (see table 2). Using second and third electron affinities of V, Au_s and Ag_s defects we find V(=/−) and V(≡/=) levels at around $E_c - 0.50$ eV and $E_c - 0.25$ eV, respectively. The ∼0.7 eV band gap of Ge implies that the V(=/−) state falls very close to the V(−/0) level, and we cannot rule out a negative-U correlation energy between them. This effect is a consequence of the strong structural relaxation of V^0 and $V^=$ when compared to V^-. Note that each electron on the t_2 split-off components shrinks the vacancy volume by ∼16 and ∼11% for V^0 and $V^=$, respectively. Therefore we have to admit that the $E_v + 0.2$ eV level that has been inferred from PACS measurements [4] could actually be assigned to a (0/=) occupancy state. Finally, the fact that Ag_s and Au_s defects lead to vacancy levels which differ by at most 0.04 eV implies that this would be the resulting error of a calculation utilizing the Ag_s marker to evaluate the Au_s levels.

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