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Calculated properties of a {113} planar vacancy aggregate in Si

J P Goss[1], P R Briddon[1] and R Jones[2]

[1] School of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, UK
[2] School of Physics, The University of Exeter, Exeter EX4 4QL, UK

E-mail: J.P.Goss@ncl.ac.uk

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Abstract

Large aggregates of self-interstitials are known to be responsible for the rod-like defects which have a {113} habit plane. In regions where there is a supersaturation of vacancies, similar defects are formed by the aggregation of lattice vacancies. We present the results of first principles calculations that show such structures to be particularly stable in comparison to isolated vacancies and stable vacancy clusters, but less stable than the {113} self-interstitial structures.

1. Introduction

Native defects in silicon play an important role in the electronic properties of semiconducting materials. For instance, the divacancy in silicon possesses a number of levels in the bandgap and acts as a deep electron and hole trap in p- and n-type materials. Although isolated interstitials and vacancies interact with other impurities forming compensating defects, in low-impurity materials it is the interaction of these native defects with each other that is of particular interest. A considerable amount of effort has been made to understand the clustering of self-interstitials, often in the context of the rod-like defects (RLDs) that contain large numbers of interstitials and typically lie in {113}-planes [1]. However, less is known about the comparable defects made up from lattice vacancies. We present here the results of first principles calculations for the vacancy agglomerate lying on the {113}-plane suggested by experiment [2].

We first outline the important theoretical and experimental data pertaining to this study, starting with the small vacancy clusters.

Individual isolated lattice vacancies (V) have not been detected experimentally due to their high mobility, but the formation energy of V has been estimated using both theory and experiment. There is considerable uncertainty in the actual value, with various estimates lying in the range of 2–4 eV [3–8]. Recent exhaustive density-functional-theory (DFT) calculations suggest a value of 3.17 eV [9]. The theoretical difficulties arising for V arise at least in part

from the subtle reconstruction of the dangling bonds, and controversy still remains regarding even the sense of the distortions [9, 10].

Unlike V, vacancy clusters have been assigned to a range of EPR centres, electrical levels, and optical transitions (see, for example, [11–14]). Besides the well known EPR centres and electrical levels associated with the divacancy, in float-zone (FZ) silicon, which is lean in impurities and particularly oxygen, one finds very stable structures made up from rings of six vacancies (V_6). These aggregates reconstruct to form systems with no dangling bonds. The reconstructions in V_6 are between second-neighbour atoms which, after relaxation, are calculated to result in bonds of length 2.63 Å, i.e. only $\sim$12% longer than the bulk bond-length, and some 31% smaller than the next-nearest-neighbour separation in bulk material. The reconstruction constitutes a rather strong effect with a profound impact on the stability, formation energy and electronic properties of the aggregate. In the absence of any impurities, and in particular hydrogen, the hexavacancy is stable to 450 °C. It is the fact that this aggregate is able to remove *all* dangling bonds that makes it particularly stable, and it is this property that we shall show is present in the form of *infinite* planar aggregate investigated in this study.

We note that, despite being free from dangling bonds, V_6 is able to capture excitons that recombine giving rise to the J-lines [14, 15], and it seems likely that other defects containing elongated reconstructed bonds are likely to also introduce bandgap states.

Over recent years, tight-binding (TB) calculations have been applied to defects from V to aggregates of several tens of vacancies. Due to the approximate way that the electrons are treated, TB calculations have a considerable speed advantage over the more accurate DFT methods, and it is possible to treat systems containing large numbers of atoms. However, the more approximate method leads to less reliable absolute formation energies, and one must view the absolute values that TB calculations yield with caution. This said, the trends are likely to be correct, and indeed TB indicates a local minimum (with respect to the number of vacancies) in the formation energy per vacancy for V_6. With this in mind, TB calculations suggest that the hexavacancy has a formation energy per vacancy of 1.90 eV [16] and 1.75 eV [17]. Since the hexavacancy is believed to be a defect that is present in irradiated FZ material, we shall use these figures as a benchmark for our current results. Note that the TB formation energies for V at 3.40 eV [16] and 3.8 eV [17] differ by 7% and 19% from the best first principles value, but the difficulties inherent to the calculation of the formation energy of V, as highlighted above, are likely to mean that all such calculated values may have rather large error bars. The formation energy per vacancy is predicted to diminish nearly monotonically, with clusters of 6, 10 and 14 vacancies yielding local minima, and hence suggestive of V_6, V_{10} and V_{14} being particularly stable structures. A cluster of 35 vacancies has a formation energy per vacancy of just 1.01 eV [16]. This indicates that the binding energy per vacancy to very large aggregates is of the order of 2 eV.

This estimate is on the lower limit of the values obtained experimentally. Recent experiments with ion-implanted samples have suggested that large vacancy clusters exist with individual vacancies being bound by 3.2 ± 0.2 eV in the bulk, with structures near interfaces binding individual vacancies less well at 2.6 ± 0.6 eV [18]. The former value is close to that obtained from the diffusion of Sb markers at 3.3 ± 0.3 eV [19], although this relies on an estimate of the formation energy of the lattice vacancy, V (3.6 ± 0.5 eV [3]). The formation energy per vacancy in these large clusters is then estimated at just 0.34 ± 0.3 eV [19], i.e. just 10% of that of V! However, the uncertainties in the various quantities render a precise estimate of the cluster formation energies extremely problematic.

A final note regarding large vacancy aggregates comes from Laplace deep-level transient spectroscopy (LDLTS) experiments. These have revealed that in ion-implanted material electrically levels around $E_c - 400$ meV are associated with extended states [13]. The precise

form of these defects is not clear from the experiments, but such an extended wavefunction might be consistent with, for instance, linear and planar aggregates of vacancies or self-interstitials.

Turning briefly to large self-interstitial aggregates, RLDs in silicon and germanium have received considerable attention due to their potential role in the transient enhanced diffusion of dopants such as boron. Although RLDs adopt a range of structures, they are based on a core defect formed by the insertion of chains of self-interstitials along parallel [110] channels in the diamond structure [1]. RLDs are mostly of the {113}-type, but a small fraction ($\sim$10% [20, 21]) occur on {111} habit planes. Empirical potential calculations [21] indicated that the {111} RLDs are lower in energy, with a formation energy per interstitial around 80% that of those with a {113} habit plane. This trend has also been found using DFT-based methods [22].

The theoretical stability of the {111} orientation rather than the dominant {113} variety seen experimentally may imply that there is some non-equilibrium driving force that predisposes the [110]-chains to assemble on the {113}-plane. Indeed, it has been suggested that this disposition for the formation of {113} RLDs may be due to the presence of *vacancy-related planar defects* on {113}-planes that then interact with self-interstitials to form the RLDs [2].

This hypothesis is supported by high resolution transmission electron microscopy (HRTEM) that suggests the existence of these vacancy-related {113} planar defects [2, 23]. The structures are seen in thin ($<$10 nm) FZ silicon wafers where a vacancy supersaturation is believed to exist, and are formed after 20 min *in situ* under the 400 kV electron beam at room temperature. Under these conditions the irradiation products are believed to be mobile.

The model for the planar vacancy-related feature is constituted from the removal of chains of atoms along [110] within a {113}-plane, so that the reconstructions yield a series of eight-member rings. In some cases two narrow layers of the eight-member rings occur together [2]. The fit of a vacancy-based model to the HRTEM image seems convincing, but due to the difficulties in fitting atomic models to HRTEM images it is not unique. Importantly, and in contrast to the RLDs, the surrounding lattice is only very slightly affected by the their presence, with the distortion estimated at 0.020 ± 0.01 nm [2]. The argument then made for the formation of the {113} interstitial-type defects is that mobile self-interstitials become trapped in the core of the vacancy defect, but they do not annihilate. Instead the combined aggregate is termed a 'zero-defect' (ZD) where the density of Si atoms equals that of the host, but where the local bonding structure is strongly perturbed. This amounts to a stacking fault on a {113}-plane.

If the transitory formation of {113}-oriented vacancy clusters is important, one would expect them to be strongly bound. We have therefore undertaken a study of the model given in [2] to evaluate the formation energy, structure and electrical properties.

2. Method

To examine the structure and properties of {113} vacancy-type defects we have used local density functional theory [24, 25]. The structures are represented using supercells based on a bulk supercell containing 44λ host-atom sites with lattice vectors $\lambda[113]\ a_0$, $[1\bar{1}0]\ a_0/2$ and $[33\bar{2}]\ a_0/2$, $\lambda = 1$ and 2. Since the model is periodic in the (113) plane, it is not necessary to extended the supercell in the other directions. The Brillouin zone is sampled using the Monkhorst–Pack scheme [26]. The k-point sampling has been varied so that the formation energy per vacancy converges to within 1%. In practice this means using a mesh of $2 \times 8 \times 2$ k-points, although we have tested the convergence with calculations involving meshes twice as dense as this. The core electrons are removed by the use of pseudo-potentials [27]. The charge density is expanded in plane waves with a cut-off of 80 Ryd, and the wavefunction basis is constituted from four independent sets of s- and p-Gaussians, and two sets of d-Gaussians, all

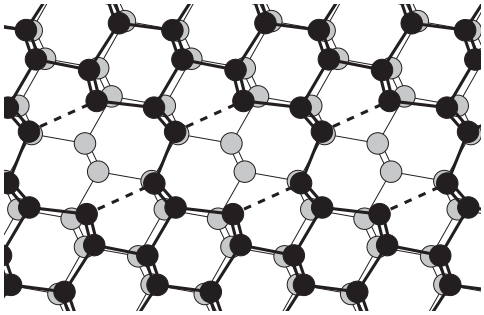

Figure 1. A schematic representation of a (113) planar vacancy aggregate projected onto the $(1\bar{1}0)$ plane. The light grey circles and lines represent the silicon sites and bonds in bulk silicon, with the superimposed black circles and lines representing the (113) vacancy aggregate. The vertical and horizontal are [113] and $[33\bar{2}]$, respectively. The second-neighbour reconstructions are shown by the dashed lines.

centred at the atomic sites. This basis set reproduces the lattice constant and bulk modulus of silicon to within 1% of experiment, and the band-structure agrees well with previously published plane-wave data [28].

3. Results

3.1. Structure and formation energy

Figures 1 and 2(a) show schematically the structure of the [110]-oriented vacancy chains after reconstruction and relaxation, but retaining the lattice vectors appropriate to the bulk cell. We calculate the formation energy per vacancy of this planar defect to be 2.1 and 1.5 eV for the 44 and 88 atom cells, respectively, which is considerably lower than the 3.3–3.6 eV of the isolated vacancy, and comparable to the similarly reconstructed hexavacancy at $\sim$1.8 eV.

The geometry, as depicted in figures 1 and 2(a), is highly strained with 'reconstructed bonds' (dashed lines in figure 1) being around 3 Å in length. The bond angles vary over a range of 95°–151°. Although the bond-lengths indicate that the reconstructions are rather weak, they are around 20% shorter than the internuclear distances of next-nearest neighbours in bulk silicon, and a visual analysis of the charge density in the planes of the reconstructions indicates that chemical rebonding is present.

3.2. Shear relaxation

The initial estimate of the formation energy corresponds to lattice vectors that may artificially constrain the defect. We have therefore introduced a series of displacements in the [113]-direction along with a series of shear components along $[33\bar{2}]$ so that the supercell lattice vectors no longer form an orthogonal set. Such a distortion might be anticipated since it tends to reduce the length of the reconstructed bonds, and hence lower the energy of the bonding orbitals associated with them. We have not explored the possibility of a shear component along the $[1\bar{1}0]$-direction because the reconstructions are wholly contained with $(1\bar{1}0)$-planes. The procedure we have adopted leads to a two-parameter energy surface. We find that the total energy is (at least locally) minimised by a combination of a small [113] displacement (a contraction) and a considerable shear. The equilibrium lattice vectors for the 44 atom cell are $[1\bar{1}0]\ a_0/2$, $[33\bar{2}]\ a_0/2$, and $\{(1-\alpha)[113] + \beta[\bar{3}\bar{3}2]\}\ a_0$, with $\alpha = 0.03$ and $\beta = 0.12$. The structure of the {113} vacancy aggregate including the optimisation of the lattice shape is depicted in figure 2(b). The small value of α is consistent with the small displacement measured

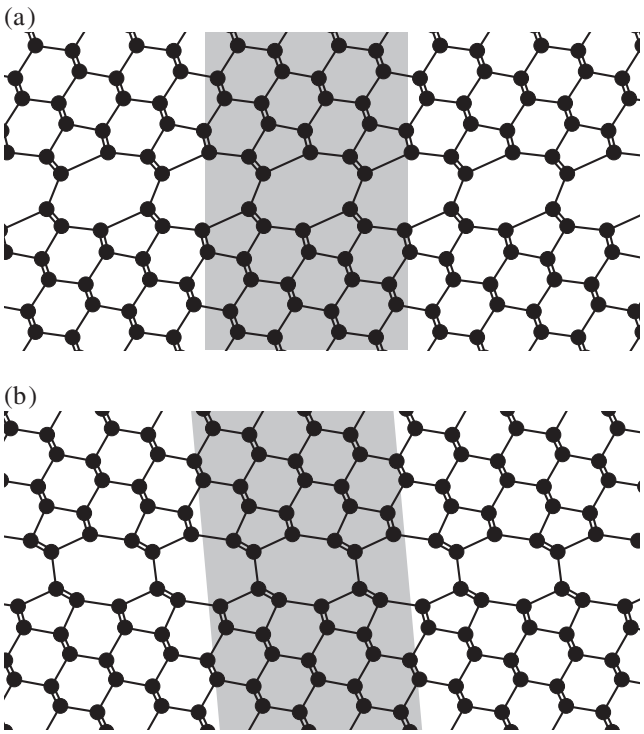

Figure 2. A schematic representation of a (113) planar vacancy aggregate projected onto $(1\bar{1}0)$-plane, the vertical and horizontal axes being [113] and $[33\bar{2}]$, respectively. (a) The relaxed geometry for fixed lattice vectors. (b) The relaxed structure including lattice vector optimisation. The shaded areas indicate one period along $[33\bar{2}]$, and for (b) also indicates the shear with respect to bulk.

from the HRTEM (0.05 nm compared to 0.01–0.03 nm from experiment [23]). The larger cell yields the same displacement in the [113]-direction (0.05 nm). The relaxation of lattice vectors leads to reconstructed bond around 2.6–2.7 Å, close to those of the hexavacancy. All bond-lengths lie within 99–115% and bond-angles within 85–134% of bulk values. To the eye, the geometry close to the vacancy aggregate is very similar for the two different supercell sizes.

The shear leads to a considerable reduction in the total energy with the minimal formation energy around 1.3 eV/vacancy in the 44 atom cell, and just 1.0 eV in the 88 atom cell. This represents a formation energy density of just 80 meV Å^{-2}. This is lower than that of the similarly bonded hexavacancy (as determined using the more approximate TB methods), and slightly lower than the large (up to 35 vacancies) clusters as quoted in [16]. Furthermore, it is just around a third that of the best estimates for the isolated vacancy [9], and represents a binding energy relative to V of around 2 eV. This extended defect therefore represents an efficient sink of the mobile vacancy.

3.3. Electronic properties

By examining the electronic density of states for the fully relaxed structure, we find that the strained Si–Si bonds give rise to empty levels in the upper part of the bandgap, as shown in figure 3. The electronic densities of states are obtained by summing over a Monkhorst–Pack mesh of $50 \times 50 \times 50$ k-points for a two-atom primitive bulk silicon cell and $15 \times 10 \times 50$ k-points for the 44 atom defect cell, so that the k-point densities are comparable. The individual Kohn–Sham levels are broadened using Gaussians of width 0.1 eV. The energy scale is defined

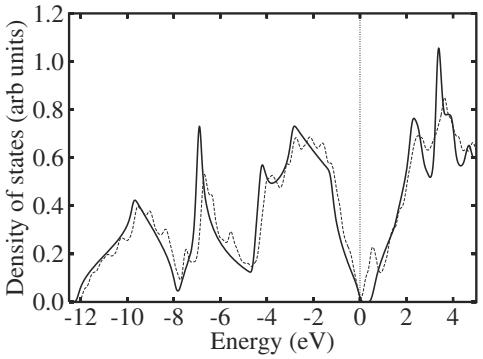

Figure 3. The electronic density of states obtained from the Kohn–Sham eigenvalues. The full curve is for bulk silicon and the dashed curve is the fully relaxed {113} planar vacancy defect.

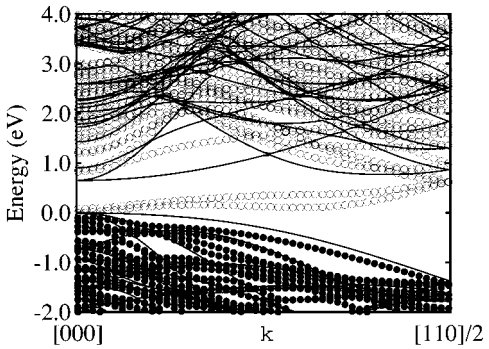

Figure 4. The Kohn–Sham band structure for the structure depicted in figure 2(b). The wavevector, **k**, is in units of $2\pi/a_0$. The filled and empty circles show the eigenvalues for the defect which are filled and empty, respectively. The black continuous curves represent the bands of the bulk cell.

such that the highest occupied Kohn–Sham levels are at zero. This indicates that, unlike the case found for the interstitial related RLDs, the planar vacancy defects are able to be negatively charged in n-type silicon, with the additional electrons populating anti-bonding combinations in the dilated bonds. A comparable analysis for the larger supercell yields very similar results.

An alternative illustration of the electronic structure is shown in figure 4. The plot represents the electronic structure along the line of the vacancy chains. The empty band giving rise to the peak in the bandgap in figure 3 can be seen to traverse the bandgap. This deep band of extended states is consistent with the LDLTS data [13], although clearly not uniquely so.

3.4. The zero-defect (ZD)

In addition to the infinite planar vacancy aggregate, we have also examined the energetics of the ZD made up from the insertion of [110]-chains of self-interstitials into the 8-member channels left by the vacancy chains (figures 1 and 2). This defect can also be viewed as essentially a rearrangement of bulk silicon where bonds have been switched by pairs in much the same way as for the {113} planar interstitial aggregates [29]. The resultant structure is shown schematically in figure 5. As with the {113} vacancy aggregate, the ZD structure is most stable subsequent to a $[33\bar{2}]$-shear. The equilibrium structure contains a range of bond-lengths between 97% and 101% of the bulk, but the bond-angles are 84–122% of the tetrahedral angle.

The formation energy per site in the defect is around 0.7 eV, or $\sim$58 meV Å^{-2}, compared to the energy of the {113} vacancy defect at $\sim$80 meV Å^{-2}. Since the ZD is essentially a stacking fault, we have also made the comparison with intrinsic and extrinsic stacking faults (ISF and ESF). ISF have experimentally been determined to have a formation energy of 3.4 ± 0.4 meV Å^{-2} [30], and theoretically ISF and ESF are around 2.1–2.4 and 1.6–2.1 meV Å^{-2}, respectively [31, 32]. Using a supercell with lattice vectors 4[111] a_0, $[1\bar{1}0]$ $a_0/2$ and $[10\bar{1}]$ $a_0/2$, which have then had either a double layer removed (ISF) or added (ESF), we obtain formation energies of 2.3 and 1.5 meV Å^{-2}, respectively. In particular, our results agree very well with [32]. The fact that the ZD is considerably higher in energy than the stacking faults is unsurprising since the deviation from bulk values for bond-lengths and angles in the ISF and ESF defects is very small in comparison to those of the ZD.

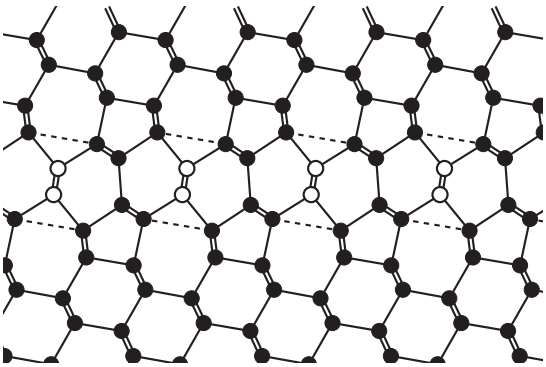

Figure 5. A schematic representation of a (113) planar ZD projected onto the $(1\bar{1}0)$-plane. The vertical and horizontal are [113] and $[33\bar{2}]$, respectively. The dashed lines indicate the reconstructions in the {113} vacancy defect, and the inserted $[1\bar{1}0]$-chains of interstitials are indicated with the white circles.

The difference in formation energies of the ZD and {113} vacancy defects tells us that the former should be thermodynamically more stable than the latter. We can also quantify the binding energy of an isolated self-interstitial (I) to the {113} vacancy defects when forming a ZD, given by $E^f(I) + E^f(\mathrm{V}^{\{113\}}) - E^f(\mathrm{ZD}) \approx E^f(I) + 0.3$ eV. A theoretical estimate of $E^f(I)$ using the same approximations as in this study is 3.9 eV [33]. Then the binding energy of individual self-interstitials to the {113} vacancy defect is in excess of 4 eV, and this represents a deep trap for mobile I. However, if the interstitials can annihilate with isolated vacancies, the energy saving is greater, so that the process of absorption of I by the {113} vacancy defects can only occur if kinetic factors favour it.

Our calculations show that, for large {113} vacancy defects able to accommodate the shear in the Burgers vector of the bounding dislocation, the ZD is a metastable defect, i.e. there is a barrier unfaulting. This, combined with the energetics obtained for {113} vacancy defects and ZDs, supports the proposed formation trajectory suggested by the HTREM experiments [2].

4. Conclusions

In summary, we have shown for that a rod-like defect structure in a {113}-plane made up from agglomerated lattice vacancies in the form of [110]-chains is a particularly stable structure, strongly resembling the model from HRTEM [2, 23]. For an *infinite* defect, the formation energy per vacancy is 1.0 eV. Within this framework, finite systems would have a higher energy due to contributions from the bounding dislocations and terminating dangling bonds in the $[1\bar{1}0]$-directions.

However, this represents a particularly stable defect in comparison to other theoretical estimates for vacancy agglomerates, but higher than those of around 0.3 eV from experiment [19]. It should be noted that the method we have employed generally underestimates the strength of reconstructed bonds, and it seems likely that our value for the formation energy is an over-estimate.

Significantly, the electronic density of states shows an empty band in the upper half of the bandgap, consistent with the observation of extended states in LDLTS experiments.

The binding energy of isolated vacancies to the {113} planar aggregate is estimated to be around 2 eV. This is lower than that calculated for isolated self-interstitials to the RLDs using the same methods [22], which yield >3 eV using a formation energy of the isolated interstitial at 3.9 eV [33].

The binding energy of I to the {113} vacancy defects to form ZDs is large, and the model proposed from experiment [2] for the preferential formation of {113}-oriented interstitial RLDs over those in the {111}-planes seems plausible. However, there remain other factors that might

also explain the apparent bias for the {113}-orientation over {111}, such as finite aggregate effects due to the bounding dislocation loop, kinetic factors, and nucleation processes.

Finally, although we have shown that the {113}-oriented vacancy aggregates are stable, low-energy structures, we note that it seems likely that their formation will be highly dependent on the details of the irradiation method, sample geometry, composition and any heat treatment. For example, in Si/SiGe structures implanted with Ge+ ions followed by annealing, vacancies form *spherical* agglomerates which assemble in the quantum wells, driven by a strain-enhanced migration mechanism [34–36].

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