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Dislocation core reconstruction in zinc-blende semiconductors

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Abstract. Using *ab initio* total-energy calculations, we computed core reconstruction energies of partial dislocations in zinc-blende semiconductors. The reconstruction energy of 30° partials was found to scale almost linearly with the experimental activation energy of 60° dislocations. The electronic structure of a dislocation shows that in an unreconstructed core, the gap states comprise a half-filled one-dimensional band, which splits up into bonding and antibonding states upon reconstruction. The energy states which lie in the electronic gap come from the core of β-partials, while those related to α-partials remain resonant in the valence band.

Dislocation mobility is known to control the plasticity of materials. In semiconductors, while dislocations have low mobility in type IV compounds, their mobility is considerably higher in type III–V and II–VI compounds under equivalent conditions. Since all of these materials have the same structure, and therefore the same set of active dislocations [1], it is important to understand the cause of such a wide range of dislocation mobilities. In semiconductors, dislocations glide conservatively in {111} planes [2, 3]. These (screw and 60°) dislocations have extended cores consisting of (30° and 90°) partial dislocation, separated by a stacking fault. In a III–V compound, dissociation into partials generates three types of dislocations: α, consisting of a 30° and a 90° partial with the cores formed by type V atoms; β, consisting of a 30° and a 90° partial with the cores formed by type III atoms; and a screw consisting of two 30° partials, one of each type. In a type IV material, α- and β-dislocations are identical.

It has been long appreciated that the cores of dislocations should be full of dangling bonds. Core reconstruction has been suggested as a mechanism by which most of these dangling bonds are eliminated. Core reconstruction should be favoured in covalent materials since the energy gain due to dangling-bond pairing is larger than the energy due to bond distortion on going from an unreconstructed to a reconstructed configuration. Recent *ab initio* calculations showed that the reconstruction of partial dislocations in semiconductors is favourable [4–6]. Since dislocation motion is controlled by the energetics of the atomic motions that happen in the dislocation core [7], it is relevant to learn how core reconstruction can affect dislocation mobility. The effect of core reconstruction on dislocation mobility is straightforward [8]; for a dislocation to move through the lattice, reconstruction bonds must be broken. This provides an additional resistance to dislocation motion, above the usual lattice resistance to interatomic slip. The stronger the reconstruction bonds are, the higher should be the resistance to dislocation motion [9].

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Dislocation velocities are controlled by thermally activated kink mechanisms, exhibiting a behaviour [2]

$$v_d = v_0 \exp\left(-\frac{Q}{k_B T}\right) \tag{1}$$

where v_0 is a constant velocity, Q is the activation energy, and k_B is the Boltzmann constant. Here we have established a direct connection between this dislocation activation energy and the core reconstruction energy of partial dislocations. This was achieved by computing the reconstruction energy of 30° glide partial (both α- and β-) dislocations in several zinc-blende materials using *ab initio* calculations and comparing them to the respective experimental activation energies of 60° glide dislocations. We focused on the 30° glide partials motivated by the experimental data on 60° dislocations, since it has been shown that it is the 30° partial which controls the dislocation mobility [10].

We considered an orthorhombic supercell with 96 atoms, where a dislocation dipole, consisting of 30° partials, was introduced [2]. The dislocation dipole contained an α- and a β-partial in a type III–V material, or two identical partials in a type IV material. The cell geometry is such that the dislocations are four lattice parameters apart in the glide plane, preventing core–core interactions. Figure 1 shows a {111} glide plane containing unreconstructed and reconstructed 30° (α- and β-) partial dislocations. Core reconstruction involves formation of bonds between atoms of the same species. Reconstruction energies of α- and β-partials were computed by taking the difference in total energies of the configurations 1(b) and 1(a) and the configurations 1(b) and 1(c), respectively.

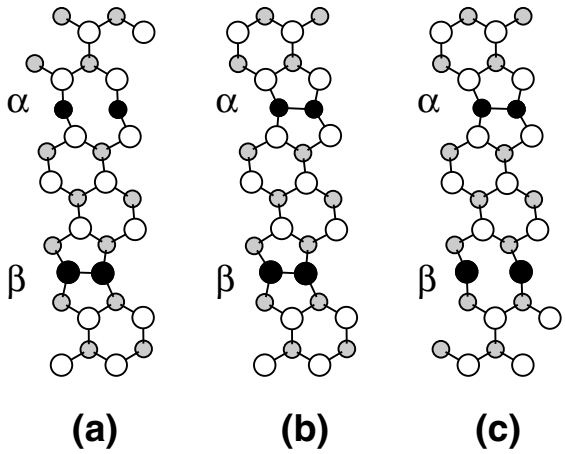

Figure 1. The atomic configuration of a (111) plane with a 30° partial dislocation lying in the [110] direction. In the figure, (a) and (c) show unreconstructed α- and β-dislocations respectively, while (b) shows a fully reconstructed dislocation. White and grey circles represent type III and type V atoms respectively. Black circles represent the atoms in the dislocation core.

Full atomic relaxation of the configurations presented in figure 1 is an enormous computational task using *ab initio* methods. To overcome this difficulty, we initially relaxed the structures with a less computationally expensive model, using interatomic potentials. These atomic relaxed configurations could be used as inputs to the *ab initio* calculations, when full relaxation could then be performed. However, for this procedure to really speed up the calculations, a reliable interatomic potential should be used, at least for dislocation core properties. One such model, called the EDIP (environment-dependent

interatomic potential), has been recently developed for silicon [11, 12], and provides a superior description of dislocation properties in Si [9, 12]. This potential, combined with a conjugate gradient algorithm, was used to generate reconstructed and unreconstructed dislocations. The relaxed structures obtained for silicon were used for all of the zinc-blende compounds, just renormalizing the lattice parameter for each compound. The reliability of this procedure was tested by checking the atomic forces on the *ab initio* calculations for the input configurations. For all compounds, the Hellmann–Feynman forces on all atoms were already below 0.2 eV Å^{-1}.

The *ab initio* calculations [13] were performed within the density functional theory and the local density approximation framework. The Kohn–Sham equations were solved by the Car–Parrinello scheme [14] using separable norm-conserving pseudopotentials [15, 16]. The valence electron wave-functions were expanded in a plane-wave basis set, with kinetic energy up to 16 Ryd. The sampling in the Brillouin zone was performed using a set of two k-points [17]. Geometric optimization of the atomic structure of all systems was performed by allowing atoms to relax until the Hellmann–Feynman forces were smaller than 0.02 eV Å^{-1}.

Table 1 presents the reconstruction energies of α- and β-partial dislocations. In all compounds, the reconstruction energies of α-dislocations are smaller than those of β-dislocations. This is consistent with experimental results [18–25] which find activation energies for 60° α-dislocations smaller than those for 60° β-dislocations. The ratio between the reconstruction energies ($E_\beta^{rec}/E_\alpha^{rec}$) is between 1.3 and 1.8. Experimental estimation for several compounds sets the ratio of activation energies (Q_β/Q_α) around 1.3 [23]. Table 1 also presents the relative distance between the reconstructed core atoms for all compounds, as compared to the respective crystalline bonds. Figure 2 displays the relation between the calculated reconstruction energies of 30° partial dislocation and the experimental activation energies of the respective 60° dislocation for the intrinsic material. The results suggest that the activation energies scale with the reconstruction energies. Our results also imply that the dislocation velocity activation energy for a certain semiconductor can be estimated only by computing the core reconstruction energy.

Table 1. The calculated reconstruction energy (E_{rec}, in eV/reconstructed bond) of 30° (α- and β-) partial dislocations and relative distance (d) between core atoms (as a percentage of a crystalline bond) for several type III–V and IV semiconductors. The table also presents the experimental activation energies (Q) for 60° ((α- and β-) dislocation velocities. For type IV materials, α- and β-results are identical, and the results are presented as α-dislocations.

	E_{rec}^{α} (eV)	d_α	E_{rec}^{β} (eV)	d_β	Q_α (eV)	Q_β (eV)
Si	0.92	5.9%			2.20 [18]	
Ge	0.64	6.2%			1.62 [19]	
AlP	0.47	1.2%	0.87	9.2%		
AlAs	0.44	8.1%	0.70	5.3%		
GaP	0.47	5.2%	0.83	−0.4%	1.45 [20]	1.68 [20]
GaAs	0.43	8.7%	0.56	1.4%	1.30 [21]	1.30 [21]
					1.00 [22]	1.40 [22]
GaSb	0.50	12.0%	0.63	−3.4%	1.30 [23, 24]	1.60 [23, 24]

We also investigated the electronic band structure of dislocations in semiconductors. The current picture of the electronic structure associated with the dislocation core considers a band in the materials gap [26]. For an unreconstructed dislocation core, the electronic state at the core is a half-filled one-dimensional band in the band gap, which splits up into filled bonding and empty antibonding states upon reconstruction. We focused our study on the case of aluminium phosphide (AlP), which was motivated by the fact that for all of the systems studied here, AlP was the material with the largest energy gap, facilitating the identification of the band structure.

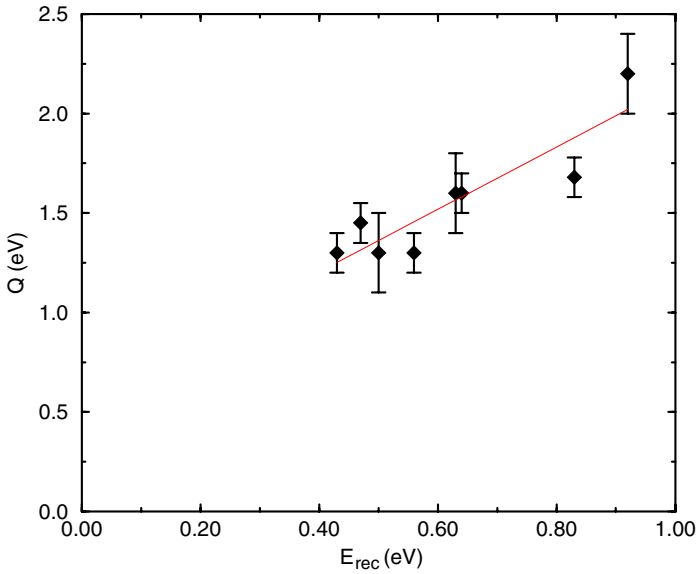

Figure 2. Calculated core reconstruction energies for 30° partial dislocation versus experimental activation energies of 60° dislocations for several type IV and type III–V semiconductors (according to table 1). Error bars represent the estimated error of the experimental data.

We computed the electronic band structure of a dislocation on the basis of the *ab initio* results obtained for the atomic structures displayed in figure 1. For that we considered a large set of k-points in the first Brillouin zone along the direction of the reciprocal-lattice vector related to the dislocation line direction. We found a very small dispersion in any direction normal to the dislocation line (lower than 40 meV). The dispersion in the electronic energy levels results from a one-dimensional band related to the dislocation line direction.

Let us consider the reconstruction of the β-dislocation. In the unreconstructed case, bonding and antibonding levels form a half-filled energy band on the top of the energy gap. On the other hand, in the reconstructed case, bonding and antibonding levels split away, forming a gap of 0.15 eV. The last occupied level comes from the Al–Al core interaction. Figure 3 shows the electronic charge distribution of the last occupied level for the reconstructed and the unreconstructed β-dislocation. In the reconstructed case, the charge distribution of the last occupied level is highly localized at the interstitial region between Al core atoms. For the unreconstructed case, the charge distribution of the last occupied level is highly delocalized inside the dislocation core. For the case of the reconstruction of the α-dislocation the situation is considerably different. The reconstructed P–P bond between the core atoms generates an energy level resonant in the valence band, 4 eV below the top of that band. In the unreconstructed case, this level moves up, remaining resonant in the valence band.

In summary, we have investigated the core properties of partial dislocations in semiconductors. We have identified for the first time a direct connection between the core reconstruction energy of partial dislocations, a microscopic property, and the activation energy of the dislocation velocity, a mesoscopic property. Considering the results obtained from our calculations, as well as the available activation energies for dislocation motion of II–VI zinc-blende semiconductors [25], which are below 1 eV, we estimate that the reconstruction energies for partial dislocations in II–VI materials are very weak, at 0.25 eV/reconstruction bond. Furthermore, we have unveiled the band structure of the dislocation core. The β-dislocations

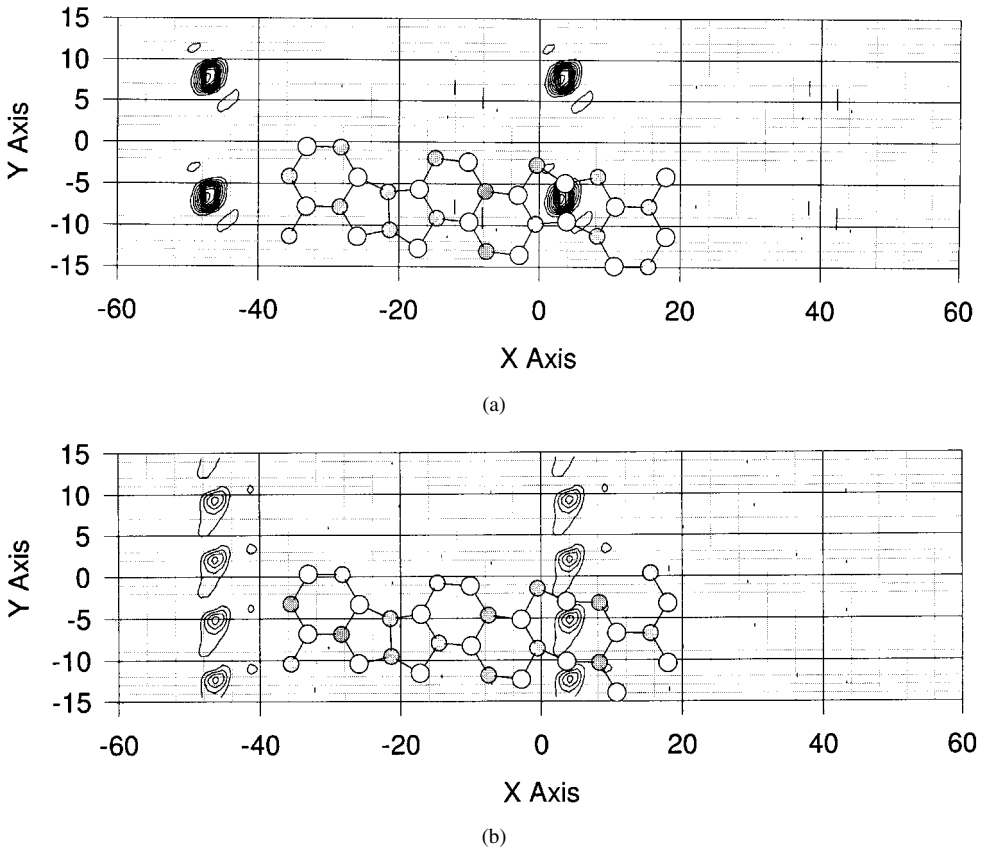

Figure 3. The electronic charge distribution of the last occupied level for the reconstructed (a) and the unreconstructed (b) β-dislocation. The figure presents the charge distribution on the {111} glide plane containing the aluminium atoms.

control the mobility of the dislocations, as result of a larger core reconstruction energy. Moreover, they control the electronic activity of the dislocations, being responsible for the dislocation-related energy levels which appear in the materials gap.

Acknowledgments

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