First Principles Calculations of the Energy Barrier to Dislocation Motion in Si and GaAs

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Abstract

The single kink formation and migration energies, F_k and W_m, of 90° glide partial dislocations in Si and GaAs are calculated using an *ab initio* local density functional cluster method. Kink migration occurs via a concerted exchange of an atom at a dislocation core with one of its glide plane nearest neighbors. By constraining these atoms to sit in high energy positions and relaxing a surrounding cluster of atoms, sufficient points in configuration space can be sampled for the energy barrier for the first step in kink pair formation to be estimated. By including an estimate of the elastic energy of interaction of kink pairs, the single kink formation energy is calculated. It is found that F_k and W_m for Si are 0.1 and 1.8 eV respectively. For the 90° α glide partial in GaAs, these quantities are 0.07 and 0.7 eV respectively, and 0.3 and 1.1 eV for β partials.

I. INTRODUCTION

It is widely accepted that the structure of dislocation cores plays a vital role in understanding the electronic and dynamical properties of dislocations in semiconductors [1]. In both Si and GaAs, the commonly occurring 60° and screw dislocations lie on {111} planes and are dissociated into partials separated by an intrinsic stacking fault [2–4]. The dissociation reaction is:

$$\frac{a}{2}[1\bar{1}0] \rightarrow \frac{a}{6}[1\bar{2}1] + \frac{a}{6}[2\bar{1}\bar{1}]. \tag{1}$$

It is likely that the partials are of the glide type [5]. This means that the core lies on the narrowly spaced {111} planes and contains lines of atoms with dangling bonds lying almost in the {111} glide plane giving rise to the possibility of bond reconstruction. If the core lay on the widely spaced planes leading to shuffle dislocations, the dangling bonds would be normal to the glide plane and reconstruction leading to the pairing of bonds would be impossible. Glide dislocations are then expected to have lower energy than shuffle ones. The two chemical species present in GaAs lead to two types of partial dislocations: the core atoms can be Ga, giving β dislocations, or As ones leading to α dislocations (Fig. 1). A screw dislocation dissociates into two 30° partials: one of Ga (β) type and the other of As (α) type. A 60° dislocation dissociates into a 30° and a 90° partial of the same type. A reconstructed bond would have to be formed between atoms of the same type.

The dislocation core structure has previously been investigated using our *ab initio* density functional cluster method for both Si [6] and GaAs [7,8]. The important conclusion, in agreement with previous work in the case of Si [9–16], is that the bonds within dislocation cores in Si and the β partial in GaAs are *strongly* reconstructed with bond lengths comparable to crystalline values. The α core in GaAs, however, is more weakly reconstructed. There are several implications of a strong reconstruction. Firstly, the dislocations are unlikely to be electrically active: the formation of a covalent bond between core atoms will lead to a great separation of bonding and anti-bonding states or between filled and empty levels. Any states in the band gap are then likely to be shallow electron or hole traps. Secondly, the reconstruction might not occur if electrically active impurities present in the core possess extra or fewer electrons than the host atom they replace. For example, N or P in Si prefer to remain three-fold coordinated with the remaining valence electrons occupying a lone pair [6,7,17] and in GaAs, a bond does not form for example between a pair of Be impurities within the core of a β dislocation [7,8]. Hence, whenever these impurities diffuse to the core, they cause a change in the reconstruction possibly leading to a pinning effect.

The third implication which we shall consider here is that bond reconstruction leads to low dislocation velocities as these bonds have to be broken for the dislocation to advance. Now, dislocations move by the thermal creation and diffusion, under an applied stress, of kinks and the magnitude of the dislocation velocity is then controlled by the kink formation energy, F_k, and the barrier to kink migration of energy W_m – assuming that there are no pinning points or strong obstacles along the dislocation line [5]. There is controversy over whether W_m is much greater than F_k [1,18–21] but strong reconstruction implies that the barrier to dislocation motion is considerable and the brittleness of the semiconductors is then understood to arise from the difficulty of breaking the reconstructed bonds.

In this paper, the first step in kink pair formation is studied and the energies of activation and formation are calculated. These quantities can be used to estimate F_k and W_m. This is the first time these quantities have been calculated using *ab initio* methods.

The local density functional cluster method used [22,23] has given bulk Si and GaAs bond lengths to within a few % of their crystalline values and has shown that the 90° partial dislocation in Si is strongly reconstructed with a core bond of length 2.43 Å compared to a bulk bond length of 2.35 Å. In GaAs using a variety of different cluster sizes [7,8], the same method gave a weakly reconstructed α core with an As-As core bond of length 2.58 Å compared to a bulk Ga-As bond length of 2.43 Å. The Ga-Ga bond in the β core is more strongly reconstructed, with a length of 2.40 Å. This strong core bond was considered to have arisen from the transfer of charge to the core from the surrounding shell of As atoms. These values are far from those given by the sum of the atomic radii of Slater [24], which are deduced from X-ray studies of metallic As and Ga compounds and they imply that the As-As and Ga-Ga bonds would be 2.30 and 2.60 Å, respectively. It appears to us that these values are not appropriate for dislocations or defects in GaAs. They predict, for example, that the Si-As bond should be shorter than the Si-Ga one whereas the *ab initio* calculations [25] show the reverse and account for the fact that the local vibrational mode of Si_{Ga} is lower than that of Si_{As}.

In section II we discuss the theory and measurements of the dislocation velocity and in section III we describe our calculations for Si and GaAs and give our conclusions in section IV.

II. THE KINK FORMATION AND MIGRATION ENERGIES

According to the model of Hirth and Lothe [5], the dislocation velocity, V_{dis}, for long dislocation segments in the high stress regime is governed by the generation and diffusion of kinks and is given by:

$$V_{dis} = \frac{\beta \nu_d \tau b^4}{kT} e^{-(F_k + W_m - TS)/kT} \tag{2}$$

where b is the primitive lattice vector and β is a geometrical factor of the order of unity. τ is the stress applied, ν_d an attempt frequency and S is an entropy term. The magnitude of V_{dis} can only be made to agree with experimental values if the entropy term, S, is of order 5-7k. Calculations of the vibrational entropy contribution indicate that such values are not unreasonable [26], although the important electronic contribution coming from the temperature variation of occupied energy levels was not considered. The activation energy for V_{dis}, Q, is the sum of the kink formation energy, F_k and the kink migration energy W_m.

The energy necessary to form a double kink of width nb depends on n and is sketched in Fig. 2. This dependence arises as the ends of the double kink can be thought of as single kinks which attract each other. For large n, the energy necessary to form a double kink is defined to be $2F_k$, *i.e.* the kinks are considered to be non-interacting. The kink-kink interaction energy is approximately described by elasticity theory [5] as:

$$E_{int} = \frac{Gb_p^2h^2}{8\pi nb}\frac{1+\nu}{1-\nu}, \tag{3}$$

where G is the shear modulus, b_p the partial Burgers vector, ν is Poisson's ratio and h is the height of the kink. For a 90° partial, $h = b_p = a/\sqrt{6}$ and taking ν to be 0.2, the interaction energy is:

$$E_{int}(n) = \frac{Gb^3}{48\pi n}. \tag{4}$$

In this paper we calculate E_1 and E_2 in Fig. 2, corresponding to $n = 1$. E_2 is the formation energy of a double kink of the smallest separation and is approximately related to F_k by:

$$E_2 = 2F_k - E_{int}(n = 1). \tag{5}$$

This assumes that the expression for $E_{int}(n = 1)$ based on elasticity theory is valid for a kink separation of about 4 Å. Calculations of the kink pair formation energies for larger n would require very much larger clusters than considered here. For Si, where b is 3.84 Å and G is 0.427 eVÅ^{-3}, we find $E_{int}(1)$ to be 0.16 eV for n equal to unity. In the case of GaAs, where b is 3.96 Å and G is 0.305 eVÅ^{-3}, $E_{int}(1)$ is 0.13 eV.

When a stress is applied, the double kinks of width nb which are formed thermally collapse back to a straight line provided $n < n^* = 0.14\sqrt{\frac{G}{\tau}}$, whereas those with n larger than n^* are forced to expand by the stress [5]. For stresses of order $10^{-3}G$, this means that $n^* \approx 4$. The migration energy W_m refers to that barrier associated with the motion of a kink with critical spacing. However, as the atomic processes involved in this migratory step are very similar to those involved in the first step, we assume that W_m is given by the average of E_1 and $E_1 - E_2$ (Fig. 2). The only previous theoretical estimate of F_k was based on interatomic potentials, *e.g.* a Tersoff potential gave 0.12 eV in Si [13].

Measurements of dislocation velocities in Si at low stresses are susceptible to errors arising from the pinning effect of impurities, but at higher stresses, values of Q around 2.2 eV for 60° and 2.3 eV for screw dislocations are found [18,27–29]. In GaAs the measurements of Q for 60° dislocations have greater scatter and range from 0.89 eV [30] to 1.3 eV for α dislocations [31–33] and between 1.24 eV [30] and 1.57 eV [34] for β dislocations. The pre-exponential factors for V_{dis} also display great variation between different groups with their ratios for α to β dislocations varying between 0.1 [30] to about 30 [31]. Q for screw dislocations is around 1.1 eV [34] or 1.3 eV [31]. All groups, however, find α dislocations to be more mobile than β ones. The similarity of the activation energies for screw and 60° dislocations suggests a common mechanism for the motion.

The experimental determination of F_k and W_m has, however, been a much more difficult procedure with different groups finding very different results. A summary of recent experimental results for Si has been given by Gottschalk et al [35]. They show W_m ranges between 1.2 and 1.8 eV, and F_k to lie between 0.4 and 0.7 eV. These values have been found from several techniques including internal friction studies and by the observation of the critical dislocation length, L_0, below which the velocity depends linearly on the segment length L [36,37]. If L_0 is determined by the mean separation of kinks in thermal equilibrium, then

$$L_0 = 2be^{F_k/kT}. \tag{6}$$

When L is smaller than L_0, kinks reach the ends of the segment before annihilation by a kink traveling in the opposite direction. The equation for V_{dis} then becomes:

$$V_{dis} = \frac{\tau abh^2\beta L}{kT} e^{-(2F_k+W_m-TS)/kT}. \tag{7}$$

The theory implies that the activation energies Q in the two regimes will differ by F_k. However, Yamashita and Maeda [38,39] find there is no difference in Q between the two regimes. They suggest instead that L_0 is determined by the separation of obstacles which act as recombination points for kinks traveling in opposite directions. The model assumes that the time needed for the line to breakaway from the obstacle is not rate determining, as this is less than the time needed for double kinks to be generated and expand to the ends of the segment. Furthermore, the density of obstacles is independent of temperature with L_0 about $400b$. In this case, Q is given by $2F_k + W_m$ and the equilibrium separation of kinks is greater than L_0. Thus F_k must be greater than 0.5 eV. However, Hull and Bean [40], also assume L_0 to be given by this model of obstacle limited kink mean free path, but find $F_k < 0.2$ eV. Hirsch et al [41] estimate W_m to be less than 1.2 eV from observations of the movement of kinks. These large discrepancies in estimates of F_k and W_m show that further studies are required.

There has been much less work carried out on determining W_m and F_k in GaAs. Maeda and Takeuchi [42] investigated the effect of electronic excitation on the dislocation velocity. They found Q in the dark to be 1.0 and 1.7 eV for α and β dislocations respectively, which are reduced by more than 0.7 and 1.1 eV respectively under electron irradiation. They argue that the recombination of excess electrons and holes generated by electron irradiation reduce the migration energy W_m which must then lie between 0.7 and 1.0 eV for α dislocations and 1.1 and 1.7 eV for β dislocations.

III. METHOD

Only a brief summary of our method will be given here, as we have discussed this in great detail in other papers [22]. We use the local density functional approach to the solution of the many-body Schrödinger equation expanding both the charge density and wave-functions in terms of a basis of Gaussian orbitals. The basis used here is similar to that used previously [8]. Norm-conserving pseudopotentials of ref. [43] eliminate the need to include core electrons. The self-consistent energy is found as well as the forces on each atom and all the atoms in the cluster relaxed using a conjugate gradient minimization method.

The clusters used in the present investigations comprise 158 atoms surrounding the 90° dislocation with composition $Si_{84}H_{74}$ for the case of silicon and $Ga_{42}As_{42}H_{74}$ for GaAs. The latter is shown in Fig. 1. H atoms are used to terminate the surface dangling bonds. In the case of GaAs, the clusters are stoichiometric and hence electrically neutral. For a β partial, there is a double line of Ga atoms along $[10\bar{1}]$ and the stoichiometry then implies that there are more As than Ga atoms on one of its (111) surfaces. This gives rise to a electrical dipole moment parallel to [111]. This dipole moment may cause additional forces on the core atoms and displace them in this direction. However, as the main rebonding pattern lies in the (111) plane, we expect this dipole to have a minimal effect on the calculated distortions. The same considerations apply to α partials.

The 158 atom cluster containing the 90° partial dislocation is relaxed to give the structure of the straight dislocation (Fig. 1). This has already been done for dislocations in Si and GaAs and has been reported in earlier papers [6–8]. In order to form a kink pair, one core atom and one of its nearest neighbors lying in the glide plane of the dislocation must be rotated through $\approx 90°$ about an axis normal to the slip line (see Fig. 3; the atoms in question are numbered 20 and 6). Of course, the rotation is not rigid, and in practice the length of the bond 6-20 might change during the motion. The double kink is actually created in a region where the stacking fault lies. There is only a small energy difference if the kink is created on the side of the dislocation where the stacking sequence is normal [44]. After the rotation, a short segment of the dislocation core has been displaced and the smallest double kink created. This structure is then relaxed using the same basis set as that used for the straight dislocation. Because the bonding pattern has now changed, the atoms do not revert to their position found for the straight dislocation. The difference in the energies between the two relaxed clusters is then E_2. It is important to realize that the double kink would not spontaneously collapse back to the straight dislocation because there is an energy barrier, $E_1 - E_2$, between the relaxed structures. This can only be overcome by thermal fluctuations. E_1 is the energy barrier that must be surmounted for the kink pair to form. For this to be calculated, the structure at the saddle point must be found. This is done by introducing two constraints, (con_1, con_2), which prevent the structure from relaxing to either the straight or the kinked dislocation. Ideally these constraints should be chosen so that the energy varies rapidly with them, and their initial and final values should refer to the straight and kinked dislocation. In practice, we choose constraints related to bond lengths so that the lengths of the bonds 6-22 and 20-21 gradually increase while those of 6-21 and 20-22 gradually decrease as we pass from the straight to the kinked dislocation. The actual constraints are (con_1, con_2) where

$$con_1 = |\mathbf{R}_{20} - \mathbf{R}_{21}|^2 - |\mathbf{R}_{20} - \mathbf{R}_{22}|^2 \tag{8}$$

$$con_2 = |\mathbf{R}_{6} - \mathbf{R}_{22}|^2 - |\mathbf{R}_{6} - \mathbf{R}_{21}|^2. \tag{9}$$

These equations are solved for one of the coordinates of $\mathbf{R}_{20}$ and $\mathbf{R}_6$, and then the other coordinates of these atoms as well as the coordinates of all the remaining atoms are relaxed using the conjugate gradient method. Energy contour plots are then constructed for the variables (con_1, con_2) and these show a saddle point often close to the origin, i. e., $(con_1, con_2) = (0, 0)$ where the 20-21 and 6-22 bond lengths are equal to those of 20-22 and 6-21. This method for obtaining activation barriers has been successfully used to treat the diffusion of oxygen in Si [45] as well as the reaction energies of adsorbed species on a surface of diamond [46].

The energy levels of the saddle point structure yield information on the effect of doping on the activation barrier.

IV. RESULTS

A. Silicon

The relaxed 158 atom cluster containing a straight 90° glide dislocation had a central Si–Si core bond of length 2.46 Å. The backbonds were 2.36, 2.44, 2.37 and 2.38 Å in the glide plane and 2.38 and 2.39 Å out of the glide plane. Since the bulk Si bond length is 2.35 Å these bond lengths give about 5% strain, and in agreement with earlier studies, show that the dislocation is strongly reconstructed.

We then investigated the kinked dislocation as illustrated in Fig. 3. The double kink has a strongly reconstructed central core bond of length 2.45 Å. The backbonds were of lengths 2.37, 2.39, 2.38 and 2.43 Å in the glide plane and 2.39 and 2.38 Å out of the glide plane. Thus the strain in the double kink is about the same as in the straight dislocation. The difference in energy between the the straight and kinked dislocation clusters, i. e. E_2, was found to be 0.004 eV: a negligible amount when considering the errors in the method. Our estimate of F_k is, from eqn. (5), thus given entirely by the elastic interaction term $\frac{1}{2}E_{int}(n = 1)$, and is then about 0.1 eV—rather close to that found from using a Tersoff potential [13]. This small value is the result of comparable bond length strain in the kink and straight dislocation.

We then investigated the barrier to the formation of the double kink using the method described above. The results of the constrained cluster calculations are shown in Fig. 4 and reveal an energy barrier to kink pair formation of 1.80 eV. This then is approximately W_m. The implication is then that the formation energy of kinks is a small fraction of W_m and our estimate for Q, the activation energy for dislocation velocity, is 1.9 eV. This is reasonably close to the observed energy of 2.2 eV. Nevertheless, F_k is at the lower end, and W_m at the higher end, of the experimental estimates discussed in section II.

The energy levels of the relaxed clusters containing the straight, kinked and saddle point dislocation configurations are shown in Fig. 5. The dashed lines represent the three lowest empty levels. The straight and kinked dislocations have band gaps devoid of deep mid-gap states consistent with strong reconstruction. The band gaps are larger in the clusters used here than in bulk because of the effect of the hydrogen atom confinement. In the case of the saddle point configuration, a filled and an empty level have been pulled into the mid-gap region from the top of the valence band and the bottom of the conduction band respectively. They arise from bonding and antibonding states of heavily strained Si–Si bonds. We now argue that the positions of these saddle point levels lead to the prediction that the barrier, E_1, in doped material is lower than in undoped material [20]. In n-type Si, we expect a shallow kink acceptor level to be occupied and the total energy of this configuration would include the energy of this state. At the saddle point, however, this level has now dropped to mid-gap (Fig. 3c) and the energy of the charged saddle point configuration would be lowered over the charged kink configuration by approximately half of the energy gap — provided changes in the Hartree and exchange-correlation energies are ignored. This is similar to the model of Hirsch [19] for the doping effect except the deep levels are associated with the saddle point configuration and not with kinks. Similarly, emptying a shallow filled kink state in p-Si would reduce the activation energy for positively charged kinks. Initial experimental investigations [47–49] showed that Q is reduced by 0.6 eV for Si:P and 0.5 eV for B doped Si in accordance with the theory. However, later experimental studies [29], although finding the same reduction in Q for n-doping, failed to find an effect for boron doping. The effect disappears above a certain temperature and it may be that this critical temperature was different in the more recent investigations.

B. The β Partial in GaAs

The same method has been applied to the two types of partial in GaAs. For the straight dislocation, the central Ga–Ga core bond of a 90° partial is strongly reconstructed with length 2.41 Å. The backbonds have lengths 2.48, 2.43, 2.54, 2.47 Å in the glide plane and 2.38 and 2.37 Å out of the glide plane. These represent strains of ≈5% about the same as found for Si.

In the case of the kinked dislocation, the central Ga–Ga bond in the double kink has length 2.42 Å, with backbonds 2.50, 2.46, 2.40 and 2.45 Å long in the glide plane and 2.34 and 2.38 Å out of the glide plane. These strains are similar to those in the straight dislocation. The difference in energy between these two clusters is 0.4 eV. This, together with the kink-kink interaction term calculated in section II gives an estimate for F_k of 0.27 eV.

The energy barrier to double kink formation is shown in Fig. 6 and gives E_1 to be 1.30 eV. The kink migration energy, W_m, is then estimated to be 1.1 eV and the activation energy for the dislocation velocity, Q, to be 1.4 eV in reasonable agreement with experimental values ranging from 1.24 to 1.57 eV.

The energy levels for the straight, kinked and saddle point configurations compared with those of a perfect 154 atom hydrogen terminated GaAs cluster are shown in Fig. 7. The straight and kinked β dislocations (Figs. 7 b, c) have a somewhat smaller band gap than the perfect cluster (Fig. 7 d). It is, however, not possible for us to be certain whether the β partial, or indeed the α partial, introduce shallow states into the band gap because of the sensitivity of the levels to the actual cluster. In contrast with Si, the saddle point configuration (Fig. 7 a) has only a filled level in the upper gap. This suggests a strong effect on Q in p-doped material. On p-doping, this level would be empty, hence reducing E_1. Now the dislocation velocity is the sum of contributions from kinks in different charge states. The theory predicts that the mobility of positive charged kinks would be greater than either neutral or negatively charged ones. Thus, as the Fermi level rises with n-type doping, the concentration of positive charged kinks becomes progressively less, and the dislocation velocity becomes dominated by neutral or negatively charged kinks with higher values of

Q. This is in agreement with experiment, as this shows that Q increases from 1.15 eV in p-GaAs to 1.3 eV in undoped material, and to 1.6 eV in n-GaAs [31,32].

C. The α Partial in GaAs

In agreement with previous results for the straight dislocation, the central As–As core bond of a 90° partial is only weakly reconstructed with length 2.58 Å. This is 6% longer than a GaAs bond. The backbonds have lengths 2.54, 2.42, 2.63, 2.43 Å in the glide plane and 2.39 and 2.40 Å out of the glide plane.

In the case of the kink, the As–As bond has length 2.54 Å, with backbonds of lengths 2.54, 2.42, 2.52 and 2.50 Å in the glide plane and 2.37 and 2.41 Å out of the glide plane. The difference in energy between these two clusters is negligible. Taking the kink-kink interaction energy into consideration, the kink formation energy, F_k, is calculated to be 0.07 eV—substantially less than that of the β partial.

The results of the constrained calculations for the activation barrier are shown in Fig. 8 and give E_1 and W_m to be 0.7 eV. Thus we find Q to be about 0.8 eV in this case. E_1 and E_2 are much smaller for α partials than β ones because of the weak core reconstruction of the former. The theory then accounts for the greater mobility of α partials, and the predicted value of Q lies at the lower end of experimental estimates of 0.89 to 1.3 eV.

The energy levels for the straight, kinked and saddle point configurations are shown in Fig. 7. The straight and kinked dislocations (Figs. 7 e, f) have energy levels similar to those of the β partial. This suggests that electron beam induced current (EBIC) contrast should be similar for both partials in the absence of impurities or defects. The saddle point configuration (Fig. 7 g), however, has an *empty* level pulled down from the conduction band bottom and lies just above the valence band top. This is quite different from the β partial case. It suggests that negatively charged kinks in α partials should, in contrast to β ones, have greater mobility than positively charged ones. In n-GaAs, this level would be occupied, hence it would cost less energy to pull it towards the valence band thus reducing E_1. Indeed, experiments reveal a reduced activation energy for n-type material for Q changes from 1.10 eV in n-GaAs to 1.3 eV in undoped material, and to 1.4 eV in p-GaAs [32]

V. DISCUSSION

The *ab initio* cluster method shows that the shortest possible double kink on a 90° partial has very low formation energy in both Si and GaAs. These small values arise because both the straight and kinked dislocations possess bond lengths strained by a similar amount. Consequently, the energy of the double kink, at least in Si and for α cores in GaAs resides in the elastic strain field. The activation barrier on the other hand is very large. It is likely that the cluster method underestimates the true formation energy, and overestimates W_m, as the cluster surface is free to relax in our calculations and it is known that, near the surface, the formation energy of defects can be reduced [50]. Nevertheless, this reduction is likely to be the same in materials with similar elastic properties and we can conclude that, whereas the formation energy of kinks in Si is comparable to those in GaAs, the values of W_m are quite different and reflect the strength of chemical bonds. W_m is greatest for Si and is least for α

partials. The errors expected from our *ab initio* method are a few tenths of an eV, and when this is taken into account the values of F_k and W_m span the ranges reported by different experimental groups. Table 1 gives our estimates of these parameters. The predicted values of the activation energy for dislocation motion, Q, are in reasonable agreement with the available results in Si and agree closely with the values of refs. [30,42] in GaAs. These results support the Hirth-Lothe model for the dislocation velocities in semiconductors.

The energy levels associated with the saddle point for kink pair activation are very different in the three cases investigated. In Si, they lie around mid-gap and the activation energy for neutral, negatively and positively charged kinks are expected to be very different with neutral kinks being the least mobile. For the β partial in GaAs, an occupied saddle point level is close to the conduction band and leads to the prediction that positively charged kinks have greater mobility than either neutral or negatively charged ones. In the case of the α partial, an empty saddle point level lies near the top of the valence band and this suggests that n-doping lowers the activation barrier. Of course, these levels also suggest strong reductions in the barrier when electron-holes pairs are present from either current injection or photo-ionization.

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REFERENCES

[1] M. S. Duesbery, and G. Y. Richardson, CRC Crit. Rev. Solid State Mater. Sci. **17**, 1 (1991).

[2] I. L. F. Ray, and D. J. H. Cockayne, Proc. Roy. Soc., A **325**, 534 (1971).

[3] A. Gomez, D. J. H. Cockayne, P. B. Hirsch, and V. Vitek, Phil. Mag, 31, 105 (1975).

[4] A. Gomez, and P. B. Hirsch, Phil. Mag, A38, 733, (1978).

[5] J. P. Hirth, and J. Lothe, *Theory of Dislocations*, McGraw Hill, New York, 2nd Edition, (1982).

[6] A. Umerski, and R. Jones, Phil. Mag. A 67, 905 (1992).

[7] R. Jones, A. Umerski, P. Sitch, M. I. Heggie, and S. Öberg, Phys. Stat. Sol. (a) **137**, 389 (1993).

[8] P. K. Sitch, R. Jones, S. Öberg, and M. I. Heggie, Phys. Rev. B, in press (1994).

[9] S. Marklund, Phys. Stat. Sol., B, **85**, 673 (1978).

[10] P. B. Hirsch, J. Phys. (Paris), **40**, C6-40 (1979).

[11] R. Jones, J. Phys. (Paris), **40**, C6-33 (1979).

[12] K. W. Lodge, S. L. Altmann, A. Lapiccirella, and N. Tomassini, Phil. Mag., **49**, 41 (1984).

[13] M. I. Heggie, and R. Jones, Inst. Phys. Conf. Ser. *Structure, and Properties of Dislocations in Semiconductors*, ed. by ?
87 Phys Rev, 367 (1987).

[14] S. Marklund, and Y. L. Wang, Solid St. Comm., **82**, 137 (1992).

[15] H. Teichler, and H. Veth, J. Phys. (Paris), **44**, C4-93 (1983).

[16] J. R. K. Bigger, D. A. McInnes, A. P. Sutton, M. C. Payne, I. Stich, R. D. King-Smith, D. M. Bird, and L. J. Clarke, Phys. Rev. Lett., **69**, 2224 (1992).

[17] M. I. Heggie, R. Jones, and A. Umerski, Phys. Stat. Sol., (a) **138**, 383 (1993).

[18] H. Alexander, and P. Haasen, *Solid State Physics*, **22**, edited by H. Ehrenreich, and J. Turnbull, Academic Press, New York, 27 (1968).

[19] P. B. Hirsch, J. Phys. (Paris), **40**, C6-117 (1979).

[20] R. Jones, Phil. Mag., B**42**, 213 (1980).

[21] P. B. Hirsch, Inst. of Phys. Conf. Ser., *Microscopy of Semiconducting Materials*, ed. A. G. Cullis, S. M. Davidson, and G. R. Booker, **67**, 1 (1983).

[22] R. Jones, Phil. Trans. Roy. Soc., London, A **341**, 351 (1992).

[23] P. R. Briddon, and R. Jones, Phys. Rev. Lett., **64**, 2535 (1990).

[24] J. C. Slater, *The Self-Consistent Field for Molecules and Solids*, McGraw Hill, New York, (1974).

[25] R. Jones, and S. Öberg, Semicond. Sci. and Technol., in press (1994).

[26] S. Marklund, Solid State Commun., **54**, 555 (1985).

[27] J. R. Patel, and A. R. Chaudhuri, Phys. Rev., **143**, 601 (1966).

[28] F. Louchet, and A. George, J. de Physique, C4, **44**, 15 (1983).

[29] M. Imai, and K. Sumino, Phil. Mag., **47**, 599 (1983).

[30] M. Matsui, and T. Yokoyama, Inst. Phys. Conf. Series, **79**, 13 (1986)

[31] I. Yonenaga, and K. Sumino, J. Appl. Phys., 65, 85, (1987).

[32] K. Sumino, Inst. of Phys. Conf. Ser., *Structure, and Properties of Dislocations in Semiconductors*, ed. S. G. Roberts, D. B. Holt, and P. R. Wilshaw, **104**, 245 (1989).

[33] H. Alexander, and H. Gottschalk, Inst. of Phys. Conf. Ser., *Structure, and Properties of Dislocations in Semiconductors*, ed. S. G. Roberts, D. B. Holt, and P. R. Wilshaw, **104**, 281 (1989).
[34] V. B. Osvenskii, and L. P. Kholodnyi, Sov. Phys. Sol. St. **14** 2822 (1973)
[35] H. Gottschalk, N. Hiller, S. Sauerland, P. Specht, and H. Alexander, Phys. Stat. Sol. (a) **138**, 547 (1993).
[36] F. Louchet, D. Cochet Muchy, Y. Brechet, and J. Pelissier, Phil. Mag., A **57**, 327 (1988).
[37] B. Ya. Farber, Yu. L. Iunin, V. I. Nikitenko, V. I. Orlov, H. Alexander, H. Gottschalk, and P. Sprecht, Phys. Stat. Sol. (a) 138, 557, (1993).
[38] Y. Yamashita, K. Maeda, K. Fujita, N. Usami, K. Suzuki, S. Fukatsu, Y. Mera, and Y. Shiraki, Phil. Mag. Letts., 67, 165, (1993).
[39] K. Maeda, and Y. Yamashita, Phys. Stat. Sol. (a) **138**, 523 (1993).
[40] R. Hull, and J. C. Bean, Phys. Stat. Sol. (a) **138**, 533 (1993).
[41] P. B. Hirsch, A. Ourmazd, and P. Pirouz, Inst. Phys. Conf. Ser. No. **60**, 29 (1981).
[42] K. Maeda, and S. Takeuchi, J. de Physique, C4, **44**, 375 (1983).
[43] G. B. Bachelet, D. R. Hamann, M. Schlüter, Phys. Rev. B, 26, 4199 (1981).
[44] K. Wessel, and H. Alexander, Phil. Mag., **35**, 1523 (1977).
[45] R. Jones, S. Öberg, and A. Umerski, Mat. Sci. Forum, **83-7**, 551 (1991).
[46] C. D. Latham, M. I. Heggie, R. Jones, and P. R. Briddon, Diamond, and Related Materials, **3**, 1370 (1994).
[47] V. N. Erofeev, and V. I. Nititenko, Sov. Phys. Sol. State. **13** 116 (1971).
[48] J. R. Patel, L. R. Testardi, and P. E. Freeland, Phys. Rev., B **13**, 3548.
[49] S. B. Kulkarni, and W. S. Williams, J. Appl. Phys. **47**, 4318 (1976).
[50] D. M. Duffy, J. H. Harding, and A. M. Stoneham, J. Appl. Phys. **76**, 2791 (1994).

TABLES

TABLE I. Calculated values of F_k, W_m and Q, in eV, and crystal type necessary for reduction in Q

	F_k	W_m	Q	type
Si	0.1	1.8	1.9	n-type, p-type
GaAs β-partials	0.3	1.1	1.4	p-type
GaAs α-partials	0.07	0.7	0.8	n-type

VI. FIGURE CAPTIONS

Fig. 1. The 158 atom cluster, $Ga_{42}As_{42}H_{74}$, containing a 90° partial dislocation with a reconstructed core. The small spheres indicate Ga, and the larger ones As. The terminating H atoms are not shown. The two lines of Ga core atoms parallel to the dislocation line along $[10\bar{1}]$ are bonded together with reconstructed bonds. The Burgers vector of this partial lies along $[1\bar{2}1]$ and is perpendicular to the dislocation line. The (100) slip plane is perpendicular to the dislocation line and to the Burgers vector and cuts through the reconstructed bonds.

Fig. 2. Schematic representation of the energy involved in the formation of a kink pair of width nb, and the migration energy, W_m, of a kink. E_1, and E_2 represent the activation barrier and formation energy of a double kink of width $n = 1$.

Fig. 3. The atoms in the glide (111) plane, i. e. parallel to the horizontal plane in Fig. 1, for the relaxed straight and kinked 158 atom GaAs cluster. The full line in the first figure is in the dislocation core along $[10\bar{1}]$ and is perpendicular to the partial Burgers vector of the 90° partial along $[1\bar{2}1]$. The double kink has moved part of the dislocation in the (111) slip plane and in the direction of the Burgers vector.

Fig. 4. Contour plot of the energy barrier, E_1 eV, to kink pair activation for the 90° partial in Si. The lower left hand corner is close to the configuration of the straight dislocation whereas the upper right hand corner is close to that of the double kink.

Fig. 5. Cluster energy levels (eV) for the (a) straight (b) kinked, and (c) saddle point dislocation structures in Si. The broken lines show the three lowest unoccupied levels. Note that there is a substantial energy gap between the filled and empty levels for the straight and kinked dislocation but two deep gap levels for the saddle point configuration corresponding to double kink activation.

Fig. 6. Contour plot of the energy barrier, E_1 eV, to kink pair activation for the 90° β partial in GaAs.

Fig. 7. Cluster energy levels (eV) for the (a) saddle point structure of β partial, (b) kinked structure of β partial, (c) straight β partial, (d) perfect 154 atom cluster, (e) straight α partial, (f) kinked structure of α partial, (g) saddle point structure of α partial. The broken lines show the three lowest unoccupied levels. Again there is a gap between the highest filled and empty states of all the dislocations except those corresponding to saddle point structures in (a) and (g). However, the possibility of electron or hole traps associated with the dislocation cores cannot be excluded.

Fig. 8. Contour plot of the energy barrier, E_1 eV, to kink pair activation for the 90° α partial in GaAs. The lowest left hand corner is close to a configuration of a straight dislocation and the upper right hand corner is close to that of the double kink.