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Stability and core structure of undissociated screw dislocations in group IV materials investigated by means of atomistic calculations

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Abstract
We have examined the various possible configurations for an undissociated screw dislocation in group IV materials (Ge, Si, 3C-SiC, diamond) by means of semi-empirical atomistic calculations. A complete structural characterization and a determination of the relative stability are performed. We found that, in contrast to the case for Ge and Si, a geometry with the presence of sp^2 atoms in the core is the most stable structure for 3C-SiC and diamond. This yields a stable screw dislocation configuration in the 'shuffle' set for Si and Ge, and in the 'glide' set for 3C-SiC and diamond.

1. Introduction

Despite recent advances in the understanding of the elementary mechanisms of plasticity in a prototype semiconductor such as silicon, further work is required to shed some light on specific domains, such as the dislocation core structures and their relation to the dislocation mobility. Atomistic modelling is a valuable tool in performing such studies, because of the reduced sizes and possible complex structures of the dislocation cores in covalent materials [1]. For silicon, the cores and several kink structures have been widely investigated [2] with these methods. Recently, an attempt to unite all this knowledge in a coherent picture to explain the observed dislocation mobility has been proposed by Bulatov *et al* [3]. However, up to now, much of the effort has been devoted to dissociated dislocations in the 'glide' set, i.e. narrowly spaced {111} planes. Recent transmission electron microscopy observations have shown that undissociated dislocations, located in the 'shuffle' set, i.e. widely spaced {111} planes, should also play a key role for low-temperature high-stress conditions [4]. In particular, perfect dislocations with screw, 60°, 30°, and 41° characters have been observed.

In a recent paper, we have investigated the core properties of screw dislocations in silicon [5]. Three different screw core structures have been obtained from the calculations, each of these corresponding to a different plane localization of the core (figure 1). Configuration A,

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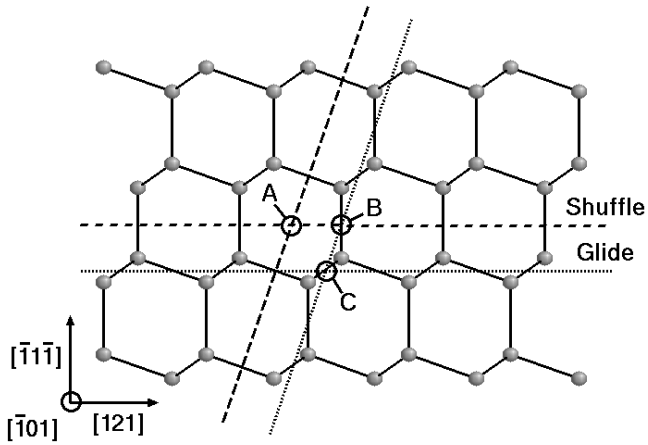

Figure 1. A ball-and-stick representation of the ($\bar{1}01$) plane of Si. The three circles A, B, and C show the positions of the line for a screw dislocation. Dashed (dotted) lines show the 'shuffle' ('glide') {111} planes.

where the dislocation belongs to two shuffle planes, is the most stable structure for silicon. We have shown that configuration B, with a dislocation belonging to both a shuffle and a glide plane (figure 1), is clearly metastable, and that the use of the Stillinger–Weber (SW) potential [6] was responsible for the different conclusions of Koizumi *et al* [7]. In this paper, we also described another core structure, C, where the dislocation is located in two glide planes. This last configuration, though higher in energy than the other two, shows an interesting feature. The atoms located in the near proximity of the dislocation line have coordination three, with almost coplanar bonds, characteristic of an sp^2 hybridization.

Our results on the stability of the core configurations were not surprising, the A structure being the usually accepted location of the screw dislocation [8, 9]. However, one may wonder whether the same energy ordering will be obtained for other cubic diamond semiconducting materials in group IV, such as germanium or diamond. Germanium is often thought of as similar to silicon, due to their very close properties. However, in the case of a screw structure, this point remains to be checked. But diamond may be the most interesting material for such an investigation, because the sp^2 hybridization, energetically unfavourable in silicon, is likely to increase the stability of the C configuration. For example, Ewels *et al* [10] have recently proposed that graphitization in carbon could occur at the 90° partial dislocation core. Finally, one interesting candidate for investigation would be 3C-SiC, i.e. silicon carbide in the cubic phase. This material is the natural bridge between carbon and silicon, two materials with different properties. Also, the presence of two species in SiC opens the way to a possible non-stoichiometric core dislocation, which could have a major influence on the dislocations mobility.

We have carried out empirical potential calculations of the screw dislocation core for several group IV materials. Results for the structure and stability of three different configurations are discussed and compared for silicon, germanium, diamond, and silicon carbide. After a brief description of the computational model, we describe the A, B, and C geometries obtained for all materials. In a second section, we show and discuss the stability of the configurations. Finally, we conclude and describe some possible directions for future work.

Table 1. Experimental and calculated elastic constants (in megabars) for the SW [6], Tersoff [11], and EDIP [13, 14] potentials. The SW parameters for silicon have been rescaled in order to fit the experimental cohesive energy of 4.63 eV.

		B	C_{11}	C_{12}	C_{44}	C_{44}^0
Ge	Experimental	0.77	1.29	0.48	0.67	
	Tersoff	0.76	1.38	0.45	0.66	0.93
Si	Experimental	0.99	1.67	0.65	0.81	
	SW	1.08	1.62	0.82	0.60	1.17
	Tersoff	0.98	1.42	0.75	0.69	1.19
	EDIP	0.99	1.75	0.62	0.71	1.12
SiC	Experimental	2.25	3.90	1.42	2.56	
	Tersoff	2.25	4.35	1.20	2.55	3.11
C	Experimental	4.42	10.79	1.24	5.78	
	Tersoff	4.30	10.66	1.13	6.39	6.73

2. Method

Interatomic interactions were described using semi-empirical potentials. Here, we have only considered potentials that have been specifically designed for the study of defects in group IV materials. On the one hand, it is worth noting that for a meaningful description of the core stability, the comparison among the different materials should be realized with the same potential, or at least potentials based on the same functional form. To our knowledge, sets of parameters for the complete set of materials investigated (Si, C, SiC, Ge), only exist in the case of the Tersoff potential [11]. It has been shown to give a correct description of a wide set of properties [12], and correctly predict the most stable A configuration for a screw dislocation in silicon [5]. On the other hand, it is equally important to use several potentials, to check quantitatively and qualitatively the accuracy of the results. Additional tests were then performed for silicon with the well known SW potential [6] and the recently developed environment-dependent interatomic potential (EDIP) [13, 14]. Table 1 shows the calculated elastic constants that we used in the elastic treatment, together with reference experimental values.

The modelling of the infinite straight dislocation can be done either with periodic or non-periodic boundary conditions in the directions perpendicular to the dislocation line [2]. In the case of periodic boundary conditions, a dipolar or quadrupolar distribution of dislocations must be considered to ensure a zero net Burgers vector in the computational cell [15, 16]. Here, we have used both techniques, with computational cells of at most 10 080 atoms. The differences obtained between the two methods are very small ($<1\%$), and much lower than the precision associated with semi-empirical potentials. Atomic structures were relaxed using standard techniques such as the conjugate gradient or damped molecular dynamics methods, until the residual forces were lower than 0.1 eV Å^{-1}.

3. Core structure

Figure 2 represents the three core configurations investigated. Geometry A shows no significant reconstruction or dangling bonds in the core, most of the distortions being supported by bonds of the ring encircling the dislocation. We observed no structural changes for different materials with the Tersoff potential. Configuration B is unusual since the largest displacements are located on the two atoms which are in the immediate proximity of the dislocation line. The

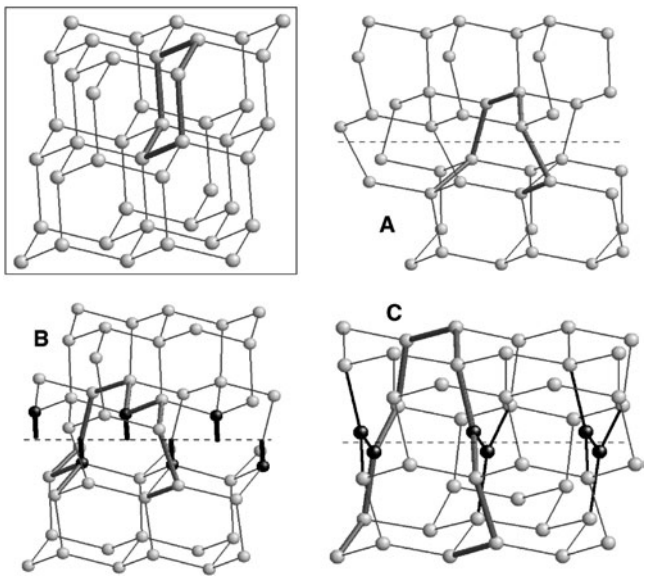

Figure 2. Ball-and-stick representations of the cubic diamond bulk (top left) and of the three screw core configurations. A six-atom ring (see figure 2) is represented by dark grey sticks, in order to show the deformation due to the dislocation and the Burgers vector. Dangling bonds (for B) and sp^2 atoms (for C) are represented by black sticks and balls. The position of the dislocation line is shown by the dashed lines.

shift along $[\bar{1}01]$ between these atoms is half of the Burgers vector (see figure 2). As a consequence, the interatomic distance is about 3.28 Å, too large for a covalent bond, and thus configuration B can be considered as composed of two rows of dangling bonds along $[\bar{1}01]$. Again, no significant changes were observed between different materials.

Configuration C bears an apparent similarity with B, because the main contribution of the distortions is also located on two atoms. However, there is a significant difference. For configuration B, the two atoms, on either side of a shuffle plane, have initially the same position along $[\bar{1}01]$, and are moved away from each other by the dislocation. For configuration C, the two atoms, on either side of a glide plane, are initially distant by half the Burgers vector, but are located at the same position along $[\bar{1}01]$ after the introduction of the dislocation. These two atoms have coordination three, the three bonds being almost in the same plane. This geometry is expected to be favoured in carbon, where an sp^2 hybridization is favoured over sp^3. We have monitored the length of the bonds between the two atoms, as well as the angle formed with neighbour bonds. With the Tersoff potential, we found for carbon a bond length of 1.40 Å which is close to the 1.42 Å length for graphite. The angle is almost 120°, expected for sp^2. For all other materials, we found a reduction of the bond length for these two atoms, but the angles tend to move away from 120°, especially for a soft element like germanium. For silicon carbide, we observed a dissymmetry in the core, due to the presence of two elements with different elastic behaviours. In fact, the sp^2 core is composed of one silicon and one carbon, and the bonds involving the Si atom are more easily stretched than those involving the C atom. Finally, a large variation in the angles and bond lengths was found for Ge. The overall C structure is conserved, but small atomic displacements seem to occur in the core.

Our results seem to indicate that a sp^2 hybridization in the core of the dislocation is stable for all the materials considered. However, though it has been shown that the Tersoff potential

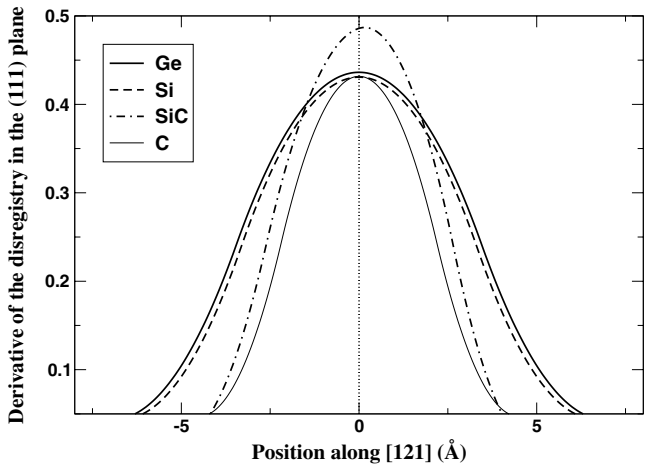

Figure 3. The derivative of the disregistry along the {111} plane for configuration B, from Tersoff calculations, and for all materials.

is able to correctly describe the transition $sp^3 \rightarrow sp^2$ [17], one has to remain cautious in the analysis. Only truly quantum mechanical calculations could unambiguously address this problem.

The core extent of the dislocation has been determined by use of the derivative of the disregistry along the {111} planes. We considered only the plane ('shuffle' for A and B, 'glide' for C) containing the dislocation line. Figure 3 shows the result obtained in the case of B, for all materials. It is clear from the figure that the spatial extents of the dislocation are reduced from Ge to C, which was expected because of the increasing hardness of the materials. They are close for Ge and Si, which can be explained by their similar properties.

The quantitative characterization of the core extent could be achieved by determining the width at half-maximum (WHM) of the derivative of the disregistry (figure 4). We observed that the reduction of the spatial extents from Ge to C is common to all configurations. One exception concerns the WHM for the C configuration: it is narrower for Ge than for Si. This peculiar results could be explained by the large angle variations and bond length variations obtained for Ge in the C geometry. It is also interesting to examine the results for SiC. In fact, it appears that the WHM for SiC can be determined directly from the average of the Si and C WHM to a good approximation. The comparison also shows that B has a much wider core than A. It is not possible to directly compare the WHM for C with the others, since the WHM determination is not done for the same plane set. However, additional information could be obtained from comparison with the geometries built from the elasticity theory (figure 4). We found that the atomic relaxation increases the extent of the B configuration, causes no changes to the WHM for A, but reduces the extent of the core of the C structure. The reconstruction of the core for the stabilization of the sp^2 structure may explain this result.

Finally, we have compared the values obtained with Tersoff, SW, and EDIP potentials for all Si structures. We found that the C configuration is not stable with the SW potential. For all other cases, very close results are obtained, the maximum WHM difference being as low as 0.2 Å. Analysis of bond lengths and angles in the core of the dislocations also shows very small differences between results obtained from different potentials. This is further evidence of the interesting fact that very similar geometries can be obtained whatever the potentials. In particular, relaxed structures used as input for *ab initio* calculations will not depend on the choice of the semi-empirical potential.

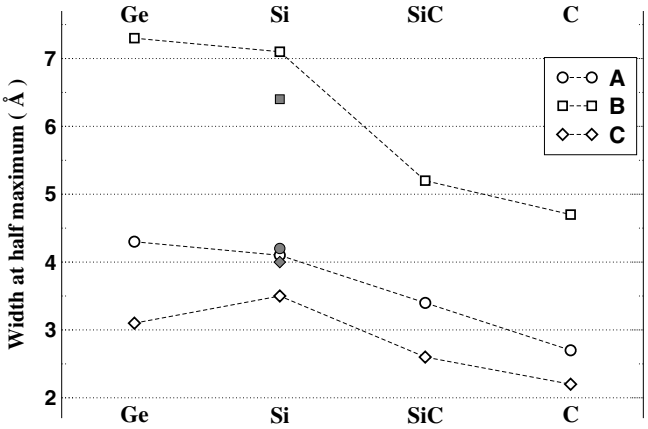

Figure 4. Variation of the derivative of the disregistry along the {111} planes for all configurations and materials, calculated with the Tersoff potential (open symbols). The results obtained from anisotropic elasticity theory are also reported for silicon (grey symbols).

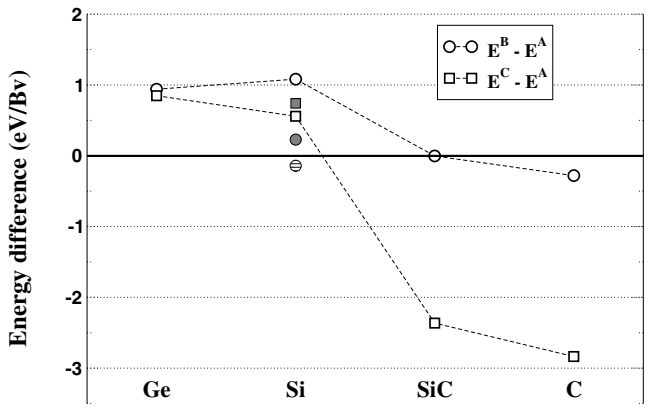

Figure 5. The variation of the energy difference between configurations B and A (circles), and C and A (squares), for all materials, calculated with the Tersoff potential (open symbols). The results obtained with the SW (striped symbol) and EDIP (grey symbols) potentials are also shown for silicon.

4. Core stability

In this section, we discuss the relative stability of the different core configurations. In a previous work, we have shown that the results obtained depend strongly on the semi-empirical potentials [5]. These results are reported in figure 5. Hence, for silicon, the B configuration was found to be more stable than the A one with SW, although with the Tersoff and EDIP potentials, the *ab initio* answer A was favoured. The Tersoff potential gives C as more stable than B, but EDIP calculations lead to the opposite conclusion. So, unlike the calculated core structures, which are almost the same for all potentials, the stabilities of different configurations should be determined with several potentials and, if possible, with *ab initio* methods.

In figure 5 we show the variation of the energy difference between configurations A and B, and also between A and C, for all materials investigated with the Tersoff potential. First we note that a similar configuration ranking is obtained for Ge and Si, with A the most stable solution,

then C and B. Secondly, it is clear from the curves that the A configuration is decreasingly favoured from Ge to C. A and B have the same energy for SiC, and B is more stable than A for carbon. But the more surprising result is the apparent stability of the C configuration over A and B for silicon carbide and diamond. The energy difference is important (almost 3 eV per Burgers vector for diamond), which tends to indicate that this is not just an artefact due to the choice of this potential. A plausible physical reason for this behaviour is based on the possible sp^2 hybridization of the C geometry. It is known that such a feature is favoured in diamond, but not in Si or Ge. For SiC, the situation is more complicated since there are two atoms (one Si and one C) with the coordination 3 in the core. Despite the large energy differences, an *ab initio* study is required for validating these results. Electronic structure calculations would also allow verification of the presence of this sp^2 hybridization of the core.

To our knowledge, there have been no experimental determinations of the core structure of dislocations in cubic SiC, because of the difficulty of growing monocrystal, or in diamond, for technical reasons. As regards calculations, the few available studies are all focused on partial dislocations in SiC [18] and diamond [10, 19]. Interestingly, a recent study by Ewels *et al* [10] indicates a possible graphitization of the core of these partials in diamond. However, they found that in all cases, the sp^2 structure is not energetically favoured compared to sp^3.

5. Conclusions

Semi-empirical potential calculations allowed us to determine the structure and stability of undissociated screw dislocations in group IV materials with the cubic diamond structure. Among the three configurations investigated, the C one shows a possible sp^2 hybridization in the core. It is particularly clear for diamond where the bond lengths and angles are very close to those of graphite. We also determined the spatial extent of the core for all materials and configurations, using the derivative of the disregistry. As expected, the core extent is reduced for harder materials. As regards the stability of the configurations, we found that the A configuration is more stable for Ge and Si, but that the C configuration with the sp^2 hybridization is favoured for SiC and diamond. It appears then that in Si and Ge, the stable screw dislocation is located in the 'shuffle' set, whereas for 3C-SiC and diamond, the 'glide' set is clearly favoured. *Ab initio* calculations are in progress for validating these results.

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