PHILOSOPHICAL MAGAZINE LETTERS, 2004
VOL. 84, NO. 11, 729–736

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First principles determination of the Peierls stress of the shuffle screw dislocation in silicon

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[*Received in final form 29 December 2004 and accepted 30 December 2004*]

ABSTRACT

The Peierls stress of the $a/2\langle 110\rangle$ screw dislocation belonging to the shuffle set is calculated for silicon using density functional theory. We have checked the effect of boundary conditions by using two models, the supercell method where one considers a periodic array of dislocations, and the cluster method where a single dislocation is embedded in a small cluster. The Peierls stress is underestimated with the supercell and overestimated with the cluster. These contributions have been calculated and the Peierls stress is determined in the range between 2.4×10^{-2} and 2.8×10^{-2} eV Å^{-3}. When moving, the dislocation follows the {111} plane going through a low energy metastable configuration and never follows the 100 plane, which includes a higher energy metastable core configuration.

§ 1. INTRODUCTION

The Peierls stress is defined as the minimal stress needed to move a dislocation from one lattice site to the next one at 0 K (Hirth and Lothe 1982). It is a fundamental quantity in the study of plasticity in materials science. Close-packed metals, ductile, have low Peierls stresses, typically $10^{-4}\,\mu$ (μ is the isotropic shear modulus; the average value for Si is 0.425 eV Å^{-3} (Hirth and Lothe 1982)), whereas values 2 to 3 orders of magnitude higher are associated with brittle covalent crystals. Experimentally, its determination is difficult since materials are brittle at low temperature. Then it is usually obtained by extrapolating measured yield strengths to the absolute zero temperature. In addition, several Peierls stresses can be defined for a given material, one for each kind of dislocation, and the separation of the different contributions in experiments is not an easy task.

The measurement is especially difficult in covalent crystals, since the brittle to ductile transition happens at high temperature, leading to rough estimation of the Peierls stress. The case of silicon, which is often considered as a model material for the study of cubic diamond and zinc blende covalent crystals and, as a result, has been extensively studied, is a good illustration. Experiments indicate a value ranging between $0.1\,\mu$ and $0.5\,\mu$ (Suzuki and Takeuchi 1989), obtained from yield strength measurements in the ductile regime. For these temperatures, it is known that dislocations are dissociated and glide along the narrowly spaced {111} planes

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Philosophical Magazine Letters ISSN 0950–0839 print/ISSN 1362–3036 online
http://www.tandf.co.uk/journals
DOI: 10.1080/09500830500041377

(Alexander 1986), thus called 'glide planes' (Hirth and Lothe 1982). It has been suggested that these partial dislocations move by nucleation and propagation of kink pairs (Duesbery and Joós 1996, Bulatov *et al.* 2001). The experimental Peierls value is then associated with the displacement of partials.

However, new information on the plasticity of silicon and other diamond cubic materials has recently emerged, concerning deformation at unusually low temperatures. Experimentally, silicon samples submitted to large shear stress components have been deformed at low temperature without failure. This has been made possible by applying a very high confining pressure or in scratch tests (Rabier and Demenet 2001, Rabier *et al.* 2000, 2001). The observed dislocation configuration differs strongly from the usually reported dissociated dislocations seen after deformation at higher temperature. The dislocations are undissociated, and thus most likely glide along the widely spaced 'shuffle planes' (Hirth and Lothe 1982), and are aligned along several favoured orientations, $\langle 110\rangle$/screw, $\langle 112\rangle/30^\circ$ and $\langle 123\rangle/41^\circ$. Rabier and Demenet pointed out (2000) that the observation of the non-dissociated dislocations fits into the analysis of Duesbery and Joos (1996), which, if extrapolated, predicts a transition from dissociated dislocations in the glide set in the high temperature/low stress domain, to undissociated dislocations in the shuffle set in the low temperature/large stress domain. Similarly, in III–V compounds with the zinc-blende structure, deformation experiments at low temperature under high confining pressure indicate that the low-temperature plastic deformation is governed by undissociated screw dislocations (Suzuki *et al.* 1998). It is then very important to characterize shuffle dislocations to understand the plasticity properties of these materials.

Despite the increasing interest, there is little quantitative information on the energetics and mobility properties of the dislocations of the shuffle set, compared to those already obtained for the partials in the glide set, which have been the subject of most studies until recently (Bulatov *et al.* 2001). For example, as far as we know, no attempts have been made to determine experimentally the Peierls stress of perfect dislocations in cubic diamond or zinc-blende materials. However, several calculations have been performed for addressing these issues. Naturally, the screw orientation is selected because, among all characteristics, it always plays a special role. Indeed, it allows for cross-slip, and in the particular case of the diamond cubic structure, it is the orientation where transition from glide set to shuffle set is possible without any diffusion. Moreover, in the observations after low-temperature deformation, it appears as one of the favoured orientations, probably indicative of significant Peierls valleys (Rabier *et al.* 2001).

The screw dislocation in the shuffle set has been the subject of recent investigations, such as stability calculations using empirical interatomic potentials (Koizumi *et al.* 2000) and ab initio methods (Arias and Joannopoulos 1994, Pizzagalli *et al.* 2003). Without going back to early elasticity-based estimates of the energetics of the screw dislocation (Celli 1961, Teichler 1967), the Peiers stress on the screw dislocation in the shuffle set has been estimated to be $0.048\,\mathrm{eV\,\AA^{-3}}$ by Joós *et al.* (1994), with the Peierls–Nabarro model. More direct atomistic calculations with the Stillinger–Weber potential by two different groups led to $0.036\,\mathrm{eV\,\AA^{-3}}$ (Ren *et al.* 1995) and $0.013\,\mathrm{eV\,\AA^{-3}}$ (Koizumi *et al.* 2000). Miyata and Fujiwara performed ab initio calculations and deduced somewhat indirectly a Peierls stress ranging from 0.14 to $0.19\,\mathrm{eV\,A^{-3}}$ (Miyata and Fujiwara 2001), about 15 times the value proposed in (Koizumi *et al.* 2000). However, these approaches suffer from some insufficiencies.

If the Peierls–Nabarro model is shown to represent planar dislocation cores well (Ren *et al*. 1995), the predicted values for the Peierls stress are more doubtful since this model considers the dislocation core as an undeformable object moving across the atomic rows. Concerning the use of the Stillinger–Weber potential, it has been shown (Pizzagalli *et al*. 2003) that it does not predict the stability of the various screw core configurations which is a necessary prerequisite to any reliable Peierls stress determination. It is also necessary to have a quantitative estimate of the effect of the boundary conditions, particularly in the relatively small cell sizes used in ab initio computations.

In this paper, we present the Peierls stress calculation of the shuffle screw dislocation using an ab initio method. In the same spirit of a previous report on the structure and energetics of this dislocation (Pizzagalli *et al*. 2003), the boundary effects which cannot be avoided in this kind of calculation were carefully determined. The Peierls stress has been calculated for both periodic and fixed conditions, and has been found in the range between 0.024 and 0.028 eV Å^{-3} when the dislocation moved in the $\langle 112 \rangle$ direction. This direction has been found to be the easiest, compared to the $\langle 110 \rangle$ direction.

§ 2. Computational methods

The determination of the Peierls stress is done by increasingly shearing the system, oriented as shown in figure 1, so that the force on the dislocation is maximum along a chosen direction. Between each shear strain increment of 1%, the atomic positions are relaxed. The corresponding Peierls stress is reached when the dislocation moves. Two selected directions, $\langle 112 \rangle$ and $\langle 110 \rangle$, have been investigated in this work. Recent ab initio calculations have shown that the configuration A,

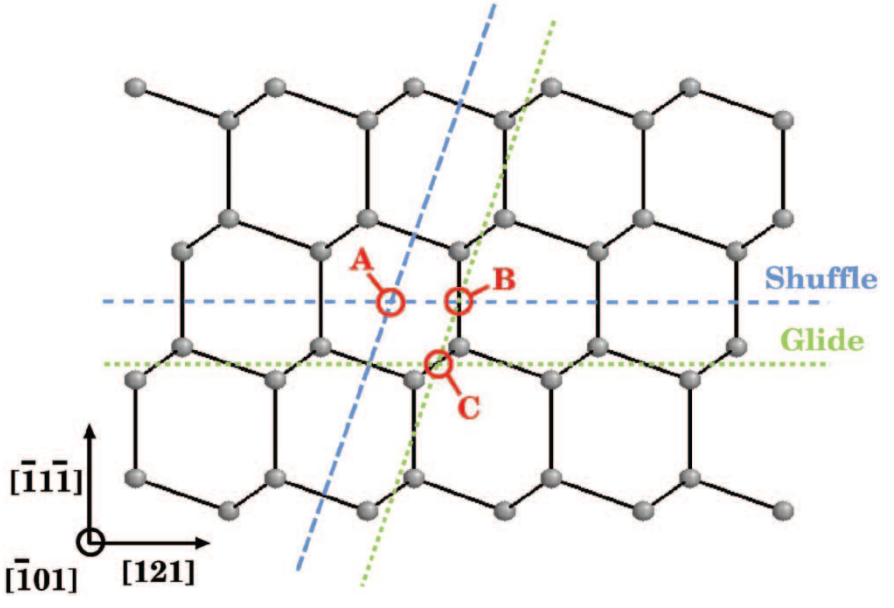

Figure 1. Ball-and-stick representation of the cubic diamond structure, oriented along axis $X = [121]$, $Y = [\bar{1}\bar{1}\bar{1}]$ and $Z = [\bar{1}01]$. Shuffle and glide sets of planes are shown, as well as the three possible stable locations A, B and C for a screw dislocation in silicon (Pizzagalli *et al*. 2003).

where the screw dislocation is located in the center of one hexagon is the most stable for Si (Pizzagalli *et al*. 2003). The configuration B, with the screw located on the long edge of one hexagon is weakly metastable. Another metastable configuration, C, is obtained for a screw located on the small edge of one hexagon. Starting from the most stable configuration A, the first direction corresponds to a sequence ABA, whereas the second one should favour a sequence ACA (figure 1).

The simulations have been performed in the framework of density functional theory (Hohenberg and Kohn 1964, Kohn and Sham 1965) and local density approximation (Goedecker *et al*. 1996), by using the code ABINIT (Gonze *et al*. 2002). The ionic interactions were described by norm-conserving Troullier–Martins pseudopotentials (Troullier and Martins 1991). We used a plane wave energy cutoff of 10 Ry and two special k-points along the dislocation line. Previous calculations with similar parameters have allowed us to accurately model screw dislocations in silicon (Pizzagalli *et al*. 2003).

Two crystal models have been constructed (Lehto and Heggie 1999). In the first one, a dislocation dipole, cut from an infinite quadrupolar distribution, is placed in the crystal unit cell, and periodic boundary conditions are used in both directions normal to the dislocation line (figure 2). In the second model, a single dislocation is placed at the centre of a cluster whose lateral surfaces are kept fixed. In both cases, periodic boundary conditions are applied along the dislocation line. We have considered these two models because, as discussed in the following, they modify differently the determined Peierls stress. In the fully periodic case the interaction of the dislocation with the surrounding ones helps its move, so tending to underestimate the Peierls stress, whereas in the cluster model the interaction with the fixed boundaries opposes the dislocation displacement and leads to an overestimation of the Peierls stress. Besides these purely mechanical effects, the two methods also show differences in the electronic structure whose effects become unimportant for cells or clusters large enough.

In case of periodic boundary conditions, we used a $12 \times 12 \times 1$ cell, i.e. 144 Si atoms. These dimensions allow a reasonable distance between dislocations, about $6|\mathbf{b}| \simeq 23$ Å ($\mathbf{b}$ is the Burgers vector, $|\mathbf{b}| = 3.84$ Å), while remaining affordable with

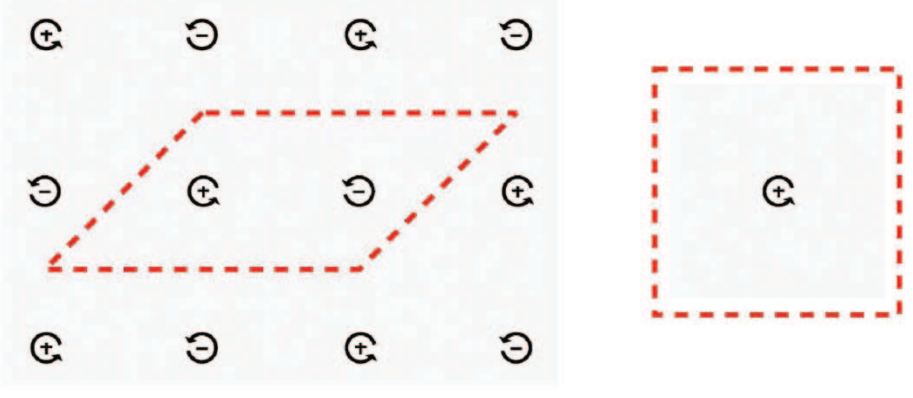

Figure 2. Models used in the simulations: oblique cell including a dislocations dipole with periodic boundary conditions (left), and cell with a single dislocation and fixed boundary conditions (right).

ab initio computations (Pizzagalli *et al.* 2003). All atoms were relaxed, the imposed deformation being kept by the periodic conditions. In case of fixed boundaries, a $8 \times 16 \times 1$ cell, i.e. 128 Si atoms, was considered and dangling bonds belonging to edge atoms were saturated by hydrogens. The system was placed in the centre of a supercell whose dimensions allowed a 3 Å vacuum left between a hydrogen and the supercell edge, and the imposed deformation was kept by relaxing only Si atoms not located on the system edges. The distance between the central dislocation and the frozen edges is then approximately 12 Å.

§ 3. Results and discussion

Starting with the periodic system, for shears up to 6% the dislocations remained in the vicinity of their initial locations. The energy of the relaxed system increased with the deformation due to the storage of elastic energy in the structure. However, when the applied deformation was equal to 7% the two dislocations of the dipole started to move closer during the relaxation. Figure 3 shows different steps of the evolution of the structure. First, the bond on the long edge of the hexagon broke, with dislocations approximately in the configuration B (figure 3b). Then the dislocations were found again in the configuration A, but in the next hexagon (figure 3c). Finally, the dislocations continued to slip closer during the relaxation (figure 3d). In fact, there is an attractive force between the two dislocations with opposite Burgers vectors, which increases as the dislocations come closer. This behaviour is different from what was obtained by Miyata and Fujiwara, where the movement stopped once the dislocations slip by one hexagon (Miyata and Fujiwara 2001). This difference may be explained by the different periodic boundary conditions used in their work, or by their larger criterion value for stopping the relaxation (10^{-3} Ry/bohr to compare with 10^{-4} Ry/bohr in our work). In the case of a fixed boundary system, we observed a similar behaviour, the dislocation moving away from the centre, but only when the deformation is equal or greater than 8%.

The stress required for moving the dislocations closer is simply the product of the imposed shear with the relevant shear modulus G (The $\langle 110 \rangle \{111\}$ shear modulus G is $1/3(C_{11} - C_{12} + C_{44})$ (Hirth and Lothe 1982) and is 0.366 eV Å^{-3} from our calculations (0.381 eV Å^{-3} experimentally)). So, in the case of periodic conditions, the calculated stress ranges between $0.06\,G$ and $0.07\,G$. However, due to periodic conditions, we have an infinite distribution of dislocations, in interaction. This stress is then not the real Peierls stress, due to these interactions. Considering that the energy varies smoothly during the ABA move, and B is a saddle point, the dislocations are expected to move once they have covered roughly half the distance between A and B. Using isotropic elasticity theory, we have evaluated the extra stress at this point to be about $-0.0051\,G$. The main contributions are coming from neighbour dislocations along the slipping direction and favour the slip, lowering the determined stress. The real Peierls stress then ranges between 0.0651 and 0.0751 G, as determined with periodic conditions. For fixed conditions, the stress ranges between 0.07 and $0.08\,G$. In that case too, the calculated stress is not the real Peierls stress. In fact, the fixed edges of the system create an extra force, opposed to the slip of the dislocation and increasing the calculated stress. Following the work of Shenoy and Phillips (1997), we estimated the extra stress to be $0.0046\,G$ when the dislocation is located at midpoint between A and B. The Peierls stress then ranges between 0.0654 and $0.0754\,G$. The agreement between values calculated using periodic or fixed conditions is very good. Therefore, we expect that our results are independent

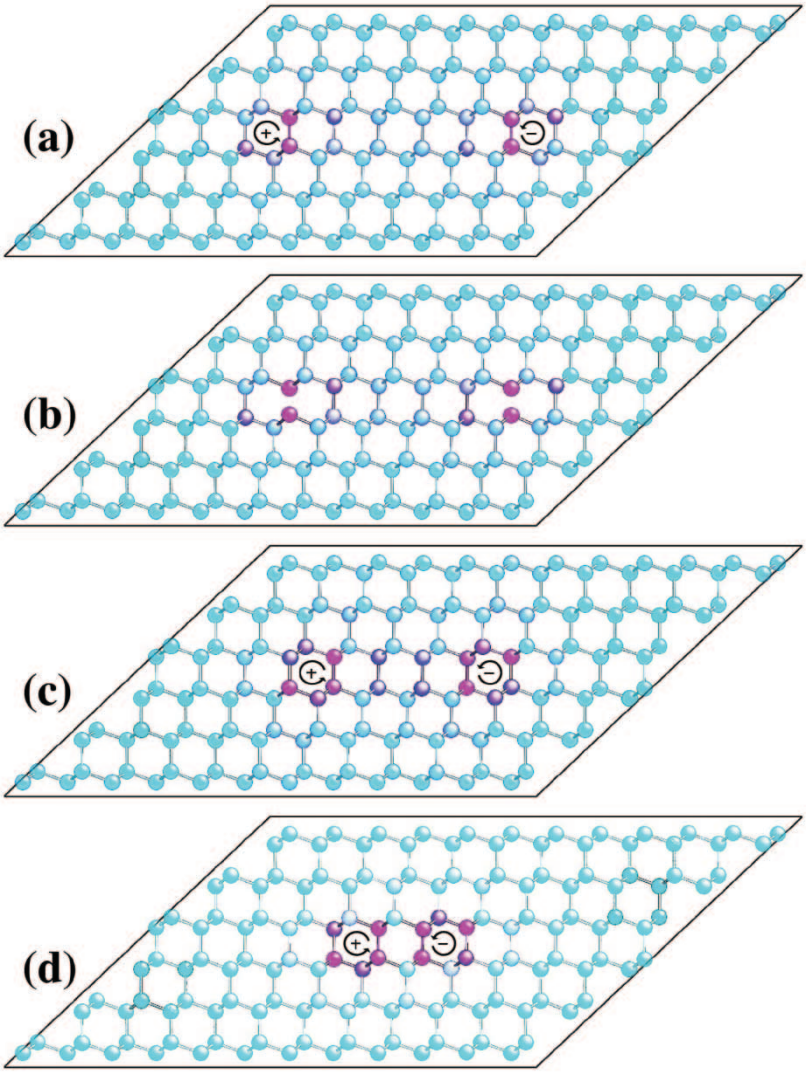

Figure 3. Evolution of the system for a shear of 7% (a) Initial configuration of one dipole, with a distance $d=6|\mathbf{b}|$. (b) The two dislocations are approximately in the configuration B, with $d \simeq 5|\mathbf{b}|$. (c) Each dislocation has moved by one hexagon, $d=4|\mathbf{b}|$. (d) $d=2|\mathbf{b}|$. The colour of atoms indicates the magnitude of calculated Von Mises stresses.

on the boundary conditions. In the present situation where the Peierls stress is relatively large, the agreement between the two methods indicates that the use of sophisticated boundary treatments, such as flexible boundaries (Rao *et al.* 1998), is not essential.

Our Peierls stress ranges between 0.0651 and 0.0754 G, i.e. between about 2.4×10^{-2} eV Å^{-3} and 2.8×10^{-2} eV Å^{-3}. We have performed atomistic simulations of the dislocation slip due to an applied stress, which is expected to be more precise than indirect methods, such as the Peierls–Nabarro model. Nevertheless, if we

compare with similar studies, we note several differences. Hence, Koizumi *et al.* determined a Peierls stress of $1.3 \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$ (Koizumi *et al.* 2000), using the Stillinger–Weber potential. Our own tests, done in the same conditions, led to a similar result, but also showed that this low value is due to an incorrect description of the ABA path energy. In fact, the configuration B, weakly metastable with a metallic behaviour along the dislocation line (Pizzagalli *et al.* 2003), is the most stable with this potential. Ren *et al.* found a much larger value, $3.6 \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$ (Ren *et al.* 1995), using Stillinger–Weber, but we have no explanation for this disagreement with Koizumi *et al.* and with our own tests. Finally, Miyata and Fujiwara have determined indirectly the Peierls stress from ab initio calculations and found a value between 14 and $19 \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$ (Miyata and Fujiwara 2001), much larger than our own value. Two possible explanations for such a disagreement can be found. The first one is related to the $10 \times 6 \times 2$ simulation cell they used. Along [121], dislocations in the cell were initially located at a $6|\mathbf{b}|$ distance, presumably giving $4|\mathbf{b}|$ between a dislocation and its periodic image. The dislocation distribution is then not truly quadrupolar. Also, along $[\bar{1}1\bar{1}]$, the distance between dislocations is only $3|\mathbf{b}|$. This leads to a strong interaction between dislocations, opposed to the dislocation slip. The second reason is related to the use of an elastic analytical model for estimating the Peierls stress from atomistic calculations. This unnecessary step is a possible source of errors.

In conclusion, we have performed an accurate determination of the Peierls stress of a shuffle screw dislocation in silicon, using first principles and two different kinds of boundary conditions. The calculated value is between $2.4 \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$ and $2.8 \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$, this range corresponding to the deformation increment of 1%. Since the uncertainty associated with the computational method is lower, we can conclude that the Peierls stress is $(2.6 \pm 0.2) \times 10^{-2}\,\mathrm{eV\,\AA^{-3}}$. This is slightly lower than the lowest experimental value (Suzuki and Takeuchi 1989). Regarding the plasticity of silicon, it has been shown that at low temperature perfect shuffle dislocations are governing. The shear applied on the system favoured the ABA path (figure 1), so that the screw dislocation remained in its shuffle plane. We also checked a possible cross-slip between shuffle and glide planes by performing simulations with an applied deformation of 10% favouring the ACA path. A slip process was obtained, the dislocations moving closer during the relaxation. However, the ABA path was again selected, instead of ACA. Therefore at 0 K, whatever the orientation of the applied shear stress, the undissociated screw keeps gliding in the shuffle set and does not spontaneously transform into a dissociated configuration in the glide set. Additional investigations have to be done to better understand the plasticity properties of silicon, and in particular the transition between shuffle mode at low temperature to glide mode at high temperature.

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