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2011 J. Phys.: Conf. Ser. 281 012002

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Dislocation cores in silicon: new aspects from numerical simulations

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Abstract. Recent theoretical investigations of the properties of dislocation cores in silicon are reviewed. New results, obtained from numerical simulations for the non-dissociated screw and 60° dislocations, are presented and discussed in relation with experiments.

1. Introduction

The plasticity properties of silicon have been largely investigated since the first studies made sixty years ago. It could therefore be surprising that nowadays there are still several important issues. What appears to be well confirmed is the occurrence of two distinct plastic regimes [1], one at temperatures higher than approximately 900°C (where Si is ductile), and the other for lower temperatures (where Si is brittle), and the fact that the plasticity is governed by dislocation core properties. This behaviour is not specific to silicon, since other covalent materials with equivalent structures have been shown to exhibit a similar characteristic [2–7]. Open questions depend on the considered plastic regime. Most of the available data refer to the high temperature case, for which the ductility of silicon allows conventional mechanical testing. Although it has first been thought that dislocations in this regime were non-dissociated and located in the shuffle set of $\{111\}$ planes in the diamond cubic structure [8], pioneering microscopy experiments unambiguously showed the occurrence of a weak dissociation. These dislocations are characterised by a $1/2\langle 110 \rangle$ Burgers vector with screw and 60° characters, and dissociate into 30° and 90° Shockley partials located in the glide set of $\{111\}$ planes. There have been many recent numerical simulations attempting to determine the core structure of partial dislocations. It is generally agreed that the 30° partial core exhibits a double period reconstruction along the dislocation line. The situation is less clear for the 90° partial since there are two possible structures which are very close in energy [9–11]. There is a general consensus that these dislocations move thanks to the thermally activated formation and migration of kinks along the dislocation line [8], with an activation energy of 2.2 eV for pure silicon. However, the elementary atomistic mechanisms responsible for this displacement are not formally known, because of the large number of possible kink configurations [12], the difficulty to compute or measure formation or migration energies with accuracy [13–19], and the likely role of topological defects along the dislocation line [20, 21]. It is therefore difficult to make the connection between kink mechanisms and the mobility law of dislocations [22, 23]. Several authors have also hinted the need to take into account the correlated motion of the partials [24, 25].

The other plastic regime is observed at temperatures approximately lower than 900 °C. Since silicon is brittle in this temperature range, experiments are usually made using a confining pressure for avoiding cracks, or in a localised area of the sample by nanoindentation [1]. In all cases, high stresses are required for plastically deforming silicon [26]. Overall, there is much less available information regarding this plastic regime, mainly because of experimental limitations. Yet the growing interest for systems with sub-micron or nanometric dimensions calls for a better understanding. In fact, in nanostructures such as nanowires or nanopillars which are often free of defects, plastic deformation has been shown to occur at large stress and low temperature [27–30]. Also, undesirable dislocations could be nucleated in silicon-based devices because of the very high stresses [31–33]. In this low temperature / high stress regime, perfect non-dissociated dislocations with orientations screw, 30° and 41° have been observed depending on the experiments [1]. The required stress for displacing dislocations has been estimated to be about 1.5 GPa [26]. Additional experiments on the physical signatures of these dislocations do not bring much more information [34]. Fortunately, many theoretical studies using numerical simulations have been done during the last decade, leading to a better understanding of dislocation properties in this regime thanks to the investigations of the stability and mobility of the dislocation cores. In this paper, we review and comment these results, which are essentially focused on the screw and 60° dislocation, and we discuss remaining issues.

2. Modelling and numerical simulations

In many materials, the Peierls-Nabarro model allows to determine basic properties of dislocation cores such as dissociation width and Peierls stress, in particular thanks to several recent improvements [35–37]. However, dislocation cores in silicon are often characterised by a complex topology, which may be different than in the bulk due to bond reorientation or reconstruction. As a result, such a model based on an approximate core description is usually not well suited for providing quantitative results [38]. Most of the recent investigations are then made using numerical simulations based on an atomistic description of the dislocations. They provide a better description of the core structure, and almost all related core quantities can be computed. The system can be modelled using semi-empirical inter-atomic potentials, or, at a more fundamental level, with electronic structure approaches such as tight-binding or first principles density functional theory (DFT). Usual potentials for silicon include the Stillinger-Weber [39] and the Tersoff [40] potentials, or the more recent EDIP [41] and MEAM [42]. Nonetheless, not everything in the garden is rosy. In fact, available potentials for silicon are not always accurate, and qualitatively incorrect results may be obtained in specific cases. Since none appears to be superior to the others, the usual remedy is to compare the results from several potentials. Conversely, DFT calculations provide robust and trustable results in the case of silicon. The only drawback is the large need in computational resources, which prevents the investigations of large systems. Several methods have been proposed in order to make an accurate treatment of dislocations in small systems. A descriptive listing is out of the scope of the present paper, but the interested reader will find valuable information in the references [21, 43, 44].

Calculations with atomistic methods usually deal with the determination of the most stable configuration for the dislocations core, or for defects along the dislocation line such as kinks or jogs, yielding structures and energies. The Peierls stress can also be numerically computed by applying a stress on the system encompassing the dislocation. These static calculations can be completed with molecular dynamics simulations which allow to monitor the system evolution at non zero temperature. Because of the severe time limitations for the latter, several methods have also been proposed for computing activated mechanisms using a static formalism. String-based approaches such as the nudged elastic band (NEB) method [45] are increasingly used nowadays. They allow to calculate transition mechanisms and their associated activation energies with accuracy within a reasonable time. Other kinds of transition state search methods have also

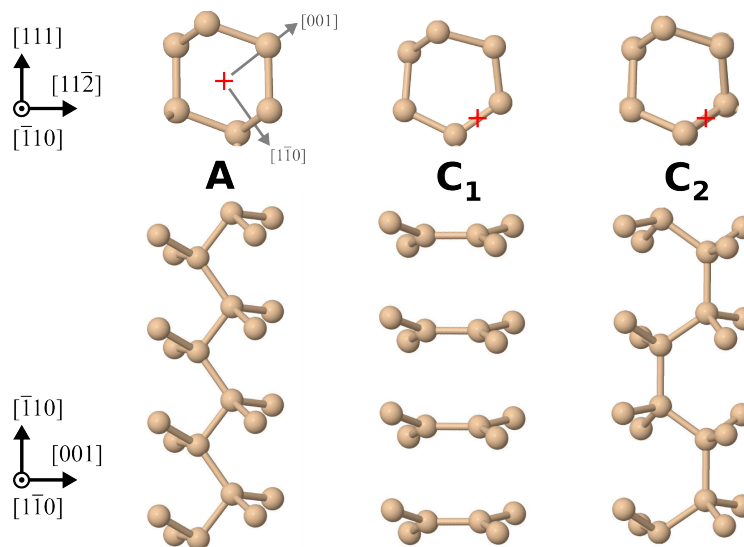


Figure 1. Three possible structures for a screw dislocation in a diamond cubic lattice, viewed along two different directions (top and bottom). Adapted from [48].

been tried [12, 46, 47].

3. The screw dislocation

We first focus on the non-dissociated screw dislocation. Although this is not always the main observed character in the microstructure, the screw usually plays a special role in the plastic deformation of materials. In 1958, Hornstra proposed two possible core structures for the screw dislocation in the diamond lattice [49]. Both core structures, labelled A and C₁ respectively, are represented in the figure 1. One is obtained when the dislocation line is placed in the centre of one hexagon, as obtained when the diamond structure is viewed along a $\langle 110 \rangle$ direction. The dislocation core therefore belongs to a shuffle $\{111\}$ plane. The second proposed configuration is located in a glide $\{111\}$ plane, and corresponds to a dislocation line passing through the centre of a hexagon small edge. Atomistic calculations using different potentials showed that A is always more stable than C₁ for silicon [50]. A third configuration has been suggested by Koizumi *et al* [51], with a core centred on a hexagon long edge, but it has been revealed to be unstable by first principles calculations [52]. Note that Celli in an early investigation already pointed that this configuration would not be stable [53]. Finally, Wang *et al* recently demonstrated that the energy of the C₁ configuration could be greatly lowered thanks to a double period reconstruction along the dislocation line [54]. This configuration, called C₂ here, is represented in the right side of the figure 1. The activation energy for this reconstruction has been shown to be low [48], which implies that the C₁ core is unlikely to occur. As a consequence, one can say that for a screw dislocation in silicon the two configurations A and C₂ are possible.

The relative energies of A and C₂ configurations have been computed within various methods [1], and it seems that C₂ is always the most stable core structure. Since a large hydrostatic pressure could be present in experiments, the effect of pressure on the stability of both configurations has been recently investigated. Although calculations revealed that the pressure has a noticeable influence on dislocation core energies and tends to favour the A core [55], the C₂ structure remains clearly the lowest energy configuration for a screw dislocation in silicon.

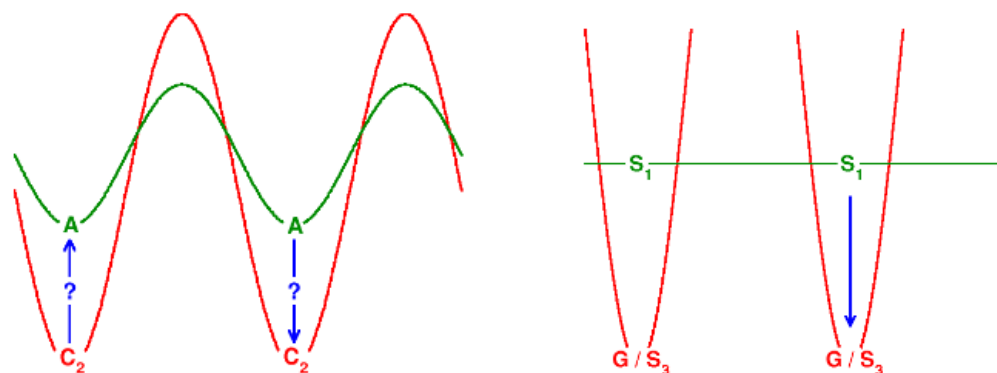


Figure 2. Schematic variation of energies for the core configurations involved in the displacement of the screw (left) and the 60° (right) dislocations.

Preliminary information on the mobility of both configurations can be gained from the value of the Peierls stress. Computed values of 4 GPa [56] and 6 GPa [54] for A and C2 suggest that the former configuration is the more mobile. Nevertheless, it is likely that the displacement of the screw dislocations in the low temperature regime is thermally activated, and activation energies for the formation and migration of kinks should be considered for a finer analysis. These quantities have been computed for the A core using NEB and DFT simulations [57], yielding values of about 1 eV for the formation energy and lower than 50 meV for the migration energy. Using these values, a theoretical comparison of the relative mobilities of the A screw and the partial dislocations showed that the former was more mobile for all stress [58], in contradiction with an early analysis [59]. To our knowledge, kink formation and migration energies are not known for the C₂ core. However, to a first approximation one could consider that the kink pair formation energy is roughly proportional to the Peierls stress magnitude, which would give a kink formation energy in the range 1.4–2.0 eV, thus much larger than values for the A core or than the ones commonly accepted for partials [22]. For the kink migration process, the obvious similarity of the C₂ core with the double period core of the 90° partial dislocation suggests close mechanism and energies for kink migration, i.e. an energy of about 1.2 eV. Therefore the C₂ dislocation core appears to be less mobile than the A core, and even than partial dislocations.

Since A is less stable than C₂ but is likely to be the core involved during the screw dislocation displacement, one can imagine a three-steps mechanism (figure 2). First, C₂ is the core configuration for a screw dislocation at rest, and the combined action of temperature and stress allows the transformation C₂→A. Then, the A core moves through the crystal. Finally, the A core is stopped for a time long enough to obtain the reverse transformation A→C₂. This issue has been recently studied by Guénolé *et al* using NEB calculations and interatomic potentials [48]. It appears that the C₁ configuration is an intermediate step of the A→C₂ transformation. But more importantly, the energy barrier that must be overcome for the A→C₂ transformation is in the same range than the energy required for the thermally activated motion of partial dislocations, and it depends only weakly on the applied stress. It is therefore unlikely that such a mechanism could be triggered for the temperatures associated with non-dissociated dislocations.

To summarise, theoretical investigations show that the most stable configuration for a non-dissociated screw in silicon is the C₂ structure. The other possible configuration A is stable too, albeit with a larger core energy. The A screw is mobile in the considered stress / temperature range, which is not the case for the C₂ core. Finally, a A→C₂ transformation would be obtained

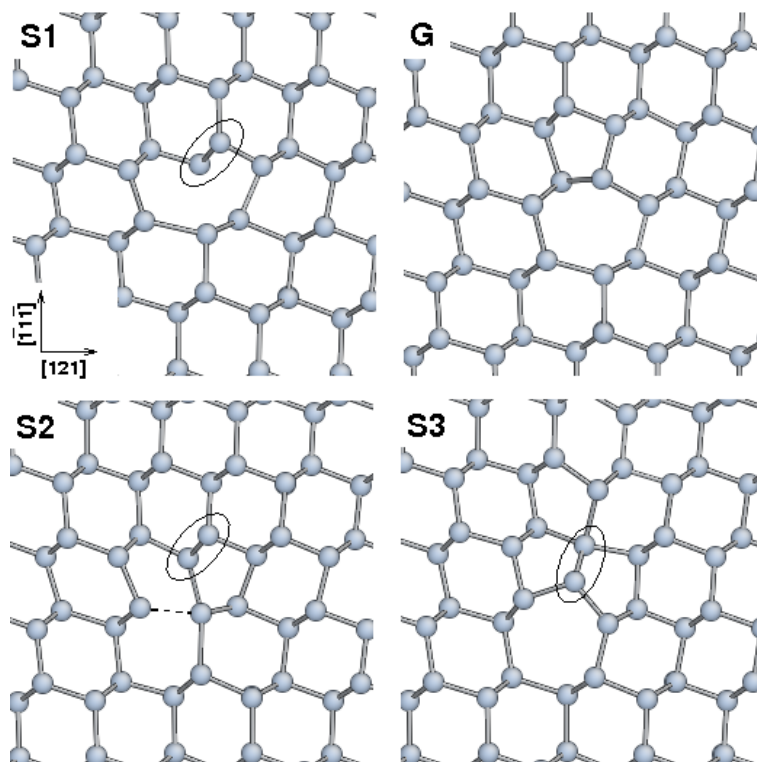


Figure 3. Four possible structures for a 60° dislocation in a diamond cubic lattice [61].

only for high temperatures, for which dissociated dislocations are observed. In a possible scenario, the core A is the likely configuration for the non-dissociated screw, and the C_2 does not play any part in plastic deformation at low temperature. This is supported by theoretical investigations of dislocation nucleation in silicon, which show the formation of the A core of the screw dislocation [60]. However, since C_2 is topologically close to partial dislocation cores, it may occur as an intermediate step during a possible transformation leading to the dissociation of the screw dislocation.

4. The 60° dislocation

The second important dislocation core in the diamond structure corresponds to a 60° orientation, which is dissociated into a 30° and a 90° partial dislocations at high temperature. However, at low temperature, 60° dislocations are not observed in the microstructure of plastically deformed silicon. One explanation is that the non-dissociated 60° dislocation is supposedly relatively mobile, and only dislocation segments for the slowest characters can be clearly observed after deformation. Additional arguments for the existence of non-dissociated 60° dislocation are given by investigations of dislocation nucleation from surfaces [60,62,63], or from interfaces of stressed systems [31,33].

Hornstra suggested one possible configuration for the 60° dislocation [49]. It is obtained when the dislocation core is located in a shuffle $\{111\}$ plane, and is characterised by an atom with a dangling bond (figure 3). It is labelled S_1 in the following. Another possible core, reported in the Hirth and Lothe textbook [8] and shown in the figure 3, corresponds to a dislocation centred on a glide $\{111\}$ plane. This G structure has no apparent under-coordination like the S_1 configuration, which would suggest a larger stability. It is worth to mention that this core exhibits a double period reconstruction along the dislocation line [61], a feature initially reported

by Blumenau and co-workers in the case of diamond [64].

Until recently, only theoretical investigations using semi-empirical potentials have been performed, and they all confirmed the much larger stability of G over the S_1 core. Still, all studies involving 60° dislocations used the configuration S_1 instead of G for the core structure [65,66]. Actually, within these potential calculations, S_1 configuration behaves as expected, i.e. it is mobile with a reasonable Peierls stress, whereas the highly stable G configuration appears to be sessile, with a large Peierls stress.

Surprisingly, to our knowledge there have been no first principles calculations of the 60° dislocation in silicon. We have then performed such calculations, which have confirmed the high stability of the G configuration [61]. But the striking result of this work is that the S_1 structure is an unstable configuration, which spontaneously evolves with an energy gain of about 1 eV/b to a so-called S_2 structure, shown in the figure 3. All tests made with different cell sizes, boundary conditions, and calculation methods, confirmed this point. The S_2 geometry is different from the one obtained in the case of diamond, since weak bonds are present into the core. Now, a slight perturbation of the S_2 structure brings the system into another third configuration, unimaginatively called S_3 (figure 3), with an extra 0.8 eV/b energy gain. The final S_3 configuration remains less stable than the G core, but with an energy difference of only 0.6 eV/b. To summarise, it appears that only the configurations G and the new one S_3 are the possible core geometries for the non-dissociated 60° dislocation. Note that this is in apparent contradiction with first-principles investigations of dislocation nucleation from surfaces, showing clearly the formation and propagation of 60° dislocations with the S_1 structure [63].

Additional clues can be obtained by studying the mobility of possible structures. We have performed molecular dynamics calculations using the EDIP and Tersoff potentials, increasing step by step the temperature and the applied stress on both G and S_3 dislocation cores [67]. Both configurations were found to be sessile even at temperatures and stresses larger than 1200 K and 3 GPa, respectively. For higher values, amorphisation occurs in the vicinity of the cores. This aspect is not surprising if one considers that both configurations are very stable, and are characterised by reconstructed bonds (especially S_3). Therefore it appears that none of the available stable configurations for the 60° dislocation are mobile in the low temperature / high stress regime. However, first principles calculations showed that if a suitable stress is applied on an unstable S_1 core, it will move and its geometry is conserved during the displacement [61]. This dazzling result explains why a S_1 dislocation core can be nucleated and displaced in a highly stressed system [63]. A crude calculation of the Peierls stress for the S_1 core yields values ranging from 1 to 2 GPa, which is in relatively good agreement with experimental estimations [26]. The dislocation displacement is obviously not thermally activated and only caused by the stress. Consequently, when the resolved stress on the S_1 dislocation core becomes too low, the $S_1 \rightarrow S_3$ transformation should occur. Since the S_1 configuration only exists in motion, the role of nucleation is essential here. This scenario is sketched in the figure 2.

To summarise these results, first principles calculations suggest that the core of a 60° dislocation in silicon is either stable and sessile, or glissile and exhibiting a transient character. This results highlights the role of nucleation in the low temperature / high stress regime, a feature which could be also dominant in the case of silicon nanostructures. Overall, the occurrence of transient dislocation cores appears to be a new finding, and tends to break the traditional pattern of theoretical investigations, where one looks first for stable core configurations before determining mobility properties. Unfortunately, an experimental confirmation will be difficult to achieve. For instance, the usual post-mortem microscopy investigations are obviously not appropriate for determining a transient dislocation core.

5. Discussion

The previous sections show that our knowledge concerning dislocation cores properties in silicon is not yet complete, despite significant advances during the last decade. In the low temperature / high stress regime, at present we know that there are two possible cores for the screw dislocation, one being more mobile than the other and likely to occur during plastic deformation. Besides, theoretical investigations suggest a glissile transient configuration for the 60° dislocation, which emphasises the role of nucleation in this regime. Little is known for the other dislocations, with 30° and 41° orientations. Geometrical arguments suggest that this original 41° orientation could be obtained by combining short segments of 30° and 60° dislocations [68], but this remains to be confirmed.

Another open question concerns the transition between the high temperature / low stress and the low temperature / high stress regimes. Our last investigations clearly showed that this transition could be triggered by nucleation only [60]. Another possibility is the transformation of non-dissociated dislocations at low temperature into partial dislocations by dissociation [69,70]. To our knowledge, there is no available information on the mechanisms and the associated activation energies for such a process. For the screw dislocation, we already proposed that a process involving first the transformation from the A core to the C_2 core followed by the dissociation of the latter, could occur for temperatures in agreement with the experimental transition.

Finally here we only focused on silicon because of the large amount of available works, and also because it is usually considered as a model material. However, it is not clear whether the results and conclusions reported in this paper can be applied to other covalent systems such as diamond, germanium, or zinc-blende compounds like SiC or GaAs (mentioning only the most common ones), although the occurrence of two plastic regimes seems to be a general feature in these systems. For instance, a tight-binding calculation of the screw dislocation in diamond points that the C_1 and C_2 configurations are quasi degenerate in energy, in clear contrast to silicon. Therefore it seems appropriate to conclude this paper by the well-known sentence, saying that additional investigations are required for a better understanding.

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