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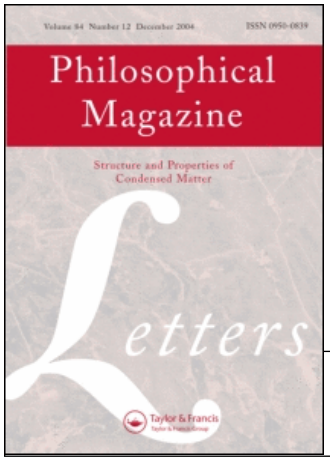

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Dislocation motion in silicon: the shuffle-glide controversy revisited

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Considering recently computed formation and migration energies of kinks on nondissociated dislocations, we have compared the relative mobilities of glide partial and shuffle perfect dislocations in silicon. We found that the latter should be more mobile over all the available stress range, invalidating the model of a stress driven transition between shuffle and glide dislocations. We discuss several hypotheses that may explain the experimental observations.

Keywords: dislocation; semiconductors; plasticity; shuffle–glide; silicon

In a seminal paper in 1996, Duesbery and Joós brought forward an explanation to the preference for dislocation motion on glide rather than shuffle planes in diamond cubic materials like silicon [1]. Using a model based on kink pair nucleation and dislocation line energy calculations, they proposed that for low stress, partial dislocations located in glide planes should be the more mobile species. On the contrary, in this paper, we show that perfect dislocations located in shuffle planes have the highest mobility, for all stresses, when kinks formation and migration energies are taken into account in the calculations.

The diamond cubic structure can be viewed as two interpenetrant face centered cubic lattices displaced by $\frac{a}{4}\langle 111\rangle$ relative to each other. As a consequence, compared to the fcc structure, there are two inequivalent families of (111) planes, the so-called widely spaced shuffle and narrowly spaced glide planes (Figure 1). Gliding dislocations, with a perfect Burgers vector equal to $\frac{a}{2}[110]$, are located in (111) planes, like in fcc materials, and so may belong to glide or shuffle planes.

Most of the experimental and theoretical studies on diamond cubic materials refer to silicon as a model. At high temperatures, i.e., in the ductile regime, all observations agree that the plasticity of silicon is governed by dissociated screw and 60° dislocations, composed respectively of two 30° or one 30° and one 90° Shockley partial dislocations [2,3]. The two partials are separated by an intrinsic stacking fault which can exist only in glide (111) planes. The 30° partial dislocation is less mobile than the 90° [4], and therefore, will govern the plastic response at high temperature. The situation is less clear at low temperature, i.e. in the brittle regime. In fact, deformation experiments performed under pressure confinement, or in scratch tests, indicate that dislocations are not dissociated [5]. Several kinds of orientations have been found, such as 30°, screw, 60°, and even an unresolved 41° dislocation. Whether these dislocations are located in shuffle or glide

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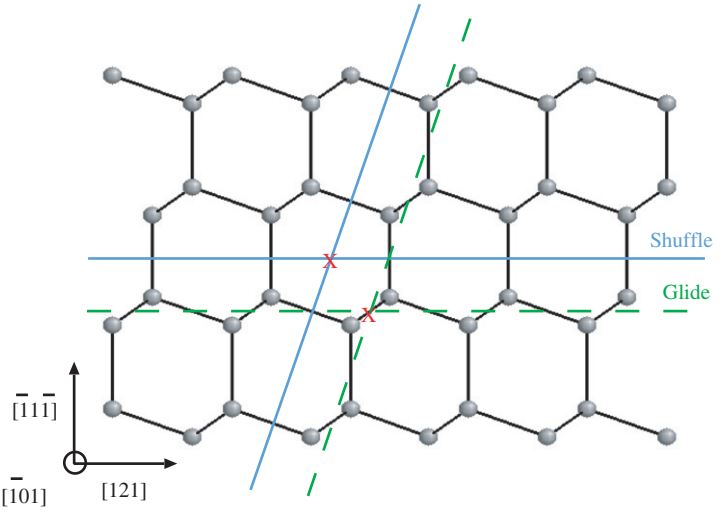

Figure 1. (101) projection of the diamond cubic structure, with the two sets of (111) planes, shuffle (full lines) and glide (dashed lines). Also shown are the two possible positions of the nondissociated screw core.

planes is not firmly established, although there is a general consensus that they belong to shuffle planes [6–9].

To understand the respective role of glide and shuffle dislocations during plastic deformation, the quantity of interest is the dislocation mobility. Simple geometrical arguments would suggest that a shuffle dislocation core is the easiest to move, because it requires to break only a single bond compared to three for the glide dislocation core. This point is confirmed by calculations of the Peierls stress, which is about at least one order of magnitude larger for partial glide dislocations than for undissociated shuffle dislocations [10,11]. However, in covalent materials like silicon, dislocations move by formation and migration of kink pairs [3]. Within this model, the line energy calculations performed by Duesbery and Joós unambiguously indicated that the free energy for the formation of a kink pairs was lower for a glide partial than for a shuffle perfect dislocation, for stress below 0.01μ (μ being the shear modulus). According to this result, in the low stress regime, glide partials should move by thermal activation before shuffle perfect dislocations, in agreement with experiments. Also, these calculations indicated that above a certain stress threshold, this behavior would be reversed. Again, this is in agreement with experiments made in the high-stress regime. Also, Rabier and Demenet have recently shown that the stress at which the glide/shuffle transition would occur is in the range 0.008–0.016μ [12], bracketting the 0.01μ value found by Duesbery and Joós [1].

The Duesbery and Joós model provides a reasonable explanation and a unified view for the two different sets of experimental results, while remaining remarkably simple. In this model, it is easier to form a kink pair on a glide partial than on a shuffle perfect dislocation because in the latter a larger line energy increase is required. However, being purely elastic, it does not include atomistic effects occuring during the migration of a kink, or in the very beginning of the kink pair formation, and it also neglects the possible

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reconstruction of the dislocation cores. Since the publication of the work by Duesbery and Joós, there have been several experimental and theoretical investigations of these atomistic effects, essentially for glide partial dislocations. For instance, many studies have focussed on core reconstructions [13–16]. Important quantities for dislocation mobility are the formation and migration energies of a single kink, F_k and W_m respectively, since they can be used for determining the dislocation velocity in the Hirth and Lothe theory of thermally activated motion of dislocations [3]. For the partial dislocations, several different measurements have been made, yielding formation energy F_k values ranging from 0.4 to 0.7 eV, and migration energy W_m values ranging from 1.2 to 1.8 eV [17]. More recently, using high-resolution electron microscopy, Kolar et al. have determined that $F_k = 0.80$ eV and $W_m = 1.24$ eV for a 30° partial dislocation [4]. Besides, many calculations have been performed, but the results are not conclusive enough because of the large scatter of computed energies [18–21]. For non-dissociated dislocations, to our knowledge, no experimental data are available for kinks. Nevertheless, kinks on a non-dissociated shuffle screw dislocation have been recently investigated by means of first principles and atomistic potential simulations, taking advantage of the Nudged Elastic Band method [22]. These calculations indicated that the kink formation energy ranges from 0.90 to 1.36 eV, whilst the migration energy is very low, and ranges from 20 to 160 meV.

Hence, in comparison with the original work from Duesbery and Joós, we have at our disposal data characterizing the formation and migration of kinks on both dissociated and non-dissociated dislocations. For the 30° partial dislocations, we consider two sets of (F_k, W_m) values. The first is the average of the various experiments reported in ref. [17], i.e., (0.55 eV, 1.5 eV). The second set are data measured by Kolar et al., i.e., (0.80 eV, 1.24 eV) [4]. For the non-dissociated screw, the average (1.13 eV, 0.09 eV) of the calculated values [22] are used. According to Hirth and Lothe [3], the energy for the nucleation of a kink pair is

$$F(x) = 2F_k - \frac{Kb^2h^2}{x} - \sigma bhx \tag{1}$$

with b the magnitude of the Burgers vector, h the kink height, x the distance between kinks, K an elastic factor [For a screw, $K = \mu(1+\nu)/8\pi(1-\nu)$, whereas for the 30 partial, $K = \mu(4+\nu)/32\pi(1-\nu)$. We used the silicon shear modulus $\mu = 68.1$ GPa $= 0.425$ eV Å^{-3} and the Poisson coefficient $\nu = 0.218$], and σ is the effective stress applied on the dislocation. The condition for propagation of the kinks is $x > x^*$, with x^* defined by $[\partial F(x)/\partial x]_{x=x^*} = 0$. $F(x^*) = F^*$, the activation energy for creating a stable kink pair, is then

$$F^* = 2\left[F_k - \sqrt{Kb^3h^3}\,\sigma^{1/2}\right] \tag{2}$$

Here, we do not consider entropic contributions that are expected to be negligible. The velocity of a dislocation is proportional to $\exp(-Q/kT)$, Q being the activation energy of the process. Q is then the important quantity for determining which of dissociated or non-dissociated dislocations are the more mobile species. According to Hirth and Lothe [3], when the characteristic length of the dislocation segment is smaller than the average distance between thermal kinks, $Q = F^* + W_m$ (regime R_1). Otherwise, Q is equal to $F^*/2 + W_m$ (regime R_2). Figure 2 shows the variation of Q as a function of σ, for both R_1 and R_2 regimes, obtained from Equation (2). There is a striking difference compared to the

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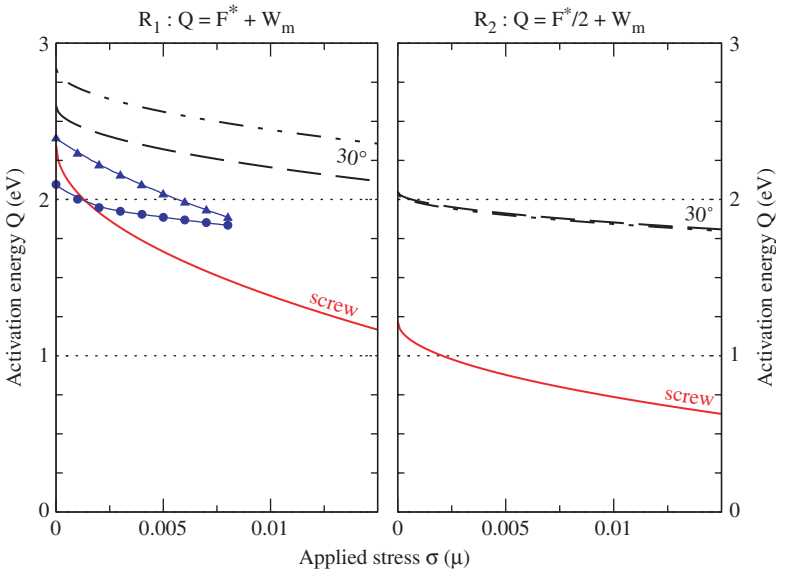

Figure 2. Activation energy for the thermally activated motion of dislocation as a function of applied stress, for $Q = F^* + W_m$ (left panel) and $Q = F^*/2 + W_m$ (right panel). For a 30° partial dislocation, two (F_k, W_m) sets of data have been used, (0.55 eV, 1.5 eV) (dashed line) and (0.80 eV, 1.24 eV) (dot-dashed line), whereas for a shuffle screw dislocation, we have considered the computed values (1.13 eV, 0.09 eV) [22] (full line). The original data from Duesbery and Joós have also been reported (circles for the 30° partial dislocation and triangles for the screw dislocation).

original data from Duesbery and Joós, also reported in the figure, that is the absence of an intersection between the 30° partial and screw dislocations curves. This suggests that the shuffle screw dislocation should be more mobile than the 30° glide partial dislocation, for all stresses.

First, it is interesting to analyze why our calculations lead to an outcome completely different from that of the previous study from Duesbery and Joós. In the expression (2), the energy decrease as a function of stress depends on the coefficient $\sqrt{Kb^3h^3}$. Since the K factors for a 30° partial and a screw dislocation are only marginally dissimilar, the main difference is coming from the $b(3/2)$ factor. Since $b_{\text{screw}}/b_{30^\circ} = \sqrt{3}$, the energy decrease as a function of stress is larger for the screw dislocation than for the 30° partial, in agreement with Duesbery and Joós [1]. So we are left with F_k and W_m, that characterizes the stress-independent formation and migration of a kink. F_k is lower for the 30° partial dislocation than for the screw dislocation, consistent with the fact that for the latter, the line energy increase is larger. Finally, the main factor comes from the large difference between migration energies. While W_m is large for partials, due to complex reorganization of atomic bonds [23], it is at least one order of magnitude lower for the screw dislocation because in that case, kink migration occurs by breaking and formation of a single highly stretched bond [22]. Therefore, it is simply the inclusion of migration energies that drastically changes the results compared to the Duesbery and Joós model.

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These results have important implications regarding the understanding of silicon plasticity, and the so-called glide/shuffle transition. The curves shown in Figure 2 indicate that if the mobility of dislocations is only controlled by formation and migration of kink pairs, the shuffle perfect screw dislocations will always be more mobile than glide partial dislocations for all stresses. Obviously, this conflicts with the model of a glide/shuffle transition driven by stress, due to Duesbery and Joós [1], based solely on the calculation of the kink pairs formation.

Before proposing arguments for explaining this discrepancy, we discuss the validity of our calculations. First, in this work we have favored a shuffle core for the screw dislocation [24], although it has been shown that a glide core is energetically more stable [25,26]. Our choice has been motivated by the fact that the glide core is necessarily reconstructed along the dislocation line, yielding a structure close to reconstructed partial dislocation cores. It is likely that the migration mechanism for a kink on the glide core is similar to what is obtained for partial dislocations, then with a migration energy of the order of 1 eV. Associated with the expected higher kink formation energy for perfect dislocations, it is reasonable to assume that a non-dissociated reconstructed glide screw dislocation should not be mobile for the temperature and stress domains usually considered.

Second, we discuss how selected energy parameters (F^*, W_m) could modify our results. It is a critical point since there is a large uncertainty on measured and calculated values, especially for the 30° partial dislocation. Using together both the lowest experimentally reported formation and migration energies, one may again expect a transition between shuffle and glide in the case of the R_1 regime (Figure 2, left panel). According to the measurements made by Rabier and Demenet, the stress value associated with the glide/shuffle transition is in the range 0.008–0.016μ [12]. Keeping the lowest experimentally reported migration energy equal to 1.2 eV, such a range corresponds to a 30° partial kink formation energy between 0.21 eV and 0.32 eV, appearing to be in agreement with some calculations [18,20], but may be too low compared to experiments. It is likely that the formation energy F_k is close to 0.7–0.8 eV, in agreement with the value obtained by Kolar et al. [4]. This is also confirmed by Cai et al. who have reproduced the experimental dislocation velocity curves in a kinetic Monte Carlo model, using the values (0.7 eV, 1.2 eV) [27], close to the data shown in Figure 2.

Third, it is also possible that the mobilities of the non-dissociated screw and 30° partial dislocations are best described by different regimes. In fact, it is not firmly established whether R_1 or R_2 dominates for 30° partial dislocations, while there is no information for non-dissociated dislocations. The most favorable case for recovering an intersection is obtained when the activation energy of the 30° partial dislocation is given by $Q = F^*/2 + W_m$, i.e., the regime R_2 (Figure 2, right panel), whereas the mobility of the screw dislocation is controlled by $Q = F^* + W_m$ in the R_1 regime (Figure 2, left panel). Unlike the Duesbery and Joós model, such a glide/shuffle transition would then be explained by a change of mobility regimes, according to the average separation between thermal kinks. Such a scenario is supported by an interesting study by Scarle et al. suggesting that the regime R_2 should be used for kink formation energies lower than 0.4–0.5 eV [28]. In this case, keeping 1.2 eV for the migration energy, the kink formation energy of the 30° partial dislocations should range from 0.17 to 0.45 eV, in order to agree with the reported stress range 0.008–0.016μ. As discussed previously, these values seem low compared to recent experiments.

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Although the possible issues described in the paragraph above cannot be ruled out completely, it appears that other arguments have to be considered in order to reconcile theory with experiments. Our investigations, as well as the study by Duesbery and Joós, are based on the assumption that dislocations move by formation and migration of kink pairs. In the following, we discuss other possible mechanisms, going beyond this simple picture, that may be at play when a dislocation moves. For instance, it has been postulated that the presence of discrete dragging points along the dislocation line could govern the dislocation mobility [29]. Such pinning points could be nonconservative jogs or locally highly stable arrangements of bonds in the dislocation core. They could also be impurities, as reported by Kolar et al. [4]. Other processes may be activated by temperature, such as local perturbations in the dislocation core structure, reducing the dislocation mobility. Such a process is possible for screw dislocations, and has been obtained for some materials [30]. In all these cases, the mobility of the screw dislocations could not be linked only to the formation and migration of kinks.

A second point concerns the character of the dislocations considered in our investigations and in the study by Duesbery and Joós. While the role of the 30° partial dislocation is firmly established, it is not absolutely sure that the plastic behavior of silicon at low temperature is governed by screw dislocations. Saka et al. have reported the presence of both screw and 30° perfect dislocations after nanoindentations [9,31]. These dislocations have also been observed by Rabier et al. in different experiments [32], in addition to a peculiar nondissociated dislocation characterized by a 41° orientation [5]. The structure of non-dissociated dislocations with 30° and 41° orientations is not known, and these dislocations might play a role during the plastic deformation. Finally, the transition between shuffle and glide modes could also be explained by the dissociation of the perfect shuffle into partial glide dislocations. Such a shuffle-glide transformation is energetically favored, explaining why the inverse transformation seems difficult to obtain [33]. In principle, given an initial distribution of perfect shuffle dislocations, one may expect to observe a thermally activated dissociation above a threshold temperature, which may depend on the applied stress. Experimentally, contradictory results have been reported. Rabier and Demenet have investigated the evolution of a population of perfect shuffle dislocations during *in situ* annealing in a transmission electron microscope with temperatures up to 685°C, without any evidence of dissociation [12]. Conversely, Saka et al., using similar apparatus and under supersaturation of interstitials, have reported a shuffle-glide dissociation for temperatures of 400°C [9,31]. These results call for additional investigations of a possible dissociation mechanism, and of the possible role of point defects in the process.

In this letter, we have revisited the so-called shuffle-glide controversy associated with the dislocation mobility in silicon. On the basis of our recent results concerning shuffle screw dislocations [22], and the available data for partial dislocations, we have shown that the model proposed by Duesbery and Joós of a stress driven transition between shuffle and glide dislocations [1] was not conclusive. Several possible scenarios are proposed as alternative explanations, and discussed in relation with available experimental and theoretical results. In the given state of knowledge, it is difficult to draw definite conclusions on this matter, and additional investigations are required for a better understanding of the relation between the structure of dislocations at the atomic scale and their mobility.

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