Test of the Peierls-Nabarro model for dislocations in silicon

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We show, using an atomistic model with a Stillinger-Weber potential (SWP), that in the absence of reconstruction, the basic assumption of the Peierls-Nabarro (PN) model that the dislocation core is spread within the glide plane is verified for silicon. The Peierls stress (PS) obtained from the two models are in quantitative agreement ($\approx 0.3\mu$), when restoring forces obtained from first principles generalized stacking-fault energy surfaces are used in the PN model [B. Joós, Q. Ren, and M. S. Duesbery, Phys. Rev. B **50**, 5890 (1994)]. The PS was found to be isotropic in the glide plane. Within the SWP model no evidence of dissociation in the shuffle dislocations is found but glide sets do separate into two partials.

I. INTRODUCTION

The Peierls-Nabarro (PN) model,[1,2] although relatively simple, has the potential of providing quantitative estimates for key dislocation properties. In that model the crystal is cut into two halves, along the glide plane, the plane which contains the dislocation line and the Burgers vector. The two halves are treated as elastic mediums, while the interface atomistically. In the original model, the restoring forces at the interface were assumed to vary sinusoidally as a function of the displacement $\vec{f}$ of one block with respect to the other with the appropriate elastic limits. Better results are expected if, instead, the restoring forces are obtained from the generalized stacking fault (GSF) energy surface, $\gamma(\vec{f})$, as was suggested a while ago by Christian and Vitek[3] and applied to bcc crystals by Lejček[4] and Kroupa and Lejček,[5] and recently by us to silicon (paper I, Ref. 6). The question is, how reliable is this model?

Silicon has been chosen as the test case because of the importance of dislocations in this system and because a first-principles GSF surface is available.[7–9] Silicon is not just the prototypical covalent semiconductor but also a thriving industry.[10] In Si the dislocations are particularly important because the cores harbor localized in-gap electronic levels which can destroy the electrical properties of a device. If they are not mobile, device logic can be made to avoid the dislocated areas. A new generation of optoelectronic devices based on strained superlattices[11] adds additional motivation to the understanding of dislocation nucleation and mobility. In spite of extensive studies of dislocations in Si, described in numerous reviews,[12–17] these two properties are not well understood.[18]

An important quantity characterizing dislocation mobility is the Peierls stress (PS), the stress required to move the dislocation from one lattice site to the next at 0 K. Due to brittle fracture it is usually difficult to obtain the PS at low temperature, especially for silicon where it is large. It is even harder to distinguish the contributions from the different dislocations. The PS can only be estimated by extrapolating the yield strengths to the absolute zero temperature. For Si this gives a value[19–21] of the order of $(0.1-0.5)\mu$, where μ is the shear modulus [the averaged value for Si is $\mu = 6.81\times 10^{11}$ dyn/cm^2 = 0.425 eV/Å^3 (Ref. 22)]. This is a rough estimate because it relies on high-temperature values of the yield strength.[23–25]

Another interesting issue for silicon is the shuffle-glide controversy.[15,16] Dislocations in silicon can be present in the glide or shuffle set configurations for which different core structures are expected. The structure is referred to as the shuffle set if the inserted lattice plane is terminated between the widely spaced {111} planes of the same index in the diamond structure, and the glide set, if between the closely spaced planes of different index (see Fig. 1). In silicon, it has been found that the glide dislocations could dissociate into two partials separated by an intrinsic stacking fault[14,26] and glide in the dissociated form.[14,27] This is not the case for the shuffle set which has no low-energy stacking fault. The dissociation into partials in this case is more complex and their motion has been argued to be akin to a shuffling motion involving movement of interstitials.[22] The direct observation of the glide of dissociated dislocations[27,28] has usually been used to argue in favor of the glide set,[29] but high-resolution electron microscopy (HREM) results are not fully consistent with the expected simple structures.[16]

Our studies in paper I of dislocations in silicon within the PN model were based on the first principles γ surfaces calculated by Kaxiras using local density functional theory.[7,8] The energies $\gamma(\vec{f})$ are generated by displacing the two halves of the crystal above and below the cut plane by arbitrary GSF vectors $\vec{f}$. In Duesbery *et al.*[7] no relaxation of the atoms perpendicular to the cut plane was allowed. In Kaxiras and Duesbery,[8] relaxed values were obtained for the unstable stacking faults γ_{US} in the glide and shuffle planes. The unrelaxed γ surfaces scaled down with those γ_{US} were used in the PN model. More recently Juan and Kaxiras[9] obtained the fully relaxed γ surfaces. The most relevant directions for the PN model are the $\langle 112\rangle$ directions in the glide plane, the direction of the Burgers vectors of the partials, and the

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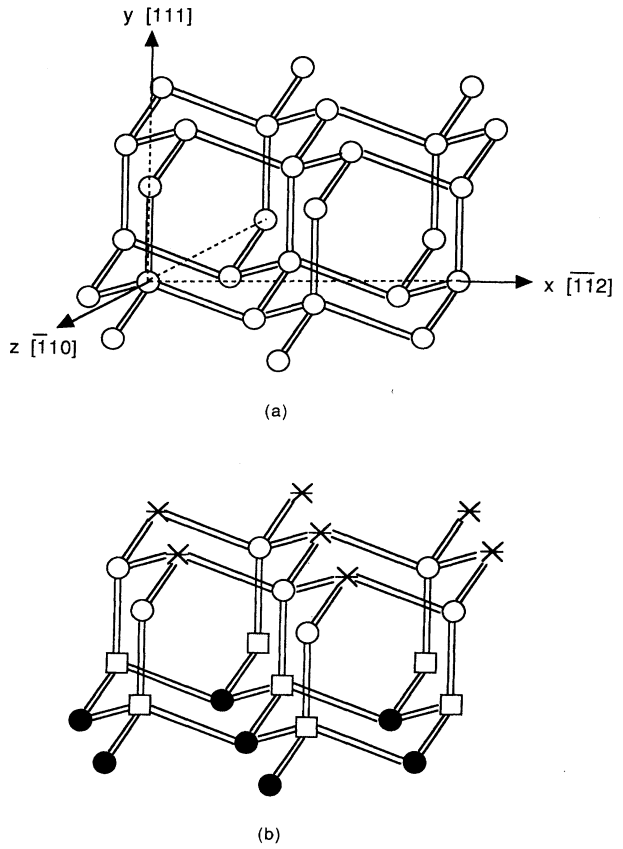

FIG. 1. (a) Four layers of perfect silicon lattice with the x, y, z directions used in the simulations. (b) The same plot but with different symbols for each layer. Solid circles, squares, open circles, and asterisks represent in the usual notation for the diamond lattice, a c plane, an A plane, an a plane, and a B plane, respectively.

$\langle 110\rangle$ directions in the shuffle plane, the direction of the Burgers vectors of the full dislocations. For the glide plane, Juan and Kaxiras find little change from the scaled γ surface, in the $\langle 112\rangle$ directions, but significant changes in the other directions. The fully relaxed shuffle plane γ surface is very similar to its scaled counterpart. The smooth variations of $\gamma(\vec{f})$ in the shuffle plane lead to low PS for the shuffle set of dislocations ($\approx 0.1\mu$) within the PN model; 0.083μ for the 60° dislocation and 0.112μ for the screw dislocation. The full dislocations in the glide plane are very narrow and have high PS. The partials, taking advantage of smaller GSF energy variations along their Burgers vector, have considerably lower PS than the full dislocations in the glide plane. These PS are of the same order of magnitude than those for the shuffle dislocations although still higher, 0.30μ for the 90° partial and 0.37μ for the 30° partial, the 90° partial having a lower PS as observed experimentally. The PN model is a zero-temperature model and no reconstruction is allowed because lattice periodicity is imposed along the dislocation line. The absence of reconstruction may artificially favor the shuffle set. Kaxiras and Duesbery have argued for an entropic effect.[8]

II. STILLINGER-WEBER POTENTIAL MODEL

To assess the validity of the PN model, we wanted to test it within an atomistic model. The Stillinger-Weber potential[30] (SWP) was chosen for several reasons; it is the most widely used empirical potential for silicon and it produces a generalized stacking fault (GSF) energy surface[7] which, overall, is similar to the one obtained from a first principles density functional calculation.[7,8] This potential has proven to be valid in many studies, such as critical layer thickness,[31] the Si surface,[32,33] silicon indentation,[34] and the phase diagram of silicon.[35] Some questions have been raised about its validity in reproducing dislocation reconstructions in Si in detail.[36] The 30° partial at least has the correct reconstruction. Bulatov, Yip, and Argon[37] made an extensive study of complexes involving 30° partials within the SWP model. The emphasis at this point is using an atomistic model which is compatible to the PN model. The Stillinger-Weber potential includes both two-body interactions V_2 and three-body interactions V_3:

$$V_2=\sum_{\substack{i,j\\ i<j}} 7.05\,\epsilon\left[0.602\left(\frac{r_{ij}}{\sigma}\right)^{-4}-1\right]\exp\left(\frac{r_{ij}}{\sigma}-1\right)^{-1}$$

$$\text{for}\quad r_{ij}<1.8\sigma, \quad (1)$$

$$V_3=\sum_{\substack{i,j,k\\ i<j<k}} 21.0\,\epsilon\exp\left[1.2\left(\frac{r_{ji}}{\sigma}-1.8\right)^{-1}+1.2\left(\frac{r_{ik}}{\sigma}-1.8\right)^{-1}\right](\cos\,\theta+\tfrac{1}{3})^2$$

$$\text{for}\quad r_{ji}<1.8\sigma \quad \text{and} \quad r_{ik}<1.8\sigma, \quad (2)$$

where r_{ij} and r_{ik} are interparticle distances, and the parameters ϵ and σ are

$$\epsilon=50\ \text{kcal/mol}, \quad \sigma=0.209\,51\ \text{nm}. \quad (3)$$

Rectangular parallelepiped crystallites of a certain number of repeat units bounded by $(\bar{1}\bar{1}2)$, (111), and $(\bar{1}10)$ planes were constructed. The dislocation line was always aligned along the $\langle\bar{1}10\rangle$ z axis with periodic boundary conditions along this axis so that effectively an infinite dislocation was studied. The atoms were displaced from their equilibrium (perfect lattice) positions as given by elasticity theory for the given Burgers vector (partial or perfect dislocations) and the position of the slip plane (shuffle or glide). The boundaries in the x and y directions were fixed while the rest of the atoms were relaxed by minimizing the atomistic potential energy as in Ref. 38. By fixing those boundaries, reconstructions are inhibited, facilitating comparison with the results of the PN model.

The stress was imposed by introducing a homogeneous shear strain over the entire region containing the relaxed dislocation.[39–41] Then, again, keeping the atoms along the x-y boundary regions fixed, the remaining atoms were relaxed. When fully relaxed, the resultant configuration was examined for any change in the location of the dislocation. Starting each time with the relaxed unstressed dislocation, the stress imposed was varied until the change in the location of the dislocation was one exact repeat lattice distance. The

corresponding stress was taken as the minimum stress required to move the dislocation. The PS for that particular dislocation and orientation was deduced by projection unto the Burgers vector. Different sizes of models with atoms from 3000 to 15 000 were tested in order to eliminate finite size effects.

III. SIMULATION RESULTS

A view of the perfect silicon lattice with our choice of axes is shown in Fig. 1(a). In Fig. 1(b) different symbols are used for each layer for ease of understanding. Solid circles, squares, open circles, and asterisks represent in the usual notation for the diamond lattice, a c plane, an A plane, an a plane, and a B plane, respectively. Shuffle dislocations are introduced between planes of the same index, i.e., between the squares (the A plane) and the open circles (the a plane), and the glide dislocations between planes of different index, i.e., between the solid circles (the c plane) and the squares (the A plane). Examples of the most relevant types of dislocations are displayed in Figs. 2 and 3 as projections along the y direction into the x-z plane, the glide plane. The z direction is chosen as the dislocation line direction. The 30° and 90° glide type partials are shown in Fig. 2 (these are the angles the respective Burgers vectors make with the dislocation line). Only the sets of atoms in the B and c planes are used for the representation. All arrows appearing on the plots are drawn from the atoms' original positions to their displaced positions on the bottom c plane. For a screw dislocation in the shuffle plane such as in Fig. 3 the planes of the same index a and A are more suitable. The dashed and solid lines show what happens to a set of atoms in the a and A planes lying above each other in the perfect lattice when the screw dislocation is introduced.

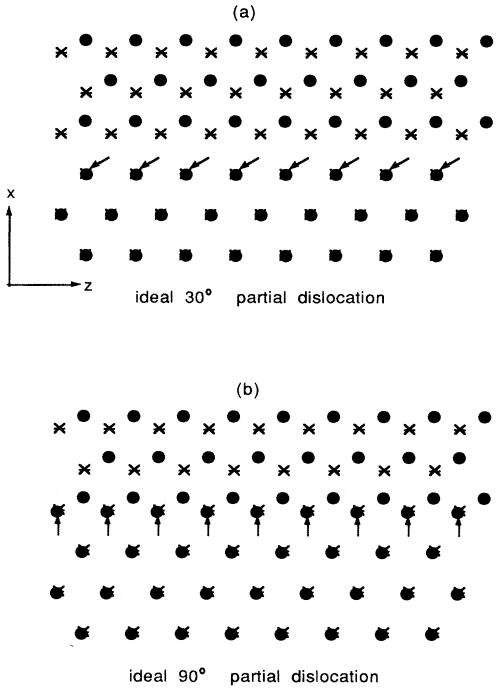

FIG. 2. (a) A silicon lattice with an ideal 30° partial dislocation in the glide plane projected normal to the (111) plane. Two layers of atoms are shown here, the B plane (asterisks) and the c plane (solid circles). (b) The same lattice but with an ideal 90° partial dislocation. All arrows appearing on the plots are drawn from the atoms' original positions to their displaced positions in the c plane.

A. Dislocation profiles

One of the important assumptions of the PN model is that the dislocation core is planar; i.e., the largest displacements are within the glide plane, the x-z plane in our case, and actually even more specifically along the Burgers vector.[22] These assumptions are clearly valid in our calculations. We illustrate this fact with the screw dislocations whose Burgers vectors lie along the z direction. Figure 3 shows the shuffle screw dislocation. The relative changes in the position of the atoms is graphically represented by the displacement of the solid line with respect to the dashed line.

Displacements along the x, y, and z directions plotted as functions of the x positions of the atoms are shown in Fig. 4. The dislocation displacements are seen to be directed mainly along the Burgers vectors for both glide and shuffle dislocations. The width of the screw shuffle dislocation is found to be 3 Å. The corresponding width of the screw glide dislocation is quite narrow, only about 0.3 Å. Those results are in good agreement with our PN model calculations.[6] There are some small displacements along the x direction for the glide screw and the y direction for the shuffle screw.

B. Peierls stress

To maintain periodic boundary conditions along the z axis the shear stress was applied within the (111) plane, the x-z plane (the Burgers vector for all dislocations lie within that plane). It was found that the PS is isotropic within that plane. In other words that the stress required to move the dislocation in any direction within that plane has the same projection unto the Burgers vector, the PS of the dislocation.

The possible effect of the finite size of the block upon the calculated PS has been tested by carrying out some calculations for different block sizes, but the differences were found to be negligible.

The results are summarized in Table I. The values from paper I (Ref. 6) for the full glide dislocations would be greatly reduced if the most recent γ surface of Jian and Kaxiras[9] had been used.

1. Shuffle dislocations

As in the PN model the shuffle dislocations have also in this calculation the lowest PS; 0.075μ for the 60° and 0.086μ for the screw dislocation compared with 0.083μ and 0.112μ in the PN model. A variety of starting positions and stresses were attempted but as expected no dissociation of the core occurred.

2. Glide dislocations

In contrast the 60° and screw dislocations of the glide set dissociate to a separation of about one lattice constant when a glide stress of the order $(0.08-0.1)\mu$ is applied to them. Since the SWP extends only to second neighbor, the intrinsic

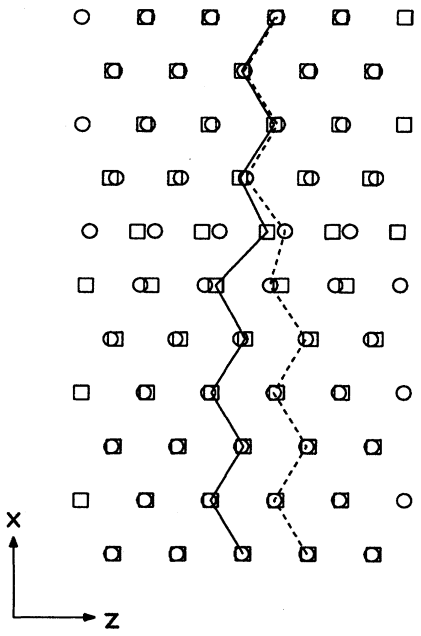

FIG. 3. A shuffle screw dislocation projected normal to the (111) plane. Two layers of atoms are shown, with the a plane (open circles) and the A plane (squares). The screw dislocation is introduced between those two planes. The relative changes in the positions of the lines of atoms in the a plane (dotted line) and the A plane (solid line) are used to calculate the displacements of the shuffle screw dislocation.

stacking fault energy is formally zero and the elastic continuum prediction of the partial separation is infinite. The much smaller observed separation is the result of the large PS. No dislocation motion is found until the stress exceeds the PS of one of the partials (see below) and then the partials can be separated further. The difference between the 60° and screw dislocations is that the first dissociates into a 30° and a 90°, while the second into two 30° partials. In short the glide dislocations can only move in dissociated form.

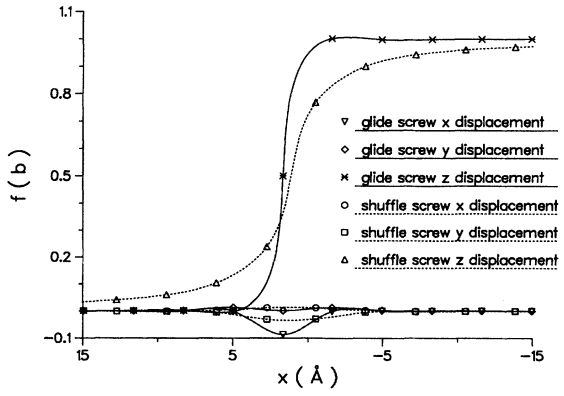

FIG. 4. Dislocation profiles of the screws. Displacements along the x, y, and z directions plotted as functions of the x positions of the atoms. The solid lines are for the glide screw dislocation and the dashed lines for the shuffle screw dislocation.

TABLE I. Comparison of Peierls stresses in Si obtained from the Peierls-Nabarro model (Ref. 6), σ_p, with those from the atomic relaxation calculation (present work), σ_b. (μ = 0.425 eV/Å^3).

Dislocation		σ_b (μ)	σ_p (μ)
glide	60°	dissociation	16.7
	screw		21.3
shuffle	60°	0.075	0.083
	screw	0.086	0.112
glide	90°	0.25	0.282
	30°	0.31	0.352

3. *Partial dislocations*

Since single partial dislocations are not observable in experiments, the PS of the partial dislocations were calculated using dissociated full dislocations, either the 30° and 30° partials (screw dislocation) or the 30° and 90° partials (60° dislocation), initially separated by an intrinsic stacking fault on the (111) plane. The results are not sensitive to the size of the stacking fault because the stacking fault energy is

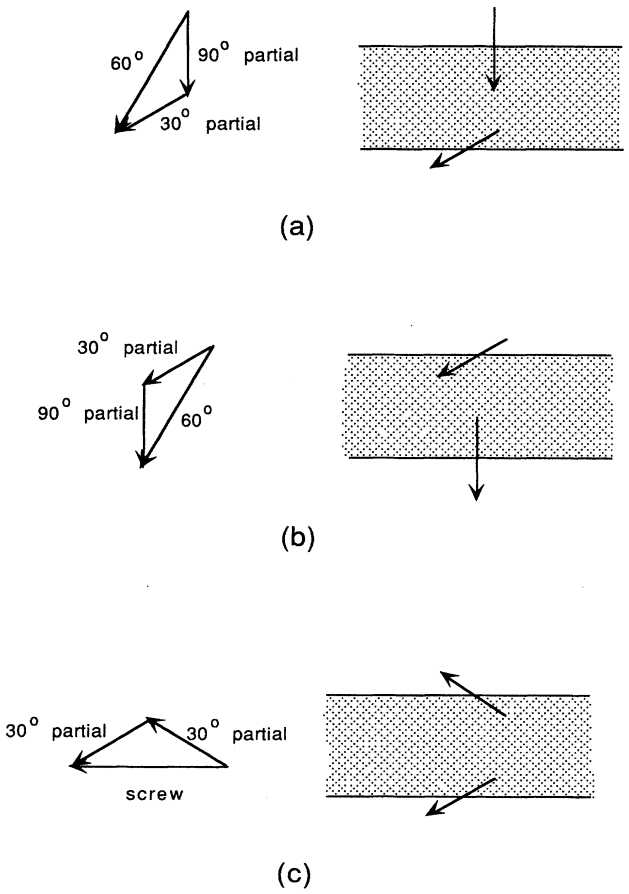

FIG. 5. (a) A dissociated 60° dislocation with a 90° partial leading. (b) A dissociated 60° dislocation with a 30° partial leading. (c) A dissociated screw dislocation with two 30° partials. The shadow areas are the stacking fault layers.

zero in the SWP model and the PS is very high. The PS were found to be 0.25μ for the 90° partial and 0.31μ for the 30° partial, to be compared with 0.282μ and 0.352μ in the PN model.

IV. DISCUSSION AND CONCLUSION

The quantitative agreement for the PS between the PN model, which does not consider reconstruction, and the SWP model, with the same constraint, is promising. A word of caution is, however, required since the two models do not have precisely the same GSF surface. But when it comes to the calculation of the PS, even order of magnitude agreements would have had to be considered as good. The dislocations in the SWP model, in the absence of reconstruction, are planar with at most a $0.1b$ displacement away from the Burgers vector direction. Under the same conditions the shuffle sets are the broadest and most mobile of the dislocations. The isotropy of the 0 K PS with the 90° partial having a lower PS than the 30° partial is in agreement with the indications of experiment. Experiment shows that under applied stress the width of a 60° glide dislocation increases if the 90° partial leads and becomes narrower if the 30° partial does.[28,42] The screw formed of two 30° partials seems to remain fairly narrow.[43,44] As seen in Fig. 5, the Burgers vectors of the partials in the dissociated dislocations are not parallel, further favoring the 90° partial through the angular dependence of the minimum stress required to move the dislocation.

This study is encouraging for the use of a PN model with GSF surfaces but several questions need to be tackled, most importantly the reconstruction of the core and its effect on the PS of the different dislocations. For the shuffle set, will reconstruction explain their absence, or are other mechanisms responsible such as the entropic effect suggested by Kaxiras and Duesbery?[8] To finish, this study also points to the usefulness of empirical potentials which reproduce the GSF surface accurately.

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