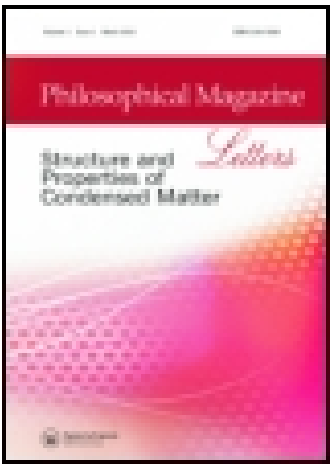

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Dislocation motion in silicon: the shuffle–glide controversy

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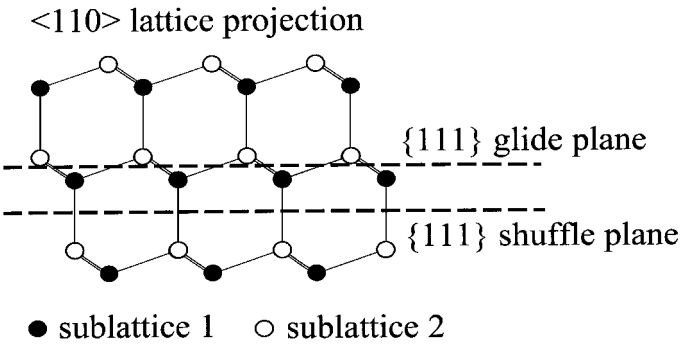
ABSTRACT

A simple explanation, in terms of the dislocation line energy, for the preference for dislocation motion on glide rather than shuffle planes in silicon and other diamond cubic materials is advanced.

Silicon and other diamond cubic (dc) structured materials form part of the essential infrastructure of the modern electronics industry. The presence and movement of dislocations in microelectronic devices can severely impair their performance. It is surprising, therefore, that one of the simplest and most fundamental questions relating to dislocation motion in the dc lattice, namely whether dislocations move on the widely spaced *shuffle* planes or the narrowly spaced *glide* planes, remains without an unequivocal answer. Theoretical arguments, without exception, predict that slip *should* occur on the *shuffle* planes. With equal unanimity, experimental observations indicate that slip *does* occur on the glide planes. This letter will suggest that there is a simple resolution to this problem.

The silicon (from here on the discussion will centre on silicon as a paradigm for the dc structure) crystal structure is built from two interpenetrant fcc cells with a mutual displacement vector of $(a/4)\langle 111\rangle$. The glide dislocations are closely related to those found in fcc crystals, with a perfect dislocation Burgers vector of $(a/2)\langle 110\rangle$ and slip plane {111}. However, there are two types of {111} plane in silicon, as shown in the $\langle 110\rangle$ lattice projection in fig. 1. The {111} planes lying between the narrowly spaced $((a/12)\langle 111\rangle)$ planes of atoms in fig. 1 are known as the *glide* planes; this terminology was introduced by Hirth and Lothe (1982) as a reminder that Shockley partial dislocation pairs can move freely on these planes. The intrinsic stacking fault which binds the partial pair can exist only on the glide planes. Those {111} planes situated between the widely spaced $((a/4)\langle 111\rangle)$ atom planes are called the *shuffle* planes. There are no stable stacking faults on these planes (Kaxiras and Duesbery 1993), so that dislocation dissociation into partial dislocations lying on the *shuffle* planes is not possible. Shockley partial dislocation pairs, which must lie on the *glide* planes, cannot move on the *shuffle* planes without the (diffusive) dragging of a row of vacancies (the so-called *shuffle*) (Hornstra 1958, Amelinckx 1979). It is important to recognize that this distinction applies only to Shockley partial dislocation

Fig. 1



Glide and shuffle planes in silicon.

pairs; perfect dislocations are geometrically free to move on either type of plane without the need for atom shuffling.

Elementary theoretical considerations suggest strongly that dislocation motion on the shuffle planes should be easier than on glide planes (Shockley 1953). For example, movement through one repeat distance on a shuffle plane breaks one covalent bond per atomic length of dislocation (fig. 1). The equivalent step on a glide plane involves the breaking of three bonds, a higher-energy process which implies greater resistance to motion. More detailed theoretical work dramatically confirms this hypothesis. Calculations of the Peierls stress for shuffle and glide dislocations using the Peierls–Nabarro (PN) model (Joós, Ren and Duesbery 1994) with generalized stacking-fault energies determined by density functional methods (Kaxiras and Duesbery 1993) indicate values nearly an order of magnitude higher for glide partial dislocations than for shuffle dislocations (perfect glide dislocations show a Peierls stress more than two orders of magnitude larger still, and therefore these will be ignored). For example, the Peierls stresses for the 30° glide partial and the shuffle screw dislocations are calculated by the PN method to be $0{\cdot}561\mu$ (μ is the $\langle 110\rangle\{111\}$ shear modulus) and $0{\cdot}103\mu$ respectively (Joós *et al.* 1994). Atomistic calculations are in fair agreement with these numbers; using the empirical Stillinger–Weber (1985) interatomic potential, comparative values of $0{\cdot}33\mu$ (30° glide partial) and $0{\cdot}091\mu$ (shuffle screw) are found (Ren, Joós and Duesbery 1995). On the other hand, *in-situ* transmission electron miscroscopy obervations (Alexander 1986) demonstrate unequivocally that dislocations in silicon are dissociated into Shockley partial pairs which move without the need for diffusion. This experimental evidence indicates that dislocation motion occurs exclusively on glide planes. Samuels and Roberts (1989) have made detailed measurements of the temperature dependence of the Peierls stress in silicon. The Peierls stress at the ductile–brittle transition temperature of 820 K is $0{\cdot}0073\mu$. Linear extrapolation of their results to 0 K, the appropriate limit for rigid-dislocation calculations, gives a value of $0{\cdot}15\mu$, roughly midway between the atomistic shuffle and glide values cited above. This lends some credence to the theoretical calculations but further emphasizes the shuffle–glide discrepancy. The observed free motion of Shockley partials leads naturally to the hypothesis that it is the dislocation dissociation itself which is

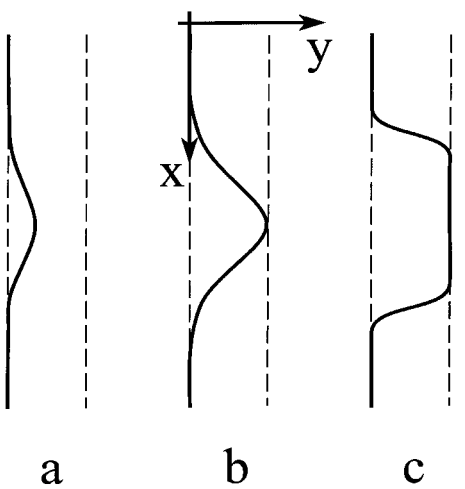
responsible for the discrepancy, but no physical reason has yet been advanced to support this speculation.

A resolution to the question comes via recognition that, in materials which exhibit significant dislocation–lattice coupling, the dislocations do not move by rigid translation, except in the strict zero-temperature limit, but rather by the nucleation and propagation of kink pairs. This mechanism is illustrated in fig. 2. A dislocation lying along a low-energy direction (the broken lines in fig. 2) develops a thermally activated bulge (fig. 2 (*a*)) which under suitable conditions may reach the adjacent low-energy site (fig. 2 (*b*)), at which point the high-energy arms of the bulge, known as kinks, can move apart (fig. 2 (*c*)), dragging the entire dislocation through a unit translation. While a full treatment of kink pair activation at the atomistic level is complex (Duesbery 1983), the demonstrated success of the quasi-elastic PN model in the treatment of dislocations in silicon (Hansen *et al.* 1995) suggests that a similar but simplified approach might serve the purpose. A suitable approach is to treat the dislocation as a linear elastic string with energy Γ per unit length lying in a periodic Peierls potential $W_{PN}(y)$ (see fig. 2) (Dorn and Rajnak 1964, Guyot and Dorn 1967). This is permissible, even though the configurations in figs. 2 (*b*) and (*c*) are of atomic dimensions in the *y*-direction, because almost all the energy of a dislocation resides in its long-range *linear elastic* field. Therefore the energy perturbation introduced by the bulge in the dislocation, which is due principally to the increased line length, can be approximated well by a linear elastic model.

In the presence of an applied stress τ the enthalpy of the bulged dislocation in excess of that of the straight dislocation is

$$U = \int_{-\infty}^{\infty} \left\{ W(y) \left[1 + \left(\frac{dy}{dx} \right)^2 \right]^{1/2} - W(y_0) - \tau b(y - y_0) \right\} dx, \qquad (1)$$

Fig. 2



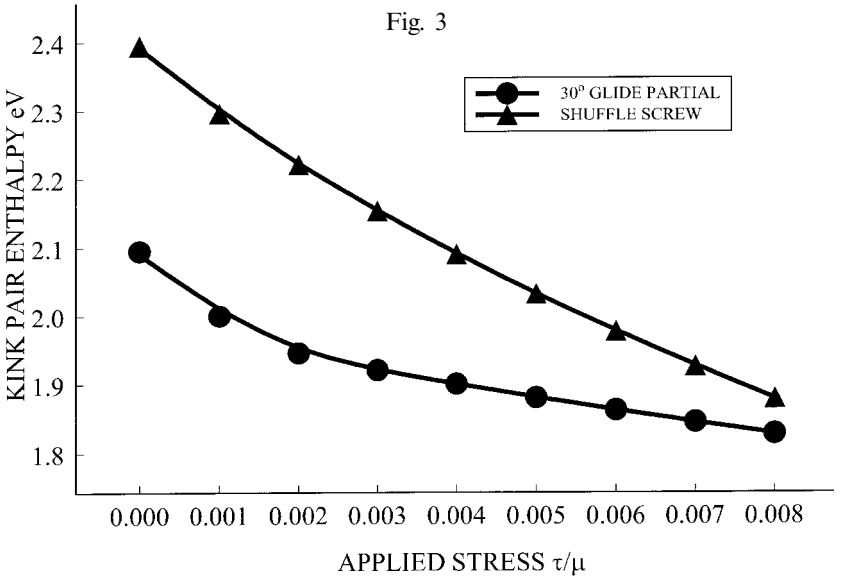
The kink pair mechanism for dislocation motion.

in which the total line energy $W(y)$ is the sum of the elastic line energy Γ and the Peierls energy $W_{PN}(y)$, b is the Burgers vector and y_0 is the position of the straight dislocation in equilibrium with the Peierls potential and the applied stress. The first two terms in the integrand of eqn. (1) represent the increase in line energy, and the third term is the work done by the applied stress. Equation (1) neglects the linear elastic interaction energy of the kinks and will therefore be a better approximation when the kinks are widely separated. Also neglected is any change in the dislocation core energy; this is expected to be small in comparison, as noted above. The integral in eqn. (1) can be minimized with respect to the shape $y(x)$ using Euler's equations. After some manipulation, an expression for the kink pair activation enthalpy can be obtained as follows (Dorn and Rajnak 1964):

$$U_{kp} = \int_{y_0}^{y_m} \left\{ W(y)^2 - \left[W(y_0) + \tau b(y - y_0) \right]^2 \right\}^{1/2} dy, \qquad (2)$$

where y_m is the point of maximum advance of the bulge. The integral in eqn. (2) is easily evaluated numerically. This has been done for the shuffle screw and 30° partial dislocations in silicon, using the values for $W_{PN}(y)$ calculated from the PN model (Joós *et al.* 1994) and a representative value of μb^2 per unit length for the elastic line energy Γ. This comparison between *total* shuffle and *partial* glide dislocations is justified because the stacking-fault energy in silicon is sufficiently low (about 50 mJ m^{-2}) that the partials behave independently (Alexander 1986). The small effect of the stacking fault on the activation process for the glide partial, the sign of which depends on whether the fault leads or trails the partial, is neglected. The results are shown in fig. 3. The activation enthalpy for the 30° glide partial is significantly smaller than that for the shuffle screw over the entire range of stresses up to that operative at the ductile–brittle transition temperature. This means that slip on the

Fig. 3



Kink pair activation enthalpies in silicon.

glide planes is expected to be preferred, in agreement with experiment. The limiting magnitudes of the calculated enthalpies at zero stress are comparable with the measured activation energy of 2·2 eV in silicon (Alexander 1986).

While the calculations are approximate, the preference for kink pair activation on the glide planes has a simple physical origin. The largest part of the activation enthalpy (2) comes from the additional length of dislocation which must be generated to form the bulge. This term depends on the line energy Γ, which is proportional to the square of the Burgers vector. Since the Burgers vector for shuffle dislocations is larger than that for the glide partials by a factor of $3^{1/2}$, the contribution of the line energy term to the activation enthalpy is proportionately larger. The magnitude of the line energy is an uncertain quantity. For straight dislocations, the line energy is given by

$$\Gamma = A\frac{\mu b^2}{4\pi}\ln\left(\frac{\Lambda}{\epsilon}\right), \tag{3}$$

where A is an elastic orientation factor of order unity, ϵ is an inner cut-off radius of the order of the lattice constant and Λ is the screening length of the dislocation substructure. It is conventional to choose an average value for Γ of $0{\cdot}5\mu b^2$ in metals, which have dislocation densities of order 10^{11} m^{-2} in the unworked state. In silicon the corresponding density is of order 10^8 m^{-2}, implying a larger screening length, and for this reason a value for Γ of μb^2 has been used. The results shown in fig. 3 are sensitive to the value chosen for Γ only in magnitude. If the value of Γ appropriate for metals is used, the enthalpies drop by about 0·5 eV, but the preference for nucleation on the glide plane remains.

This letter has advanced an elastic mechanism based on simple physical considerations in explanation of the observed preference in silicon and other dc materials for slip on the glide, rather than shuffle planes. To the best of the present authors' knowledge, no other explanations have been put forward. There may be other factors involved in the kink mechanism for dislocation motion in silicon which have not been considered here. For example, no consideration has been given to the role of the kink migration energy, which has been implicitly assumed to be substantially smaller than the nucleation mechanism. Detailed atomistic calculations (Bulatov, Yip and Argon 1995) using the Stillinger–Weber potential have identified a low-energy kink migration mode with an activation energy of 0·22 eV, consistent with this assumption. Electromechanical effects, including dislocation core reconstructions, have been ignored. These are likely to play a greater part in doped material than in pure silicon but may be of significance. Core reconstructions are necessary only for glide partials and would lower the ground-state energy, thereby favouring motion on the shuffle planes.

Acknowledgments

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