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Atomistic Determination of Cross-Slip Pathway and Energetics

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The mechanism for cross slip of a screw dislocation in Cu is determined by atomistic simulations that only presume the initial and final states of the process. The dissociated dislocation constricts in the primary plane and redissociates into the cross-slip plane while still partly in the primary plane. The transition state and activation energy for cross slip as well as the energies of the involved dislocation constrictions are determined. One constriction has a negative energy compared to parallel partials. The energy vs splitting width for recombination of parallel partials into a perfect dislocation is determined. The breakdown of linear elasticity theory for small splitting widths is studied. [S0031-9007(97)04444-X]

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The mechanical properties of metals are, to a large extent, controlled by the complicated structure and dynamics of dislocations and other defects. Linear elasticity theory is well suited to describe the long range elastic interactions between such defects but breaks down for processes involving dislocation cores. Such cases may require a treatment of all the atomic degrees of freedom.

Cross slip is the mechanism by which a screw dislocation changes glide plane and it plays an important role for plastic deformation, e.g., the onset of stage III in mechanical deformation. Several possible mechanisms have been proposed for the thermally activated cross slip [1–5], and recently the model proposed by Friedel [2] and Escaig [5] (FE) has been treated with linear elasticity theory [6,7]. During the cross-slip process the dislocation cores overlap, and the estimates of the activation energy vary appreciably depending on the cut-off procedures at the dislocation cores [6,8,9].

In this Letter we describe the results of an atomistic approach to the problem of cross slip of a dissociated screw dislocation in Cu. We use a path technique to determine the minimum energy transition path and the corresponding activation energy for cross slip. No presumptions about the actual cross-slip mechanism are made, and, furthermore, the atomistic approach enables a proper treatment of the dislocation cores.

The simulations show that cross slip proceeds in the following manner: Initially the dislocation is dissociated into two parallel Shockley partials in the primary glide plane. The partials bow in towards each other and recombine in a constriction which then redissociates in the other glide plane, the cross-slip plane. The redissociation creates two twisted constrictions on the dislocation, thus situating the dislocation partly in the primary plane and partly in the cross-slip plane. Finally the constrictions move apart, and the cross-slip process is complete with parallel partials in the cross-slip plane. This cross-slip mechanism corresponds qualitatively to the FE model. The twisted constrictions show a remarkable difference not discussed earlier with elasticity theory: One constriction has a negative energy compared to parallel partials. Simulations of straight dislocations enable determination of the energy vs splitting width for recombination of parallel partials into a perfect screw dislocation.

We consider a screw dislocation with Burgers vector $\mathbf{b} = \frac{1}{2}[110]$ in Cu, and denote the length of the perfect Burgers vector b. The computational cell is a parallelepiped of height h with the screw dislocation at the center. The cell can be seen as a stacking of (110) planes in an $\ldots ABAB\ldots$ sequence along the dislocation line, with $(\bar{1}11)$ planes and $(1\bar{1}1)$ planes as the nonorthogonal sides of the cell. Periodic boundary conditions are applied in the direction of the dislocation line, whereas the {111} surfaces are free. The side length of the computational cell perpendicular to the dislocation is denoted w. The largest system had $w = 37$ b (9.5 nm) and $h = 100$ b (26 nm) and consisted of 184 900 atoms.

The atomic interactions are described with a many-body potential derived from the effective-medium theory [10]. The potential reproduces the elastic constants and the intrinsic stacking-fault energy of Cu very well [9].

The simulated cross-slip process starts and ends in two equivalent configurations with parallel Shockley partials in either of the two possible glide planes, Figs. 1(a) and 1(f). Because of the high dimensionality of the configuration space ($\approx$550 000 degrees of freedom), it is highly nontrivial to identify the transition path and the corresponding transition state. We approach this problem with a configuration-space-path technique [11,12] in which the entire transition path is determined simultaneously. In this approach an initial guess for the transition path is relaxed according to the calculated forces until the

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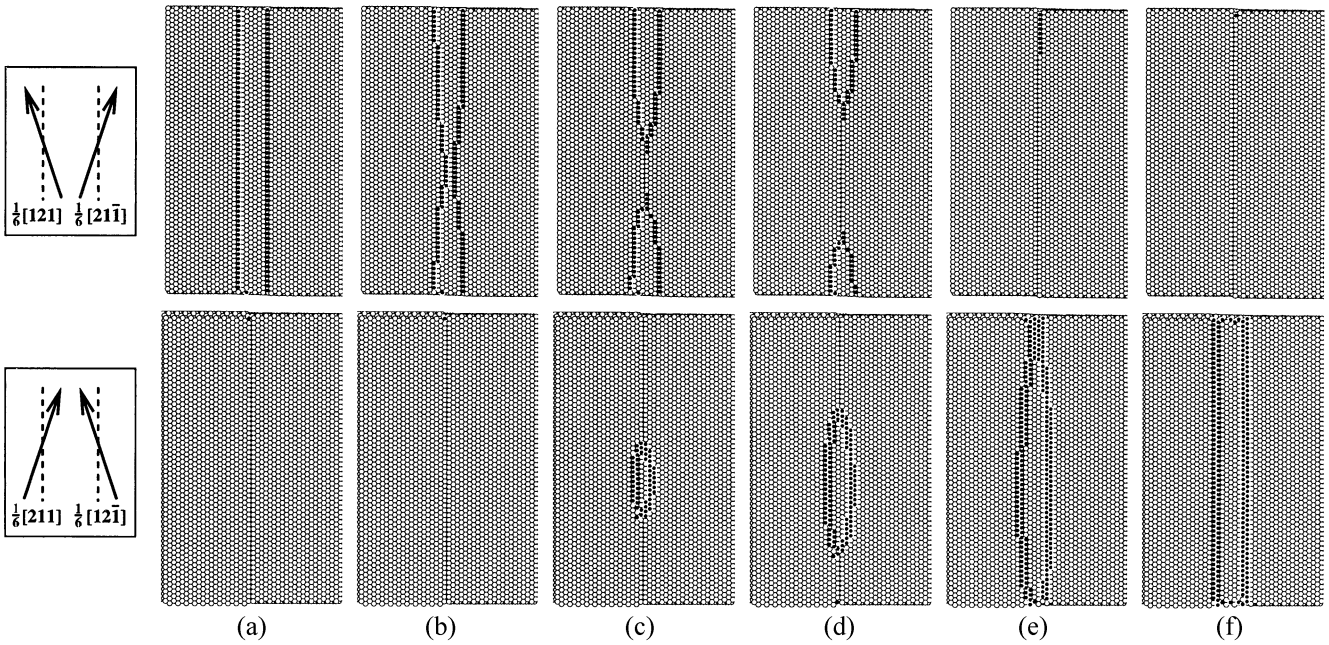

FIG. 1. Minimum energy transition path for cross slip of a screw dislocation. Top: primary glide plane $(1\bar{1}1)$. Bottom: cross-slip plane $(\bar{1}11)$. The Burgers vectors in each glide plane are indicated to the left. (a) Starting configuration with parallel Shockley partials in the primary glide plane. (b) Recombination into a constriction entirely in the primary plane. (c) Redissociation in the cross-slip plane. The upper constriction is screwlike, and the lower is edgelike. (d) Transition state with half of the dislocation in either glide plane. (e) Single plane constriction entirely in the cross-slip plane. (f) The cross-slip process is complete, with parallel Shockley partials in the cross-slip plane.

minimum energy path with vanishing forces perpendicular to the path is obtained. We use the nudged-elastic-band method [12] in which the path is represented by a sequence of replicas of the system. Each replica is relaxed perpendicular to the path using an energy minimization technique [13] keeping the replicas equidistantly spaced in configuration space. The initial path is a straight line in configuration space between the initial and final states discretized into 18–34 replicas of the system. It should be noted that no constraints on the cross-slip process are imposed, besides the specified initial and final states.

We have investigated cross slip for varying heights of the computational cell. In the first set of simulations h is either 60 or 100 b and the width is $w = 37$ b. These heights are large enough to allow the partials to be flexible in their glide planes, and thus to adopt nonstraight configurations. For the system with $h = 100$ b the path of 18 replicas consists of a total of 3.3×10^6 atoms. The smaller height ($h = 60$ b) allows simulation of 34 replicas (3.5×10^6 atoms) in the path, to check the influence of the number of replicas on the saddle point (activation) energy. The second set of simulations have $h = 5$ b (1.3 nm). The partials are kept straight, thereby enabling determination of the energy of the dissociated screw dislocation as a function of the splitting width. The simulations are carried out on a parallel computer, with each CPU handling 1–4 replicas.

Figure 1 shows the cross-slip process from the simulation with $h = 60$ b and 34 replicas in the path. The crystals have been cut through to display the primary glide plane in the top row and the cross-slip plane in the bottom row. The atoms close to the dislocation cores have been colored black, using a topologically based dislocation finding algorithm [14]. The cross-slip process is initiated by formation of a constriction in the primary glide plane, Fig. 1(b). The dislocation is still entirely in the primary plane, i.e., there is no sign of redissociation in the cross-slip plane as can be seen in the lower pane. We note that the initial configuration space path, in principle, possesses lattice translational symmetry along the dislocation line. However, small amounts of numerical noise in the atomic coordinates of the initial path are sufficient to break the symmetry, leading to the spontaneous constriction formation. In Fig. 1(c) the constriction in the primary plane has dissociated into two twisted constrictions creating a small loop in the cross-slip plane. Since the partials are no longer straight, their characters vary along the dislocation lines. We distinguish between the constrictions and denote the lower constriction "edgelike" and the upper constriction "screwlike" because of the characters of the partials close to the constriction. Figure 1(d) shows the transition state with half of the dislocation in either glide plane. The constrictions move apart, but due to the periodic boundary conditions they meet and form another single plane constriction, Fig. 1(e). The cross-slip process is complete in Fig. 1(f) with two parallel Shockley partials in the cross-slip plane. Figures 1(e) and 1(f) are equivalent to Figs. 1(b) and 1(a), respectively. The calculated minimum energy transition path agrees qualitatively with the mechanism proposed by Friedel [2] and Escaig [5].

For $h = 100$ b and $h = 60$ b the activation energies are 3.2 and 3.1 eV, respectively, independent of the number of replicas in the path. The activation energy for the smaller height is lower since the interaction between the constrictions is attractive. The energy of the single-plane constriction [Figs. 1(b) and 1(e)] is $\approx$1.6 eV.

It is interesting to examine the energetics in detail. To do so we plot the energy contributions from each (110) plane pair (AB) in the $\ldots ABAB \ldots$ stacking sequence along the dislocation line. The energy of an AB pair is the sum of the energies of all the atoms in that pair. The results for the four systems shown in Figs. 1(a)–1(d) are shown in Fig. 2. The AB pair energy of the initial configuration (a) is constant along the dislocation line and defines the zero point of the energy scale. The system with the constriction in the primary glide plane (b) shows a peak in the energy plot located $\approx$3 b below the actual position of the constriction. This is caused by the asymmetry of the dislocation characters on either side of the constriction. Below the constriction the partials acquire edgelike character, whereas above the constriction they are like screw dislocations. The asymmetry causes the energy plot to be asymmetrical and offsets the energy peak towards the edgelike part. Note that the energy of the screwlike part just above the constriction is lower than the energy of the two parallel partials with equilibrium splitting width. For a discussion of the influence of the dislocation characters on the energetics we refer to Ref. [9]. When the dislocation redissociates in the cross-slip plane two constrictions are formed. The constrictions are symmetrical with respect to the dislocation character on either side of the constriction, and the associated peaks in the energy plot [curves (c) and (d)] correspond exactly to the location of the constrictions. The edgelike constriction (to the left in Fig. 2) has a positive energy ($\approx$4 eV), whereas the screwlike constriction (to the right) has a *negative* energy (≈ -1 eV) compared to two parallel partials [15]. Hence, a configuration with a screwlike constriction on the dislocation is energetically favored over two parallel partials. The negative energy of the screwlike constriction is not included in the original approach by Escaig [5], because of the use of a simple line-tension model. The simulations [6,7] of the FE model calculate the cross-slip activation energy as the energy of the entire transition state, and the difference between the constrictions is not discussed. One can speculate that an alternative cross-slip mechanism could be cross slip of a screw dislocation terminated at a free surface, initiated by the formation of a screwlike constriction at the free surface. Such a cross-slip event has been observed in simulations, but the energy barrier for this process is at present not known [9].

The energy of the single plane constriction [Figs. 1(b) and 1(e)] has been calculated with linear elasticity theory [16,17]. The results for Cu are 2 eV (Ref. [16]) and 1.1 eV (Ref. [17]), which could be compared to our result of 1.6 eV. The present result for the cross-slip activation

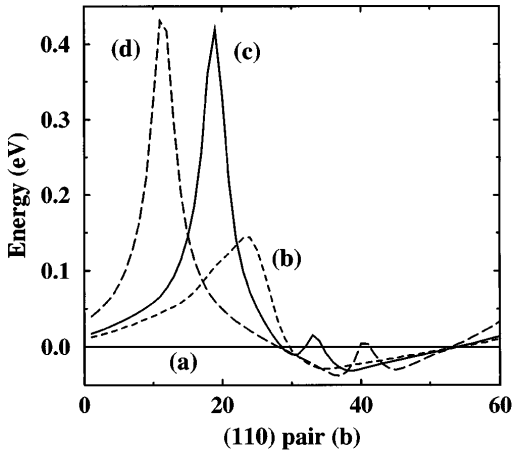

FIG. 2. Energy contribution from individual (110) plane pairs to the total energy of the four configurations shown in Figs. 1(a)–1(d). The energy of the parallel partials (a) defines the zero point of the energy. The energy of the single constriction (b) is 1.6 eV. Notice the asymmetry of the energy plot caused by the asymmetry in dislocation character below (edgelike) and above (screwlike) the constriction. After the redissociation into two constrictions, the energy increases to 2.9 eV (c) and 3.1 eV in the transition state (d). For (c) and (d) notice the qualitative difference between the two kinds of constrictions. The edgelike constriction has a positive energy, whereas the screwlike constriction has a *negative* energy.

energy is roughly 10% higher than the 2.9 ± 0.1 eV expected from simulations of isolated constrictions [18]. This is easily explained by considering the initial and final states. Ideally, these states should be systems with equilibrated partials perfectly centered in either glide plane. The true minimum energy configuration of such a system is, of course, a perfect crystal *without* the dislocation, and the dislocation is therefore balancing on a potential saddle point at the center of the cell. However, the time for displacement of the dislocation away from the center is much longer than the time for the relaxation of the dislocation core itself. This means that it is possible to obtain relaxed initial and final configurations with the dislocation displaced only very little ($\sim$1 b) away from the center of the crystal. Using a simple image dislocation construction for a parallelogram shaped computational cell of equal side length, it is possible to estimate the elastic energy associated with the displacement of the dislocation, and correct the activation energy accordingly. We have found that the displacement of the dislocation in the two glide planes was $\approx$0.9 b and this leads to a small ($\approx$0.2 eV) correction of the activation energy. The corrected activation energies become 2.9 and 3.0 eV for $h = 60$ b and $h = 100$ b, respectively, in good agreement with the result of simulations of single constrictions [9], and in reasonable agreement with simulations based on elasticity theory [6].

The simulations with short computational cells, $h = 5$ b, had 34 replicas in the path. For this height the periodic boundary conditions prevent the partials from bowing in towards each other, and cross slip therefore

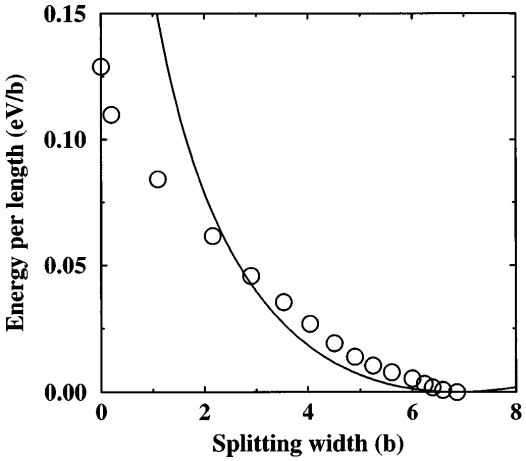

FIG. 3. Energy per length versus splitting widths for straight partials. The circles are the results from the simulation. The full line is the result from linear elasticity theory.

takes place in a homogeneous manner. The energy versus the splitting width d for recombination of two parallel Shockley partials into a perfect screw dislocation can then be found [19]. The results are shown in Fig. 3. The energy difference between Shockley partials separated by their equilibrium splitting width d_0 and recombined partials is $\Delta E = 0.13$ eV/b. A cross-slip mechanism including a segment of recombined perfect dislocation of some length in the primary plane has been proposed [1]. To complete the cross-slip process the perfect segment is suggested to bow out in the cross-slip plane under a shear stress. Within elasticity theory [17], the energy of a configuration with a perfect segment of length s can be estimated as $E_{SS} = E_0 + s\Delta E$, where E_0 is the energy of the single plane constriction. With our values for E_0 and ΔE we obtain a maximum length of the perfect segment of $\sim$(3 eV $-$ 1.6 eV)/(0.13 eV/b) = 11 b, too short to make the mechanism work for any reasonable shear stress.

Linear elasticity theory provides a simple expression for the energy as a function of the splitting width for straight partials

$$E_{\mathrm{el}}(d) = -K_i[\ln(d/d_0) + 1 - d/d_0], \qquad (1)$$

where K_i is the prelogarithmic interaction term between partials. In isotropic elasticity theory $K_{i,\mathrm{iso}} = \mu b^2/16\pi = 0.11$ eV/b, with Poisson's ratio equal to 1/3. More generally K_i is related to d_0 and the stacking-fault energy γ by $K_i = \gamma d_0 = 0.15$ eV/b, and this value can be seen as the anisotropic result. Relation (1) is plotted as the full line in Fig. 3 with $K_i = 0.15$ eV. For splitting widths less than 1 b the logarithmic divergence stemming from the use of singular dislocations dominates. For splitting widths larger than 2 b the agreement is quite good, and the small discrepancy is readily explained. Relation (1) is derived under the assumptions of constant stacking-fault energy and nonoverlapping dislocations. A plot of the displacements over the glide plane shows, however, that the partials do in fact overlap for all splitting widths.

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[1] G. Schoeck and A. Seeger, *Report on the Conference of Defects in Crystalline Solids, Bristol, 1954* (The Physical Society, London, 1955), p. 340.
[2] J. Friedel, in *Dislocations and Mechanical Properties of Crystals,* edited by J. C. Fisher (Wiley, New York, 1957).
[3] R. L. Fleicher, Acta. Metall. **7**, 134 (1959).
[4] P. B. Hirsh, Philos. Mag. **7**, 67 (1962).
[5] B. Escaig, in *Dislocation Dynamics,* edited by A. R. Rosenfeld *et al.* (McGraw-Hill, New York, 1968).
[6] M. S. Duesbery, N. P. Louat, and K. Sadananda, Acta. Metall. Mater. **40**, 149 (1992).
[7] W. Püschl and G. Schoeck, Mater. Sci. Eng. **A164**, 286 (1993).
[8] G. Saada, Mater. Sci. Eng. **A137**, 177 (1991).
[9] T. Rasmussen *et al.*, Phys. Rev. B **56**, 2977 (1997).
[10] K. W. Jacobsen, P. Stoltze, and J. K. Nørskov, Surf. Sci. **366**, 394 (1996); K. W. Jacobsen, J. K. Nørskov, and M. J. Puska, Phys. Rev. B **35**, 7423 (1987).
[11] R. Elber and M. Karplus, Chem. Phys. Lett. **139**, 375 (1987).
[12] G. Mills, H. Jónsson, and G. K. Schenter, Surf. Sci. **324**, 305 (1995).
[13] The dynamics is ordinary molecular dynamics with the following modifications. Only the forces perpendicular to the path are used to relax the path. Along the path the replicas are kept separated by spring forces between the replicas. To minimize the energy the following scheme is applied. If the dot product between the force and the momentum is less than zero, the momentum is zeroed. Otherwise, only the component of the momentum parallel to the force is used.
[14] J. Schiøtz, Ph.D. thesis, Technical University of Denmark, 1995.
[15] The constriction energy is defined as the sum of energy contributions from (110) pairs closest to this constriction.
[16] A. N. Stroh, Proc. Phys. Soc. London Sect. B **67**, 427 (1954).
[17] W. Püschl, Phys. Status. Solidi B **162**, 363 (1990).
[18] Unpublished results. The simulations of single constrictions are described in Ref. [9].
[19] The splitting widths are found by fitting two Gaussian distributions to the pressure in the glide plane, and defining the width to be the distance between the centers of the two Gaussian distributions.