Destabilization of dislocation dipole at high velocity

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Under mechanical deformation of very high strain rates, it is expected that dislocations may move very fast (being subsonic, transonic, or even supersonic). As a result, two dislocations may approach each other at high velocities. Our earlier analyses of linear elasticity indicate that a dipole is destabilized when the approaching velocity is high enough—even below the speed of sound. In this letter, using the molecular dynamics method, we demonstrate that a dipole indeed can be destabilized above a critical velocity, and stable below that. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1421425]

In solids under very high strain rate deformation, as high as 10^5-10^6 per second, dislocations are expected to move very fast.[1] With the advent of high-speed computers, the dislocation dynamics simulations[2–5] have become a feasible means of revealing the microstructure formation and evolution of dislocations. In all these approaches of dislocation dynamics, the long-range elastic interactions of dislocations are reasonably well treated—although based on isotropic elasticity. However, the short-range interactions are far from being well established. Not knowing the details of dislocation–dislocation interaction at short distances, various phenomenological rules have been assumed—some are confirmed by experimental observations of the final dislocation structure. The other aspect of dislocation interactions—velocity dependence—is also largely unknown in dislocation dynamics simulations. In an attempt to address the velocity dependence, we have formulated the dipole stability as a function of approaching velocity of two dislocations, based on the linear elasticity theory.[6] Our study indicates that a dislocation, approaching the other one at a high speed, overshoots the stable dipole configuration. In this linear elastic formulation, idealized assumptions—such as the dislocation dragging coefficient being constant—have been made. A rigorous atomistic study of this dipole destabilization process would provide a more definite conclusion and a deeper insight.

Recent molecular dynamics simulations in tungsten[7] have shown that a transonic dislocation is possible. The realization of such a transonic dislocation makes it possible for two dislocations to approach each other at very high velocities, although still below the speed of sound. The dipole destabilization reported in Ref. 6 has been questioned in several workshops (see the workshop report, Ref. 1, as an example). The major concern is whether the destabilization is physically possible at high velocities, since the dragging could become extremely viscous. To address this concern, we study the dipole stability at the atomic level.

The molecular dynamics simulation cell is similar to that used in Ref. 7, and is schematically shown in Fig. 1. Like before,[7–9] tungsten is taken as a prototype of metals in this study. The negative dislocation is generated by adding two extra (211) planes along the [111] direction to the lower half of the simulation cell, and the positive dislocation is created by pushing the piston at the speed of 75 m per second. The glide planes of the two dislocations are separated by $\sim 14b$—b being the Burgers vector. Before the two dislocations (positive and negative) reach the 45° configuration, the top piston is removed from the simulation cell—the atoms right below the left part of the top piston are also removed. This setup eliminates the effects of external stress during the dipole formation, and further slow down the dislocations by allowing the strained crystal to relax. If the destabilization is realized with this effect, it is more likely to be the case when the slowdown effects are absent. The piston at the bottom part is still fixed, and the periodic boundary condition is applied along the direction into the paper. During the simulations, the temperature is kept below 35 K, to eliminate the effects of thermal fluctuations. This temperature control is accomplished by applying the Langevin force to atoms in the dynamic region.[10] In each simulation, the position of a dislocation at each moment is defined as the coordinate—along the [111] direction—of the most distorted extra half plane.

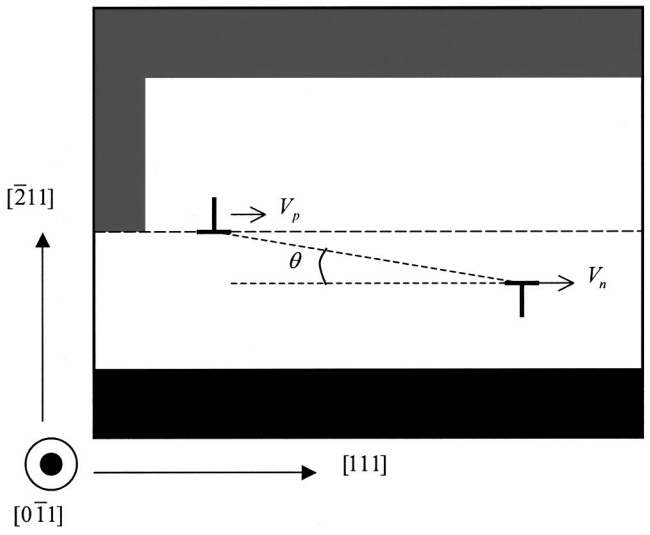

FIG. 1. Schematic of simulation cell, with crystal orientations, velocities of positive (V_p) and negative (V_n) dislocations, and relative angle indicated. The light shade indicates the top piston, and the dark shade the bottom piston.

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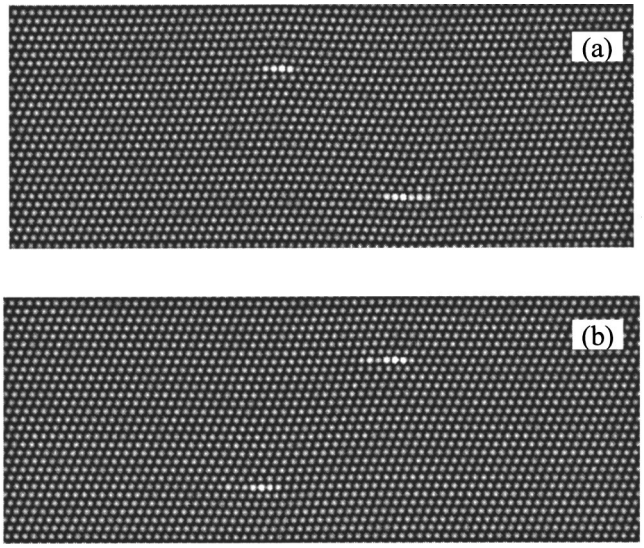

FIG. 2. Snapshots of a portion of the (011) cross section with the relative angle being (a) 45° and (b) 135°, when the relative velocity is $0.93C_t$ at 45°. The dislocation positions are indicated by the locations of the lighter atoms, and dislocation on the top is positive while the one at the bottom is negative.

The velocity is simply the derivative of the position as a function of time.

Two snapshots, corresponding to the 45° configuration, at which the relative velocity is $0.93C_t$—the speed of sound C_t being 2850 m/s,[7] and the final 135° configuration, are shown in Figs. 2(a) and 2(b). Once the dipole configuration at 45° is overshot, it is considered destabilized—other dislocations will interfere in the ensuing interactions. In another simulation, the relative velocity is $0.89C_t$ when the two dislocations are at the 45° configuration. Finally, the two dislocations stabilize at the 45° configuration, after an overshoot. A critical velocity, therefore, exists and its value is between 0.89 and $0.93C_t$ for the simulated configurations. Returning to the question raised in Ref. 6, we have shown that the strong dragging does affect quantitatively the dipole destabilization—not so many oscillations as in Ref. 6, but it does not change the conclusion on the existence of the destabilization. To test the effects of other parameters, we have simulated this process at different separations of glide planes. The critical velocity is found to go up with the separation of two glide planes. This is due to the larger amount of energy dissipation due to dragging over longer distance, when the separation is larger.

Details of relative angle and relative velocity of the two dislocations in Fig. 2, as a function of time, are shown in Figs. 3(a) and 3(b). Note that the 45° configuration is taken to be the starting point of time—about 9 ps in Fig. 3—in our analyses. This choice takes the advantage of supersonic dislocations to study the behavior of fast, but subsonic, dislocations. In the lower velocity case, it is interesting to note that the relative angle has gone up to 105°—much beyond 90°; but eventually, the relative angle goes back to 45°. Because of the finite speed of stress field propagation, the positive dislocation experiences in reality the stress field of negative dislocation at angle θ ($\theta<90°$), although the apparent angle is 105°. The distance involved in the propagation is on the order of nanometers, and the time picoseconds, in our simulations.

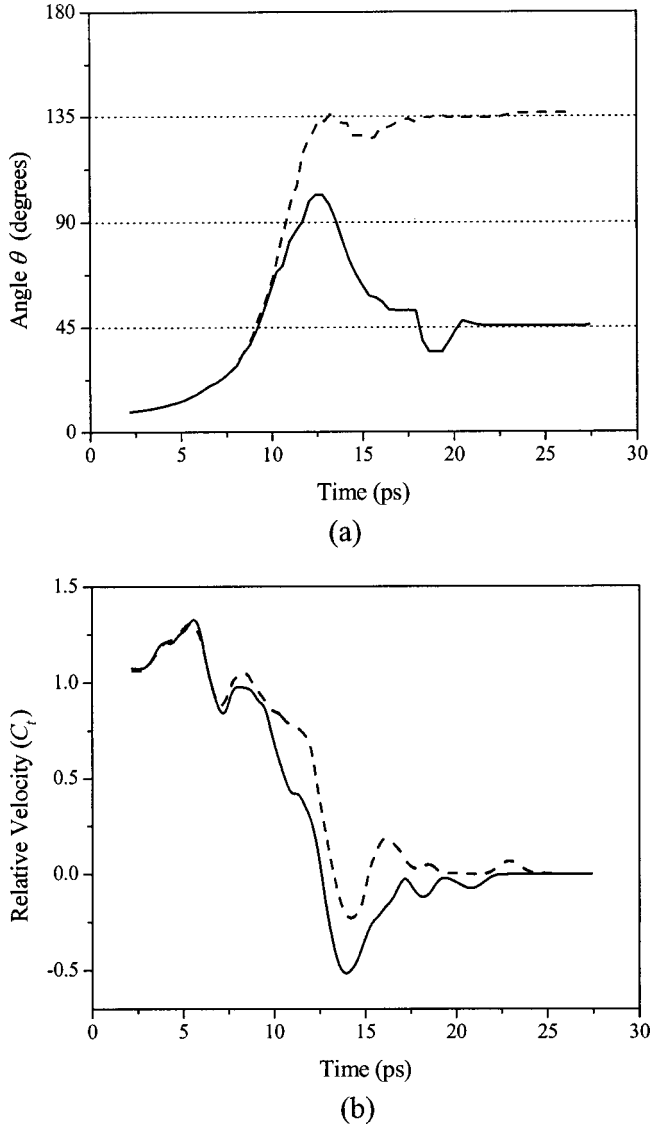

FIG. 3. (a) Relative angles of the two dislocations and (b) corresponding relative velocities, as a function of time. The broken line represents the case of higher relative speed, and the solid line the lower relative speed.

More rigorous elastic analysis is beyond the scope of this letter and will be published separately. However, an analysis of possible artifacts in the simulations is necessary. The first concern is the boundary conditions. The removal of the top piston before the two dislocations reach 45° is to eliminate unknown external stresses in the two simulations. As a result, the surface effects exist, but they are similar for both cases, during the interaction of the two dislocations. Because the glide planes are horizontal, the top and bottom surfaces contribute little image shear stress along the moving direction of the dislocations. Because the two dislocations are near the center of the simulation cell during their interaction, the image shear stress is on the order of $0.003\,\mu b^2/2\pi(1-\upsilon)$, μ being shear modulus and υ Poisson's ratio. This value is comparable to the elastic interaction of the two dislocations at 2° away from their stable configurations (at 45° or 135°). Therefore, the free surfaces will not substantially alter the phenomena observed.

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