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STEADY STATE DISLOCATION MOTION VIA MOLECULAR DYNAMICS ★

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Nonequilibrium molecular dynamics is applied to the generation and steady propagation of edge dislocations. "Normal" propagation at about one-third the longitudinal sound speed, transonic propagation at nine-tenths that speed, climb, and multiplication are all observed.

The old idea [1] that plastic flow occurs through dislocation motion became accepted when Gilman and Johnston observed this motion directly [2]. Static calculations, both in the triangular (two-dimensional) and close-packed (three-dimensional) lattices have established the least-energy dislocation-core structure [3, 4]. More recently, with the help of fast computers, efforts have been made to simulate the motion of dislocations numerically. In an interesting series of papers, Weiner [5] has studied the generation and propagation of dislocations in a square lattice of particles interacting with noncentral forces. These noncentral forces are used primarily to lessen the computational work. Similar forces have also been used by Celli and his coworkers in analyzing, analytically, the propagation of a screw dislocation in a simple cubic lattice [6].

We have developed a method of following the steady progress of dislocations through crystals in which central forces are used. Such forces have been successful in describing the equilibrium and nonequilibrium properties of simple insulators, such as argon, and are conceptually the simplest model for explaining the equilibrium and nonequilibrium properties of real materials [7].

The central forces and the close-packed structure insure mechanical stability and have recently been used to study fracture [8]. The close-packed triangular lattice structure is, for long waves, elastically isotropic. This feature of the lattice makes it particularly appropriate for comparisons with (isotropic) continuum elasticity calculations. Further, the frequency distribution [9], free energy [10] and surface-mode distribution [11] are all known analytically for this lattice.

Our own calculations are usefully thought of in three distinct phases: generation, relaxation, and propagation. A dislocation core is generated by choosing particle coordinates as predicted by macroscopic elasticity theory [12]. This initial choice is then relaxed, by adding viscous dissipation to the solution of the equations of motion. During the relaxation process extended Hooke's law forces are used, with an attraction extending to $1.40d$, where d is the stress-free interparticle spacing. The static core configurations were examined to verify the well-known logarithmic dependence of energy on number of particles [4]. Next, a crystal was generated which would make it possible to observe steady motion of the dislocation. This was done by adding many columns of fresh particles to the region adjacent to the dislocation core. Finally the entire structure was relaxed. During the relaxation a shear strain was simultaneously induced. At each time step, and after solving the equations of motion for the particles, an algorithm of the form:

$$r_n = [n\, r_{\mathrm{flat}} + (M - n)\, r_n]/M\,,$$

was applied to the upper and lower boundary rows of particles. The strained coordinates desired for these particles after M time steps, r_{flat}, were chosen to correspond to a uniform shear. Thus the top of the crystal was shifted to the right, relative to the bottom. During the M-step relaxation process the energy of the system reaches its minimum value subject to the fixed-boundary constraint.

The edge dislocation is then propagated by chang-

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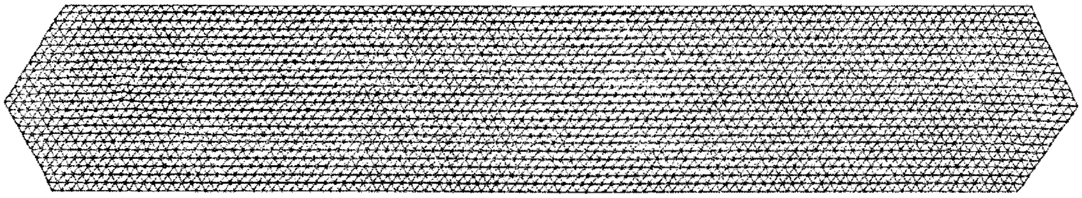

Fig. 1. A 2580-particle crystal containing an edge dislocation moving at a velocity 1/3 the longitudinal sound speed. The forces rise to a maximum at $1.15d$ and then vanish at $1.30d$. The initial strain is $4/\sqrt{3} \times 23$. The final strain is $2/\sqrt{3} \times 23$.

ing the extended Hookean forces to piecewise linear forces which rise to an attractive maximum and then fall continuously to zero. The maximum-force distance was varied from $1.1d$ to $1.2d$. The attractive forces then fall continuously to zero, vanishing at a distance ranging from $1.2d$ to $1.4d$. A typical 2580-particle crystalline with a single edge dislocation is shown in fig. 1. The dislocation propagates from right to left at approximately one-third the longitudinal sound speed. Fixed-stress, as opposed to fixed-displacement, boundary conditions can also be used in such calculations, but boundary deformation by Rayleigh waves leads to nonsteady propagation, making the plastic flow more difficult to analyze.

Several kinds of results have been obtained. At low levels of shear stress, and with a range of forces which is not too short, "normal" propagation of the dislocation occurs. The dislocation moves across the crystallite steadily with a fluctuation in speed between lattice sites of order 10%. The average velocity can typically be determined within about 1% in this case. These low-velocity "normal" results can be roughly described by the relation

$$v/c = 0.47 \exp[-0.028G/\sigma] ,$$

where c is the transverse sound velocity and G is the shear modulus. The average stress driving the dislocation motion, σ, is computed by averaging the shear stress ahead of the dislocation with that behind it. The stresses differ due to the stress relaxation induced by the dislocation motion. This relaxation amounts to a reduction in shear strain of b/h where $b(=d)$ is the Burger's vector of the dislocation and h is the height of the crystallite.

At higher stresses, or with shorter-ranged forces, interesting nonlinear effects are seen. Dislocation climb, in which the "extra plane" of particles grows

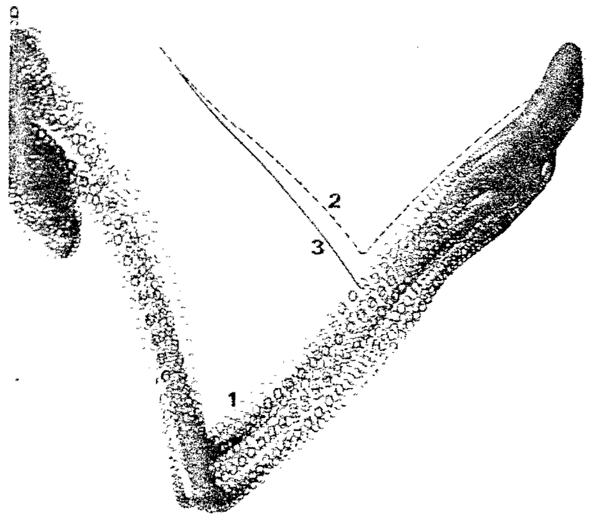

Fig. 2. Motion in the region of the dislocation core. The particles' displacements are plotted according to (1) molecular dynamics, (2) elasticity theory for the infinite plane, (3) elasticity theory for a finitewidth strip [dislocation velocity = $0.345d\,(\kappa/m)^{1/2}$]. Trajectories for 21 successive particles lying just above the dislocation slip plane are shown. The motion proceeds along these trajectories from right to left.

by abstracting particles from the lattice results in a set of nearly-evenly-spaced vacancies appearing in the crystallite. Typically the dislocation "climbs" at about one-tenth the propagation velocity. New pairs of dislocations are sometimes generated at high stress, and occasionally dislocations deform to form pentagonal or hexagonal voids in the crystal, bringing the motion to a halt. Under certain circumstances unusually high velocities have been observed. For example, with a shear stress of 0.0682 (in units of the nearest-neighbor Hookean force constant κ) and a maximum force at $1.14d$, transonic propagation at 89% of the longitudinal sound speed was observed.

This flatly contradicts the predictions of linear elastic continuum theory that dislocations cannot be accelerated beyond the transverse sound speed. Both Weiner's model calculations and Mitchell's experiments [13] have yielded propagation velocities in or near the transonic regime.

In order to compare these results with the predictions of elastic theory we show the displacement of typical particles in the core according to the predictions of molecular dynamics and elasticity theory. It should be noted that the elastic-theory predictions are qualitatively correct. In detail the figure shows that the actual dynamical trajectories have a considerably greater amplitude than the theoretical prediction. Also the front to back symmetry of the elastic predictions is absent in the dynamical trajectories. Two different elasticity-theory solutions are shown. One is the classical solution, as given in Hirth and Lothe's text [12], giving the displacements in a static dislocation embedded in an infinitely extended continuum. The other elastic solution gives the fully-dynamic motion of an edge dislocation in a finite-width strip. This solution was arrived at simultaneously and independently by two groups of workers [14] and makes it possible, for the first time, to compare elastic theory and molecular dynamics for the same material and boundary conditions. The new solution, coupled with the steady-state propagation technique described here, opens the way to the formulation and solution of dynamical flow problems which can be compared directly with atomistic calculations.

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