PLASTIC DISLOCATION MOTION *VIA* NONEQUILIBRIUM

MOLECULAR AND CONTINUUM DYNAMICS

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PLASTIC DISLOCATION MOTION *VIA* NONEQUILIBRIUM MOLECULAR AND CONTINUUM DYNAMICS*

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The classical two-dimensional close-packed triangular lattice, with nearest-neighbor spring forces, is a convenient standard material for the investigation of dislocation motion and plastic flow. Two kinds of calculations, based on this standard material, are described here:

Molecular Dynamics simulations, incorporating adiabatic strains described with the help of *Doll's Tensor*, and

Continuum Dynamics simulations, incorporating periodic boundaries and dislocation interaction through stress-field superposition.

I. INTRODUCTION

Continuum mechanics cannot furnish a complete understanding of the flow and wear of solids. Though the continuum picture *does* properly incorporate the conservation of energy and the increase of entropy it lacks a description of the microscopic lattice structure, and the defects present in the lattice. A satisfactory understanding of flow and wear can only emerge from models incorporating the creation, interaction, motion, and annihilation of crystal defects. Neither the static nor the dynamic structure of lattice defects is contained in a purely macroscopic continuum theory. Such a theory predicts, for instance, stress-field divergence in the dislocation-core region where a precise knowledge of the (finite) forces is necessary for accurate dynamical calculations.

At the same time, the vast number of lattice defects, and the complexity of their mutual interactions, make it necessary to develop a descriptive continuum picture in which stress, strain, and defect density *do* play fundamental roles, replacing the underlying atomic and electronic coordinates and momenta. This change of scale, from microscopic to macroscopic, can only take place through an understanding of microscopic defect physics.

Although experimental shockwave physics is developing rapidly[1], the resolution of structural probes is still limited to lengths and times somewhat larger than atomic spacings and vibration periods. In view of the experimental difficulties involved in probing, quantitatively, the microscopic scales of dislocation cores, vacancies, and crack tips, and in determining from these, indirectly, the form of the forces between the interacting atoms and electrons, *computer experiments*, as opposed to laboratory experiments, represent a much simpler path to understanding lattice defects. Computers are required to supplement theoretical analysis because even the classical N-body problem is complex.

Computer simulations are limited to regions perhaps 100 atomic spacings wide, and to times of 1000 vibration periods, so that an enormous extrapolation remains to be made between the microscopic computer experiments and the macroscopic scales of interest in engineering practice. Even so, recent work on the rapid shock deformation of fluids[2] and solids[3] shows convincingly that computer simulations can establish defect configurations and deformation mechanisms.

The scale gap, between microscopic computer experiments and macroscopic laboratory experiments, makes it worthwhile to develop "intermediate scale" simulation techniques. On the intermediate scale the defects themselves, rather than the underlying atoms and electrons, are treated individually.

These intermediate-scale simulations have meaning only to the extent that the assumed defect properties are firmly supported by atomistic calculations.

Operational intermediate-scale theories of plasticity, based on dislocation dynamics, are not yet in existence. On a slightly more macroscopic level, where dislocations are described by a local density function, some very promising work *has* been done. Werne(4) and Stout(5), both at Livermore, have developed macroscopic theories from this basis. Werne's work is more thorough. He has incorporated his model for plastic flow, based on dislocation density, into continuum solid-mechanics simulations of simple mechanical tests. A long-range goal of our present work is to assess the accuracy of the assumptions used in macroscopic simulations such as Werne's.

Surprisingly little simulation work has been carried out with dislocations in view of the tremendous theoretical effort(6-9) that has been expended on characterizing dislocation structure, interaction, and motion. Undoubtedly the initial motivation for the theoretical work was understanding plastic flow in metals. Much theoretical work is now pursued with the apparent goal of mathematical elegance, not physical relevance, so that despite dozens of texts and thousands of articles, we still do not know why dislocations travel at the speeds they do and we cannot predict how many will be present in a particular flow. There is too little contact between the engineers carrying out solid mechanics calculations describing real materials and the "applied" (meaning purely theoretical) mathematicians dwelling in the archives of continuous functions. The work described here is part of a long-term program to help bridge the gap between the two disparate points of view, experimental and theoretical.

The microscopic atomistic computer simulations should be viewed as experiments in their own right, on unusually well-defined materials with reproducible properties. The limitations on these computer experiments are nicely complementary to those constraining real laboratory experiments, so that by achieving correlations between the two classes of experiments, one may achieve understanding of real materials.

Because crystal dislocations are the simplest entities responsible for plastic(meaning irreversible) flow, we have chosen to study these lattice defects in detail. Figure 1, taken from a dynamical microscopic simulation, shows an edge dislocation propagating through a triangular-lattice crystal. The top and bottom boundaries of the crystal are held fixed, so that the force driving the dislocation motion is the irreversible conversion of stored strain energy into heat. The dislocation can be seen most easily by viewing Figure 1 obliquely. The defect corresponds to a place, near the righthand side of the figure, at which a diagonal line of close-packed atoms comes to an end.
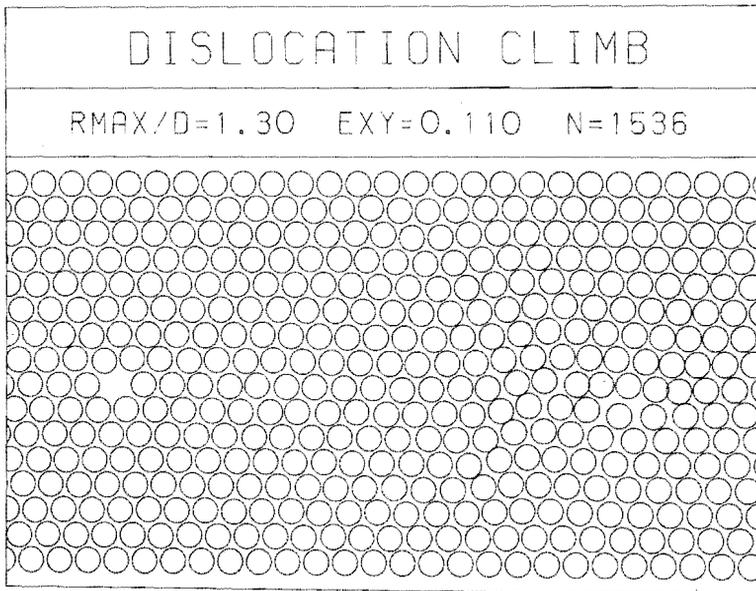
Figure 1.   Edge dislocation propagating in a triangular-lattice crystal.

In three-dimensional crystalline materials both edge dislocations, such as that shown in Figure 1, and screw dislocations can occur. In two-dimensional crystals only edge dislocations can exist, for screw dislocations involve out-of-plane displacements. The edge dislocations are mathematically more complicated, at least from the standpoint of continuum elasticity, but we consider them here because they dominate plastic flow in three dimensions as well as in two. We limit ourselves to the two-dimensional case, for simplicity, ignoring the complications associated with three-dimensional geometry, electrons, and quantum dynamics. Even so, the calculations we describe challenge even present day computers.

Prior to the advent of fast computers peculiar models, such as that of Frenkel and Kontorova, were analyzed. Such models were chosen to simplify the analytic work, but bore only a slight resemblance to many-body systems composed of similar interacting particles. These artificial models persist today, largely due to inertia and lack of imagination. Some work has been carried out on dislocations in atomic lattices. Celli's work on three-dimensional screw dislocations(10-11), and Weiner's work on a two-dimensional material with angle-dependent forces(12) exemplify recent efforts.

At present there is a flurry of interest in dislocations. This interest was generated by ill-founded speculation that these defects are present, in large numbers, in melting two-dimensional solids. Fortunately thoughtful calculations are beginning to emerge(13-15), so that the temporary pedagogical

setback suffered by melting theory will ultimately be more than offset by our enhanced understanding of dislocations in solids.

In characterizing complex phenomena it is useful to have a standard material for study, both simple and reproducible. In three-dimensional equilibrium and transport calculations, first the hard-sphere potential, and later the Lennard-Jones 12-6 potential have played this role. In this paper we choose, as our standard plastic material, a triangular lattice in which neighboring particles interact with suitably truncated Hooke's-Law springs. Much is already known about this system--that work is summarized in Section II. Sections III and IIII are devoted to atomistic descriptions of dislocations, first individually, and then in groups, using classical molecular dynamics to solve the equations of motion for the underlying crystal lattice. In Section V we describe a method for treating the mutual interaction and motion of many (hundreds) dislocations using continuum dynamics. This intermediate-scale simulation incorporates interaction information from the single-dislocation molecular dynamics work.

The main novel features of the dislocation work described here are (i) the use of Doll's Tensor in solid-phase adiabatic flows, (ii) the use of periodic boundary conditions in the continuum calculations, (iii) the direct measurement of the equation of motion for dislocations--velocity as a function of stress, and (iiii) the incorporation of kinetic stress-linked creation and annihilation of dislocations.

II. THE TRIANGULAR LATTICE, A STANDARD MATERIAL FOR PLASTIC FLOW

The theoretical microscopic analysis of metal plasticity is complicated by several unpleasant facts. The crystals contain electrons, which must be described by quantum mechanics, and typically include impurities, grain boundaries, and microcracks, all in an inhomogeneous anisotropic matrix. So far a useful computational quantum dynamics has not been developed. Considerable effort is still being devoted to equilibrium quantum fluid properties(16). Accordingly, *classical* mechanics must be used in atomistic dynamic simulation. Even with this simplification, the force laws which have proved useful in correlating equilibrium fluid and solid properties would require extremely large systems for quantitative plastic flow simulations. Numerical studies, using the Lennard-Jones 12-6 potential, indicate a relatively large 10% change in dislocation velocity as the crystal width is increased from 12 to 18 atomic spacings(17). The corresponding *three*-dimensional crystals, with 10,000 atoms, represent the practical limit for present day simulations.

Because the simulations required to test approximate theories are time-consuming and relatively expensive, a voluminous and imaginative literature has developed around the idea that dislocations are responsible for plastic flow. Much of this work bears little connection either to experiment or to well-defined mechanistic simulations. We believe that the numerical techniques necessary to advance our theoretical understanding of plasticity *do* now exist. Rather than working directly with experimental data--from systems with unknown atomistic forces--or with calculations based on *ad hoc* models, we propose to explore a mechanistic model system with forces chosen for simplicity. We choose to study an elastic structure which is (i) stable, (ii) isotropic, and (iii) relatively free of boundary effects. The *triangular* lattice with nearest-neighbor Hooke's-Law springs is mechanically *stable* because any deformation causes some of the springs to stretch, creating a restoring force. The nearest-neighbor square lattice lacks this feature. The triangular lattice is elastically *isotropic* too. The inherent four-fold invariance associated with shear deformation and the physical six-fold symmetry of the lattice are consistent only for a shear modulus which is independent of angle. The *minimization of boundary effects* is empirical, and depends, as discussed on the next page, on the form of the forces.

Because linear dynamical equations are particularly simple to analyze, we choose interatomic forces which are linear in the displacement δ from the minimum-energy rest length d_o:

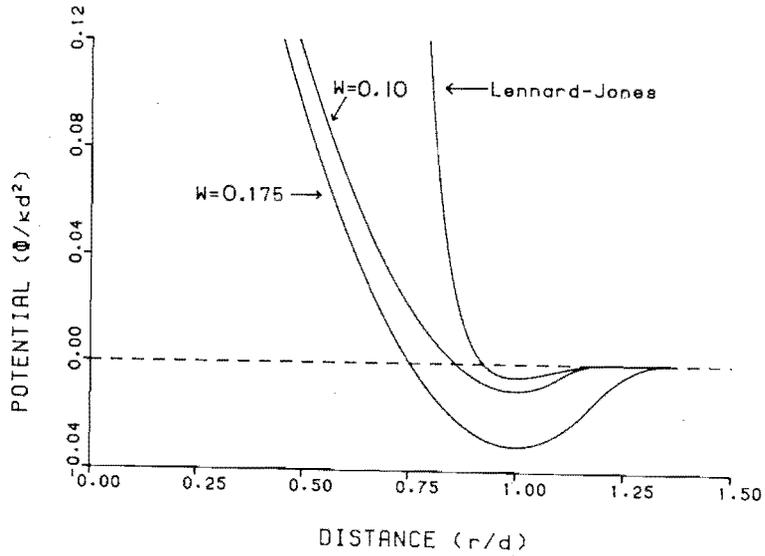$$F \equiv -\kappa\delta \quad \text{for} \quad \delta \equiv r - d_o < w. \tag{1}$$

Figure 2. Two Hooke's-Law pair potentials and the truncated Lennard-Jones pair potential. The distance and energy scales depend upon the fixed length d and the interatomic force constant κ. The parameter w, expressed in units of d, gives the "width" of the Hooke's-Law bowl.
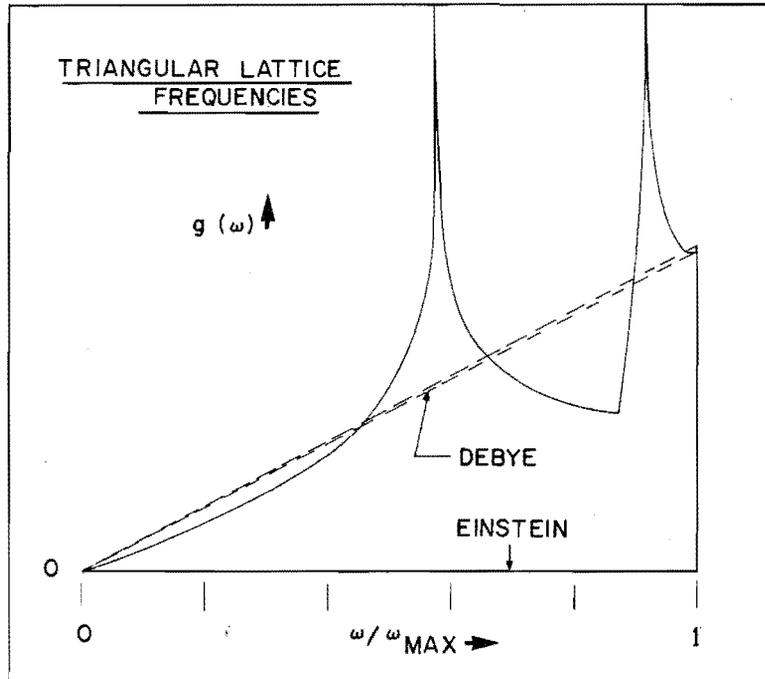

Figure 3. Distribution of vibration frequencies for the stress-free, two-dimensional triangular lattice. The Einstein approximate distribution consists of a single frequency. The Debye approximate distribution consists of either a single linear branch, of the type shown in the figure, or a combined distribution, obtained by adding two such branches together.

The Hooke's-Law force must be cut off at a distance somewhat greater than d_0 to avoid the complication of second-and-higher-neighbor interactions. We do this by continuing the force beyond the distance of greatest attraction, $d_0 + w$, where the stretch in the spring is w, to a final stretch of 2w, where the force vanishes:

$$F \equiv -\kappa(2w - \delta) \quad \text{for} \quad w < r - d_0 < 2w. \qquad [2]$$

The parameter w, which gives the range of the force, remains to be chosen. Which value of w is simplest? We have chosen $w = 0.15d_0$ because this value leads to simple defect structures and to relatively small boundary effects. This value is not very different from that suggested by the attractive-force maximum in the more-realistic Lennard-Jones 12-6 potential. The Lennard-Jones potential inflection point(force-law maximum) occurs just beyond a stretch of $0.1d_0$. The pair potentials corresponding to the force law [1]+[2] are compared with the truncated 12-6 potential in Figure 2.

What properties of the triangular lattice are already known? Dean(18) worked out the dependence of the vibrational frequencies on wavelength and direction(the "dispersion" relation), giving, implicitly, the complete frequency distribution. The calculated distribution of frequencies, at the stress-free density, is shown in Figure 3. This distribution has two quali-tatively interesting features shared by two-dimensional crystals(19). First, the frequency distribution diverges, weakly, at two characteristic frequencies. Second, the mean-squared displacement of an atom about its lattice site, computed from the frequency distribution, diverges!

$$\langle r^2 \rangle = (2kT/m)\langle \omega^{-2} \rangle \to O(\ln N), \qquad [3]$$

for large N-atom crystals. This well-known divergence is a consequence of the relatively large number of low-frequency modes. According to the two-dimensional Debye model(correct for long waves) the number of frequencies in a range dω about ω is proportional to ω. Thus the average of ω^{-2}, over all frequencies, diverges logarithmically in the low-frequency limit.

A more detailed look (See Figure 4) indicates that this divergence is too weak to have macroscopic consequences. The *relative* rms displacement, relative to a macroscopic length that scales with crystal size, *does* approach zero, as $N^{-1/2}$ for large N.

Dean's zero-stress calculation can be generalized to other densities(20). The results are surprising. First, the thermal contribution to the pressure computed classically, from the density-dependence of the vibrational frequencies, is negative(21). Thus the crystal *contracts* on heating. The negative contribution of the thermal motion to the pressure increases in magnitude
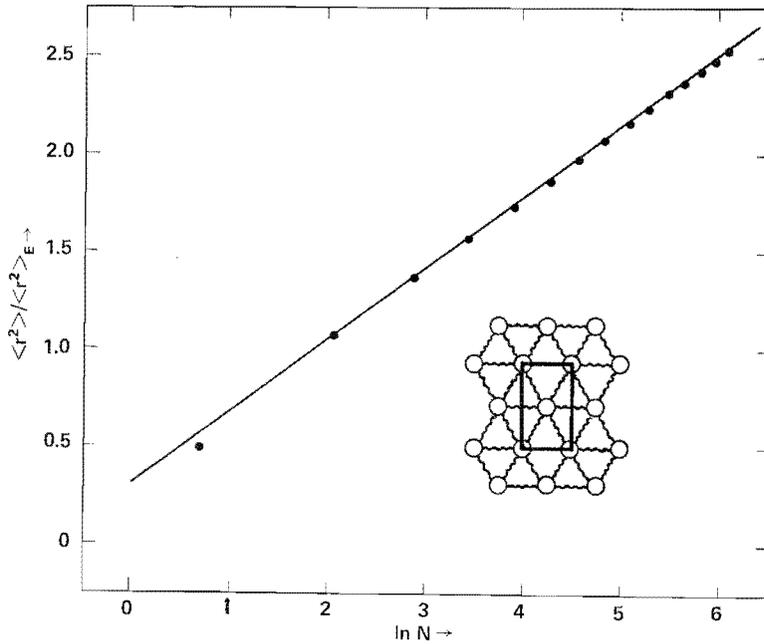
Figure 4. Mean-squared atomic displacement, relative to the Einstein-model prediction, for periodic triangular crystals with the unit cell illustrated.
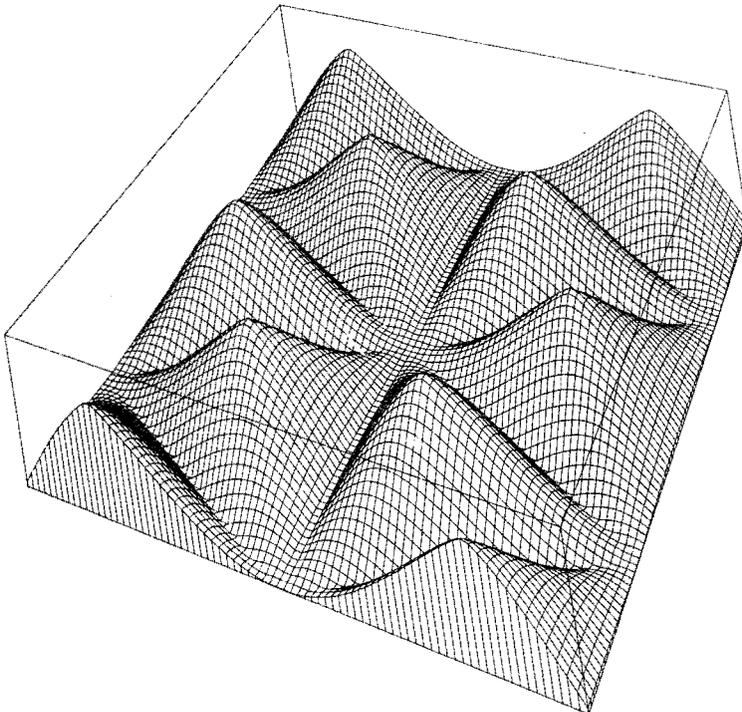

Figure 5. Frequency(low branch only) *versus* k-vector at the instability density in the triangular lattice. There are six zero-frequency valleys.

with increasing density and *diverges* at a density 16/9 times the stress-free
density. Under these conditions an investigation of the dispersion relation
(See Figure 5) reveals that *all* the transverse shear modes corresponding to
the parallel motion of close-packed rows of atoms develop zero frequency, so
that the resistance to shear disappears at high density. It is interesting
that this high-density mechanical instability is the same mechanism suggested
for *melting* on the basis of movies made of the highly anharmonic motion of
two-dimensional hard disks(22). The Hooke's-Law mechanical shear instability
seen in Figure 5 is *not* melting and is actually headed off by an intervening
solid-solid phase transition. The details of the phase diagram depend on w.
For the case we have chosen to investigate in detail, $w = 0.15d_0$, the tri-
angular lattice recrystallizes in a square lattice(where second-neighbor
interactions stabilize the high-density form).

The high-density instability just described is not peculiar to the tri-
angular two-dimensional lattice. The three-dimensional cubic and hexagonal
close-packed lattices both exhibit similar instabilities, at a density 1.728
times the stress-free density.

Two- and three-dimensional crystals also become unstable at low density.
First of all, *thermodynamic* stability precludes states of tension. Such
states are unstable relative to two-phase mixtures including a low-density
gas. Second, even if the gas phase were excluded, to allow tension, the nu-
cleation of vacancies would severely limit the tensile states that could be
achieved. The importance of vacancies in the solid phase can be estimated
from the Einstein model, in which the vibrations of each particle are computed
independently of the motion of its neighbors. This simple picture includes,
approximately, the competition between the increased energy of atoms neighbor-
ing a vacancy and the free energy of mixing, including the pressure-volume
work required to insert a vacancy into an otherwise-perfect crystal. At zero
pressure, the Einstein model predicts a vacancy fraction of

$$(n/N)_{Einstein} = (27/8)exp(-3\kappa w^2/kT), \qquad [4]$$

which, with an estimated melting temperature of $0.01\kappa d_0^2$, is 0.004 at the melt-
ing point. Both Cook and Huckaby have explored improvements on the Einstein
estimate. Cook's work(23) predicts a larger fraction(1.27 times larger) by
taking into account the effect of the vacancy on the vibrational free energy,
obtained from the force-constant matrix(24). Huckaby(25) used the systematic
cell-cluster theory approach, including two-, three-, ... particle correla-
tions in the crystal free energy. Huckaby's estimate is nearly twice that of
the Einstein estimate [4]. Neither of these calculations takes the effect of
pressure into account. This effect is easily included(26), and the corres-

ponding Einstein calculation suggests that, even at very low temperatures, the relaxation of tensile lattice energy would overcome the increase in lattice binding energy due to the introduction of vacancies, at a density about 5% less than the stress-free density.

The frequency distribution for a defect-free crystal can be used to find the macroscopic elastic equation of state. Because explicit calculation of the solid-phase Hugoniot shockwave equation of state(17) shows that thermal contributions are small, we quote here the Lamé constants, λ and η, Poisson's ratio, $\lambda/(\lambda+2\eta)$, and the longitudinal and transverse sound speeds, all calculated for a static, zero-temperature lattice:

$$\sigma = (\sigma_{eq} + \lambda\nabla\cdot u)I + \eta(\nabla u + \nabla u^{\dagger}) \; ;$$
$$\lambda V_{o} = (3N\kappa d_{o}^{2}/8)(5\rho^{1/2}-4) \qquad ;$$
$$\eta V_{o} = (3N\kappa d_{o}^{2}/8)(4-3\rho^{1/2}) \qquad ;$$
$$\lambda/(\lambda+2\eta) = (5\rho^{1/2}-4)/(4-\rho^{1/2}) \quad ;$$
$$c_{1}^{2} = (\kappa d_{o}^{2}/8m\rho)(12-3\rho^{1/2}) \qquad ;$$
$$c_{t}^{2} = (\kappa d_{o}^{2}/8m\rho)(12-9\rho^{1/2}) \qquad . \qquad [5]$$

The vanishing of the shear modulus η and the transverse sound speed coincides with the shear instability at $\rho = 16/9$, where we use ρ to indicate the density relative to the zero-stress density, $\rho \equiv V_{o}/V$.

The thermal properties of the lattice, ignored in equation [5], can be described exactly, using the strain-dependence of the frequency distribution function(27), or, approximately, in terms of the Einstein and Debye models. According to any of these approaches, the thermal part of the pressure can be expressed in terms of the "Grüneisen gamma", $-\gamma \equiv d\ln\omega/d\ln V$, averaged over the distribution of normal-mode frequencies. In the Einstein case:

$$\gamma_{E} = (4-8\rho^{-1/2})^{-1}. \qquad [6E]$$

Two different versions of the Debye model can be used. If two separate branches, one longitudinal and one transverse, are added together:

$$\gamma_{S} = (3/8)[(3-12\rho^{-1/2})^{-1}+(3-4\rho^{-1/2})^{-1}]. \qquad [6S]$$

In the more conventional Debye model, with all the frequencies combined to give a single distribution, a different gamma results:

$$\gamma_{C} = 2\gamma_{S} - \gamma_{E}. \qquad [6C]$$

Figure 6 compares the three approximate treatments [6] with the exact gamma calculated from the density-dependent frequency distribution function. In view of the two singularities in that function(See Figure 3), it is not
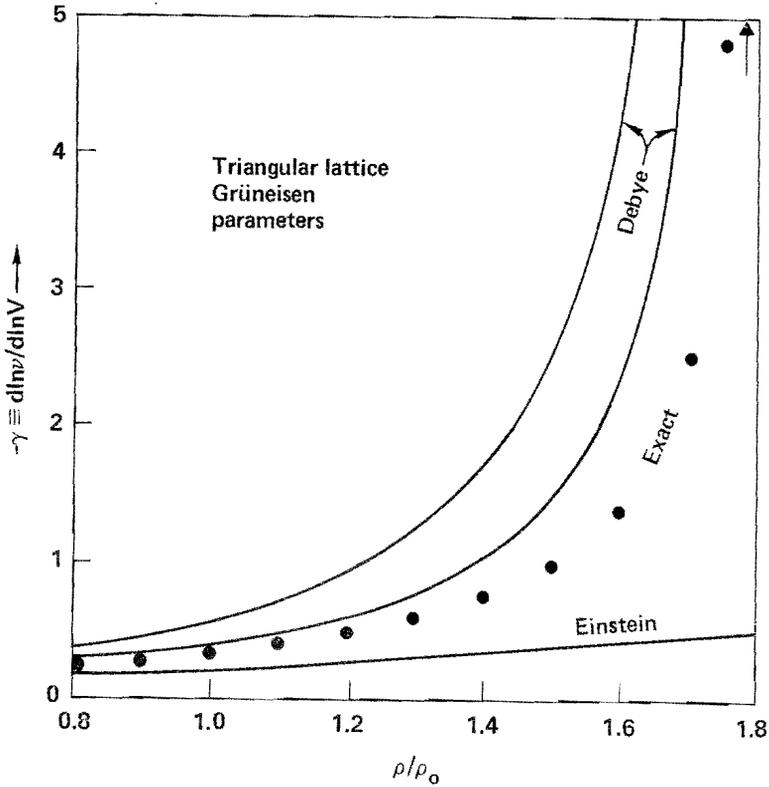
Figure 6. Comparison of three approximate models for the Grüneisen gamma [6] with an exact calculation from reference 20. The vertical arrow at the upper right indicates the instability density. The abscissa is $V_0/V \equiv \rho/\rho_0$.

surprising that all the approximations are poor. Analysis(20) near the instability density, with $\delta\rho \equiv (16/9) - \rho$, shows that the pressure diverges as $\delta\rho^{-1/2}$. The Debye models, on the other hand, predict incorrectly $\delta\rho^{-1}$.

Brittle fracture has also been investigated for our Hooke's-Law model triangular lattice(28). Both the velocity and the entropy associated with brittle-crack motion and structure have been characterized(See Figure 7). It was found that cracks, like dislocations, propagate at speeds near the sound
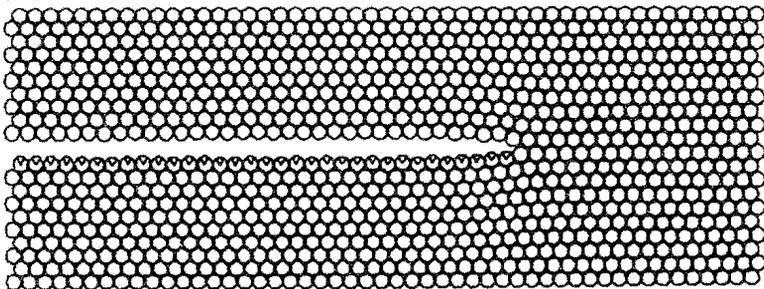

Figure 7. Brittle crack propagating in a triangular-lattice crystal.

speed, provided that the stress is sufficiently great. Some approximate lattice models have incorrectly predicted that crack propagation is reversible. The dynamical computer experiments show that cracks can propagate in a regular, orderly way, but heal only with difficulty. Because brittle cracks require tension for stability, they are not expected to be important in high-pressure flows.

The fracture work just described led to an interest in surface(Rayleigh) waves because continuum theories of fracture use superposed Rayleigh waves to represent traveling cracks. The Rayleigh-wave investigation revealed the expected dispersion, with high-frequency waves trailing low-frequency ones, as well as the unexpected result that the zero-stress dispersion relation has the same form as that found for the one-dimensional harmonic chain.
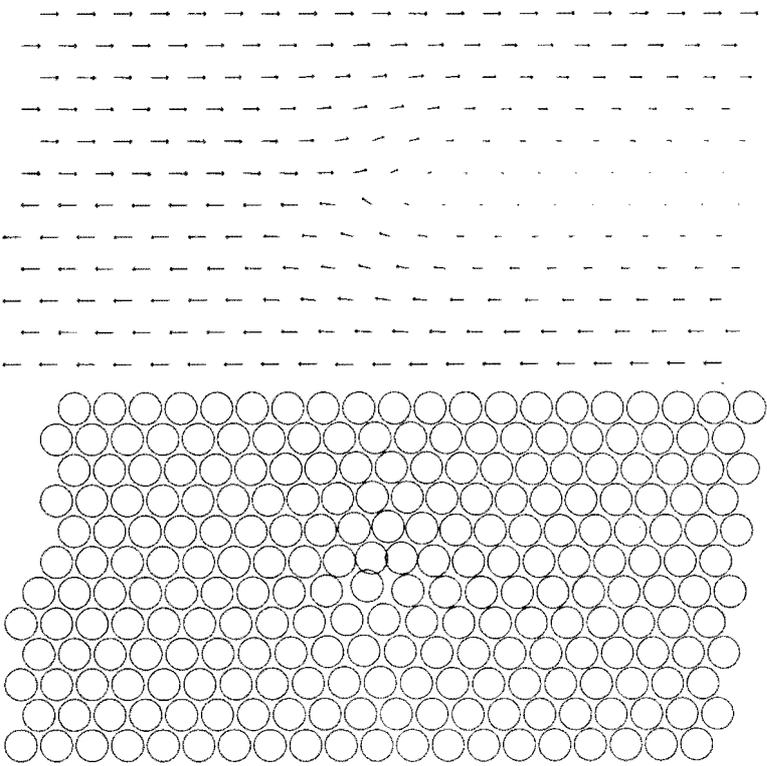
Figure 8. Continuum displacement field, in a strip with fixed boundaries, for an edge dislocation in an elastic strip(30). By propagating to the right, the dislocation reduces the shear strain by d/h, where d is the lattice spacing and h is the crystal height. At the top of the figure the continuum solution is shown, plotted as a series of displacement vectors computed for the points of a triangular lattice. At the bottom of the figure the solution is shown again, but with circles used to indicate the locations of the displaced lattice points. This continuum solution is a useful approximation to the displacement field found in atomic crystals using the relaxation methods discussed in Section III.

III.   PROPERTIES OF SINGLE EDGE DISLOCATIONS *VIA* MOLECULAR DYNAMICS

The static structure of defects such as dislocations can be determined by a straightforward modification of molecular dynamics. Including a frictional force, proportional to each particle's velocity, or alternatively, setting particle velocities equal to zero whenever the kinetic energy reaches a maximum, are two useful methods. Calculations for crystals containing a single dislocation indicate that the dislocation core structure varies in a qualitative way as w/d_o varies from 0.10 to 0.18, with the simplest structure occuring near 0.15. For this reason we have adopted that value for plasticity calculations. Substantially smaller or larger values of w/d_o lead to more complex core structures with increased dependence on system size. Similar calculations for the truncated Lennard-Jones 12-6 potential, which incorporates realistic anharmonicity, are sensitive to system size too[17].

The dislocation simulations are easily initiated by using the elastic-theory displacements for a continuum, but applied at the sites of a perfect lattice, as shown in Figure 8. Eshelby[29] derived the displacements for a dislocation, at $(x,y) = (0,0)$, moving at velocity $(v,0)$ in an infinitely-extended continuum:

$$u_x = (d/\pi)(c_t/v)^2[\tan^{-1}(\gamma y/x) - \alpha^2\tan^{-1}(\beta y/x)] \quad ;$$
$$u_y = (d/\pi)(c_t/v)^2[\gamma\ln(x^2+\gamma^2y^2)^{1/2}-(\alpha^2/\beta)\ln(x^2+\beta^2y^2)^{1/2}] \quad ;$$
$$\alpha^2 = 1 - (1/2)(v/c_t)^2; \ \beta^2 = 1 - (v/c_t)^2; \ \gamma^2 = 1 - (v/c_l)^2. \quad [7]$$

Static-lattice displacements follow from the low-velocity limit of [7].

In practice, it is necessary to specify boundary conditions in any computer simulation. A particularly convenient choice(See Figure 8) involves fixing the top and bottom crystal boundaries. With crystal height h and Burgers' vector b=d the crystal energy density far from the dislocation is $(\eta/2)[\varepsilon\pm(d/2h)]^2$. Passage of the dislocation reduces the shear strain by exactly d/h. Thus motion of the dislocation a distance d reduces the stored elastic energy by exactly ηd^2, and generates an equivalent heat, initially in the form of lattice vibrations localized near the dislocation core. The irreversible dislocation motion, converting work into heat, proceeds at constant energy, without any work being done because the boundaries are held fixed. The lattice deformation is more complicated if fixed stress, rather displacement is used as a boundary condition. See Figure 9.

The several annoying difficulties present in Eshelby's solution of the linear elastic equations are all absent in the molecular dynamics simulations: (i) there is no divergence of the dislocation energy density at infinity; (ii) there is no ambiguity in the relative displacement of atoms just below
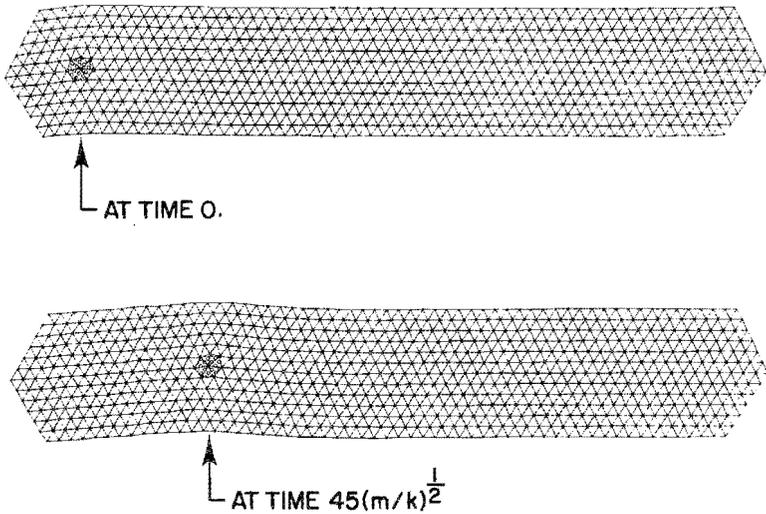
Figure 9.   Propagation with w=0.18d and constant stress of 0.04κ.   Note the Rayleigh waves generated by the moving dislocation.

and just above the glide plane(present in Eshelby's solution because d is taken infinitesimal); (iii) there is no divergence of the dislocation energy density for small distances; and (iiii) the solution of the equations of motion is, unlike Eshelby's, irreversible.   Dynamical instability in the equations of motion prevents a dislocation from converting heat back into work.

The dynamical calculations show that, for a cold crystal, velocity varies nearly linearly with strain(See Figure 10).   The indifference of the calculations to the chosen timestep, for small enough steps, indicates that the approximation of the differential equations of motion by equivalent difference equations is valid.   For large enough strains new phenomena appear.   Vacancy formation is shown in Figure 1.   In the anharmonic Lennard-Jones 12-6 case two distinct branches of the velocity-strain relation have been observed(See Figure 10).   It is possible that the high-speed branch corresponds to the isolated high-speed solution of the continuum equations of motion found by Eshelby.

The single-dislocation simulations provide detailed particle trajectories for comparison with the corresponding predictions of continuum dynamics. To make the comparison it was necessary to generalize Eshelby's solution to the fixed-boundary case(30).   Figure 11 shows that, apart from reversibility, the continuum trajectories closely resemble the atomistic trajectories, for Hooke's-Law atoms.   In the anharmonic case the agreement is relatively poor.

In the next two sections we discuss microscopic and macroscopic generalizations of the single-dislocation calculations to many dislocations.
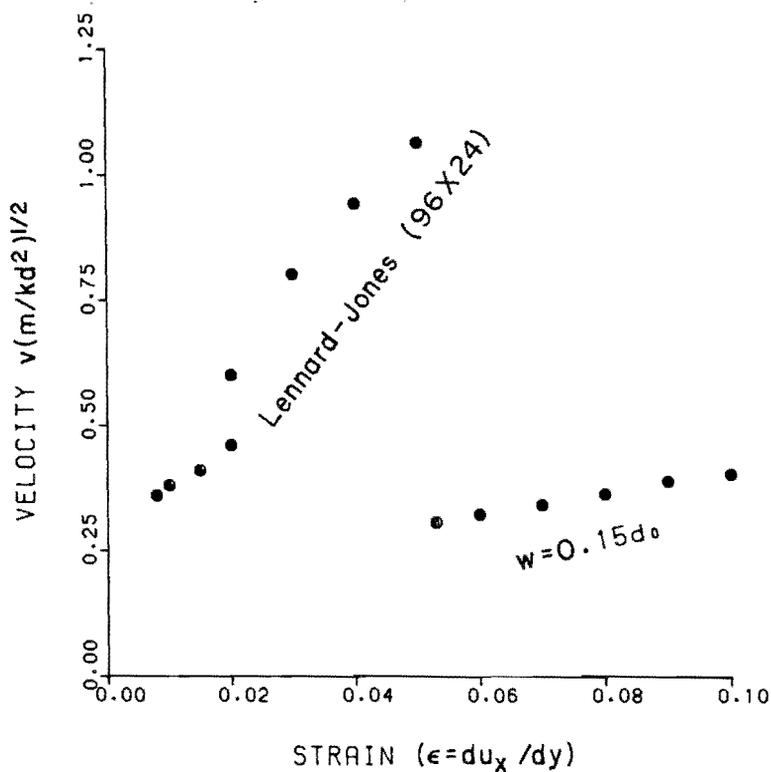
Figure 10.   Velocity *versus* strain in Lennard-Jones and Hooke's-Law crystals.
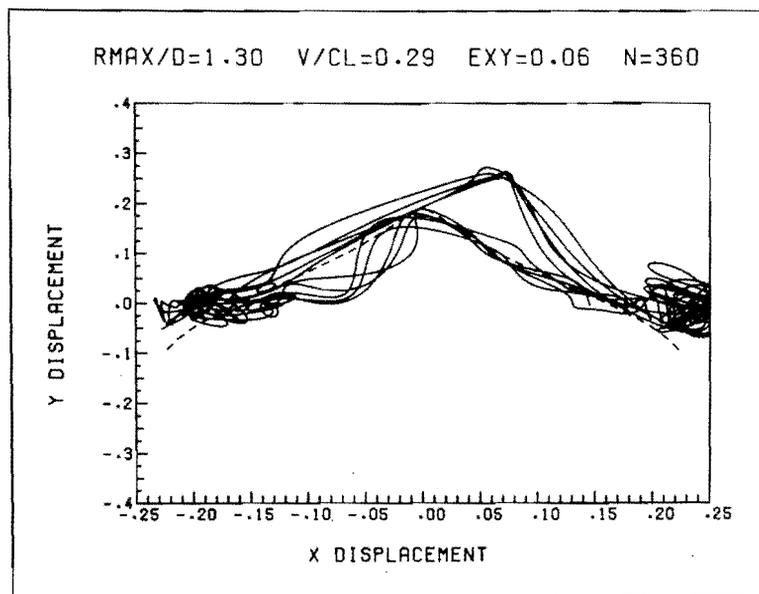

Figure 11.   Motion of atoms adjacent to an edge dislocation's glide plane. Dashes are the continuum solution. Full lines are molecular dynamics trajectories for 10 successive particles as the dislocation passes by.

IIII. EDGE DISLOCATION INTERACTIONS *VIA* NONEQUILIBRIUM MOLECULAR DYNAMICS

In computer simulations of bulk properties it has been usual to make the system boundaries *periodic* to minimize edge effects. This is necessary with long-range interactions, such as the long-range interaction between two dislocations, which varies as 1/r. A typical periodic system, containing dislocations, is illustrated in Figure 12, where the basic volume, with 125 interacting atoms, is shown surrounded by six displaced, but otherwise
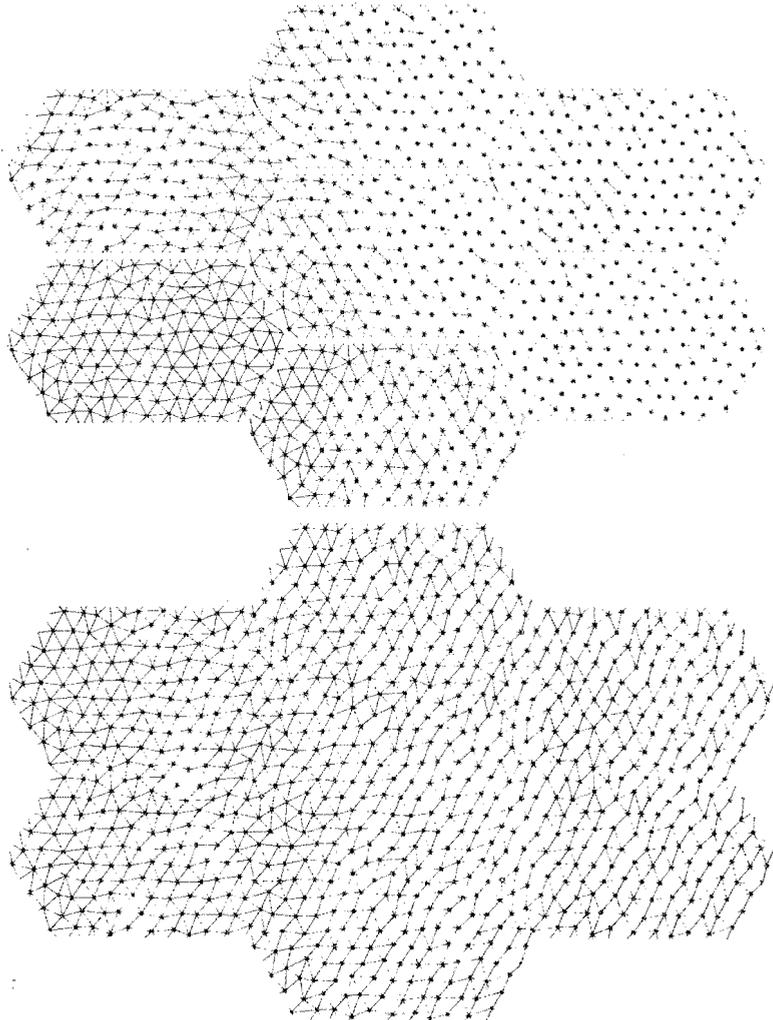

Figure 12. Periodic boundary conditions, used to eliminate edge effects in atomistic simulations. At the top seven identical copies of a 125-atom system are shown. At the bottom these copies have been joined to emphasize the periodic geometry. Careful inspection of the figure will reveal three separated dislocations and a dislocation pair. The defects can be found by locating atoms linked to five or seven(rather than six) neighbors.

identical images of that same volume.

It might appear necessary to manipulate actual physical boundaries, such as those in Figures 7 and 9, to impose stress on a system. In fact, it *is* possible to strain a *periodic* system, without boundaries, in an adiabatic way, by carrying out a continuously-varying deformation of the coordinate system in which the atomistic molecular dynamics takes place. The equations of motion which correspond to such adiabatic deformations, described below, have been used to determine the shear and bulk viscosity coefficients of fluids(31).

Adiabatic irreversible deformations are carried out by including a perturbation coupling Doll's Tensor(32,33), $\sum qp$, where q and p are the atomic coordinates and momenta, to the strain-rate tensor, ∇u, where u is the macroscopic stream velocity. The microscopic Hamiltonian, from which the equations of motion follow, has the following form:

$$H \equiv \Phi(q) + K(p) + \sum qp : \nabla u; \quad \dot{q} = \partial H/\partial p; \quad \dot{p} = -\partial H/\partial q. \qquad [8]$$

A uniform dilation of the system with $d\ln V/dt = 2\dot{\varepsilon}$, corresponds to the strain-rate tensor shown just to the right. If the system were instead undergoing a *shear* deformation, expanding in the x direction and contracting in the y direction, then the strain-rate tensor would include a minus sign in the lower

$$\nabla u = \begin{pmatrix} \dot{\varepsilon} & 0 \\ 0 & \dot{\varepsilon} \end{pmatrix}$$

$$\nabla u = \begin{pmatrix} \dot{\varepsilon} & 0 \\ 0 & -\dot{\varepsilon} \end{pmatrix}$$

righthand entry. It is easy to verify that the equations of motion [8] distort the system in a way consistent with the specified strain-rate tensor. It is also true that the "external" work which must be expended to cause the distortion is exactly that consistent with macroscopic thermodynamics:

$$dE/dt = V\sigma : \nabla u, \qquad [9]$$

where E is the *internal* energy of the volume V which has strain rate ∇u, and where the microscopic stress tensor σ contains both kinetic and potential contributions:

$$V\sigma \equiv \sum(-pp/m) - \sum(rF)_{ij}. \qquad [10]$$

The exact thermodynamic relation [9] serves as a useful check on the numerical integration of the equations of motion [8]. In most of our work the strain rate varies sinusoidally with time so that the parameters characterizing a calculation include the initial thermodynamic state, the amplitude, and the frequency of shear. The periodic system shown in Figure 12 has, after one-half cycle of adiabatic shear, reached a temperature near the melting temperature and contains several dislocations (recognizable as nearby atoms with five and seven neighbors). The temperatures are defined by the kinetic part of the internal energy, $(N-1)kT \equiv \sum p^2/2m$.
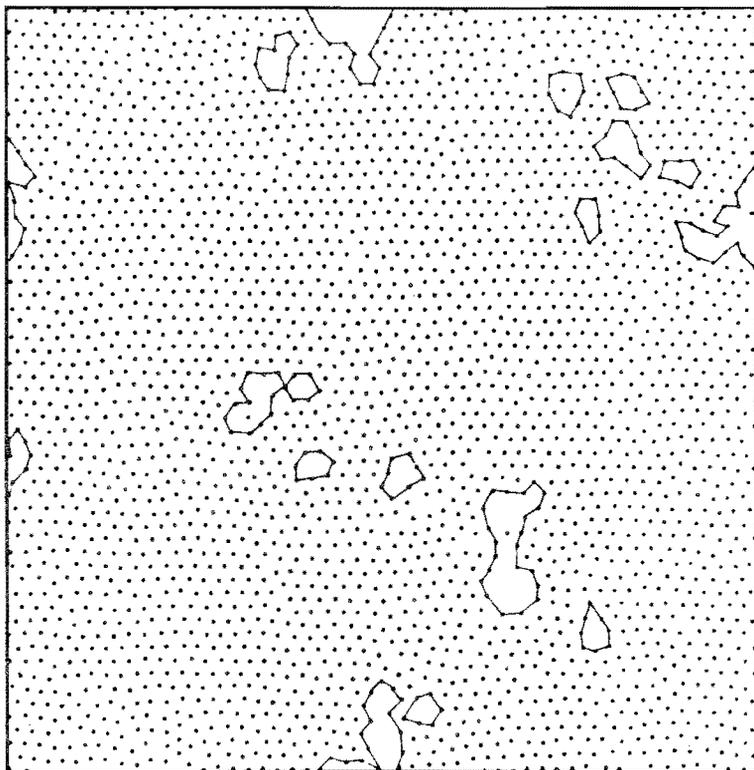
Figure 13.   A configuration, from reference 14, created by rapid heating of a
Lennard-Jones 12-6 crystal, near the solid-phase triple-point density, to a
temperature just below the triple-point temperature.   The many dislocations
and voids seen in the figure are artifacts and do not correspond to equili-
brium defect concentrations.   Compare with figure 2 of reference 13.

Equilibrium thermodynamics suggests that the number of dislocations in
a crystal can be expected to be very small.   The elastic energy of a dislo-
cation is of order $(\kappa b^2/4\pi\sqrt{3})\ln j$, where j is the number of lattice planes
separating two neighboring dislocations; this energy exceeds the kinetic
energy per particle, at the melting point, by an order of magnitude, for
reasonable densities of dislocations.   Nevertheless, some computer simula-
tions have shown large numbers of dislocations.   See Figure 13 above.   It is
interesting that Toxvaerd's calculation(13), under nearly identical thermody-
namic conditions, shows no dislocations.   Thus the defect population is a
sensitive function of thermodynamic path.

With the Doll's-Tensor perturbation providing adiabatic flow, the prin-
cipal difficulty in interpreting the results of molecular dynamics simulations
is the irreversible heating of the crystal due to dislocation motion.   This
heating can be avoided by using isothermal molecular dynamics(34), rescaling
the atomic momenta to make the kinetic internal energy a constant of motion.

Denis Evans has recently described a LaGrange-multiplier method for imple-
menting dynamic constraints in the microscopic equations of motion.

We are presently carrying out a systematic exploration of the constitu-
tive properties of Hooke's-Law solids under adiabatic shear. This project
involves, in addition to studying the usual number-dependence, analyzing the
dependence of the energy, stress, and plastic strain on the temperature,
amplitude, frequency, and dislocation density. Analyses of the deformed
structures in terms of triangles(these would be tetrahedra in three dimen-
sional problems), such as those shown in Figure 12, make it possible to iden-
tify dislocations and vacancies and to define local stresses and strains. The
identification of local variables proceeds by using a bilinear fit within each
triangle. It was shown previously that the energy and stress calculated in
this way are identical, for small deformations, with those calculated directly
from the Hooke's-Law spring forces(28).

V. EDGE DISLOCATION INTERACTIONS *VIA* NONEQUILIBRIUM CONTINUUM DYNAMICS

From the intermediate-scale continuum viewpoint, dislocations are point
defects which react to local stress. The nonequilibrium molecular dynamics
simulations indicate that the motion has negligible inertia, so that a simple
first-order equation of motion, giving dr/dt in terms of local variables, can
be used. How should the periodic boundaries be treated? Li(35) showed that
it is possible to work out the stress field for an infinite static column of
edge dislocations. This calculation can easily be extended to the dynamic
case by using the sums discussed on page 670 of reference 7 together with the
stress-tensor components displayed on pages 166-7 of that reference. In
practice the convergence of the column and row sums is sufficiently rapid
that only a few adjacent columns or rows need to be summed to obtain an ac-
curate representation of the stress due to an infinite hexagonal array of
moving dislocations. That stress can then be used in conjunction with the
intermediate-scale equation of motion(from Figure 10, for instance) to simu-
late the motion of many interacting dislocations. In keeping with the under-
lying approximation of linear elasticity, the Burgers' vector is assumed to
be infinitesimal, so that the macroscopic shape of the crystal is unchanged
in these calculations. External stress can be superposed on that due to the
interacting dislocations. The strain measured in these calculations, by
summing the effects of the moving dislocations, is plastic strain.

Whenever two dislocations approach each other closely, the interaction
between them diverges. Physically we expect that two such dislocations will
either annihilate or form a new dislocation *via* Burgers'-vector addition. We

have observed both processes in atomistic simulations. In intermediate-scale continuum dynamics we allow a dislocation reaction to occur whenever two dislocations approach within one Burgers'-vector length d of each other. If we indicate the six kinds of dislocations possible in the triangular lattice by the integers 1-6, numbered counterclockwise, then the matrix of possible reactions has the form shown at the right:

$$
\begin{array}{c}
 \\
1 \\
2 \\
3 \\
4 \\
5 \\
6
\end{array}
\begin{array}{c}
1\ 2\ 3\ 4\ 5\ 6 \\
\begin{pmatrix}
- & - & 2 & 0 & 6 & - \\
- & - & - & 3 & 0 & 1 \\
2 & - & - & - & 4 & 0 \\
0 & 3 & - & - & - & 5 \\
6 & 0 & 4 & - & - & - \\
- & 1 & 0 & 5 & - & -
\end{pmatrix}
\end{array}
$$

By studying the nonequilibrium molecular dynamics simulations described in Section IIII the creation rates for these defects can also be expressed as functions of the strain, strain-rate, and dislocation density.

Once we complete the current study of soft potentials, the more complicated problems of anharmonicity and three-dimensional plastic flow can be attacked with confidence. We believe that this program will ultimately lead to a comprehensive understanding of plastic flow, by linking together the microscopic, intermediate, and macroscopic descriptions of plasticity through computer simulations.

VI. ACKNOWLEDGMENTS

Warning:

In the Figures d and d_o are used interchangeably to indicate the stress-free interparticle spacing. In Figures 9 and 10 the force constant κ appears as k. In Figure 2 the length w is given in units of d_o. The relation linking the two frequencies ω and ν is $\omega = 2\pi\nu$. Finally, u is used to indicate both the elastic displacement(Equations [5] and [7]) and the stream velocity(in Section IIII) while the variable ρ is everywhere dimensionless and indicates the ratio of the density to the stress-free density.

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