High-Strain-Rate Plastic Flow Studied via Nonequilibrium Molecular Dynamics

William G. Hoover, Anthony J. C. Ladd, and Bill Moran
Department of Applied Science, University of California at Davis, Davis, California 95616, and
Lawrence Livermore National Laboratory, Livermore, California 94550

(Received 27 April 1982)

Recent experiments at strain rates reaching 0.1 GHz suggest a power-law dependence of solid-phase shear stress on strain rate. Novel nonequilibrium molecular dynamics simulations of plastic flow have been carried out. These steady-state isothermal calculations appear to be consistent with the present-day experimental data and suggest that the flows of metals can be described by a single physical mechanism over a range of strain rates from 10 kHz to 1 THz.

PACS numbers: 46.30.Jv, 05.20.Gg, 05.70.Ln, 61.70.Ga

It is well known that plastic flow in crystals proceeds through defect motion. There is an extensive body of experimental and theoretical work detailing evidence for this view.[1] At the same time there has been little success in correlating theoretical models with experimental data in a quantitative way. There are two reasons for this. First, the theory is relatively simple, for mathematical reasons, and omits nonlinear effects which are known to be important but difficult to estimate. Second, experiments have, until recently, been restricted to relatively slow deformations, below 1 kHz, where grain structure, impurities, and other material-dependent properties obscure the universal flow behavior expected at higher strain rates.

The use of clever experiments has extended the range of experimental data by another five orders of magnitude in strain rate. Asay *et al.* propagate plane shock waves in metals, and follow the detailed progress of these waves using the laser interferometry method pioneered by Barker.[2,3]

Several similar shock-wave experiments, with different sample thicknesses, establish that steady plastic waves are formed and that the rise time can be measured, optically, at pressures up to about 1 Mbar. Analysis of the wave shapes suggests that the shear stress increases roughly as the square root of the strain rate.[3] A theoretical model, based on the idea of shear bands, with heat flowing from the bands according to a diffusion equation, is consistent with such data.[3]

We have generalized earlier nonequilibrium molecular dynamics calculations to the systematic study of solids under shear. Related calculations have been carried out, over the past ten years, by several groups.[4] Our most successful work incorporates nonequilibrium shear deformation directly into the equations of motion, while simultaneously maintaining constant temperature. "Constant temperature" is not inconsistent with the existence of shear bands in the computer work. Only the average temperature, averaged over the entire system, is fixed.

The shear deformation is conveniently treated with Doll's tensor[5] equations of motion:

$$\dot{x}=(p_x/m)+\dot{\epsilon}y;\quad \dot{y}=(p_y/m);\quad \dot{z}=(p_z/m);$$
$$\dot{p}_x=F_x;\quad \dot{p}_y=F_y-\dot{\epsilon}p_x;\quad \dot{p}_z=F_z, \tag{1}$$

where the forces, F_x, F_y, and F_z, are derived from the interparticle potentials. The strain rate, $\dot{\epsilon}$, is the derivative of the macroscopic x velocity with respect to y. The momenta are defined relative to the local macroscopic velocity. Periodic boundaries are used to eliminate edge effects. Equations (1) satisfy the microscopic analog of the first law of thermodynamics,

$$\dot{E}\equiv-\dot{\epsilon}P_{xy}V, \tag{2}$$

so that a solid deforming in this way will gradually heat up and melt. In order to avoid this complication we obtain steady-state isothermal deformation by using a new[6] velocity-dependent force chosen to satisfy the constraint equations

$$d(p_x^2)/dt=d(p_y^2)/dt=d(p_z^2)/dt=0. \tag{3}$$

These are implemented by modifying (1) as follows:

$$\dot{p}_x=F_x-\zeta_x p_x;\quad \dot{p}_y=F_y-\dot{\epsilon}p_x-\zeta_y p_y;$$
$$\dot{p}_z=F_z-\zeta_z p_z. \tag{4}$$

The friction coefficients ζ_x, ζ_y, and ζ_z are explicit functions of the coordinates and momenta which can be identified from the constraints (3):

$$\zeta_x=\sum F_x p_x/\sum p_x^2;\quad \zeta_y=\sum(F_y-\dot{\epsilon}p_x)p_y/\sum p_y^2;$$
$$\zeta_z=\sum F_z p_z/\sum p_z^2. \tag{5}$$

It is remarkable that these equations are stable and well behaved even for very small systems.

Numerical calculations demonstrating this stability were carried out for the smallest system possible, three one-dimensional mass points connected with Hookean springs using periodic boundary conditions. In this case, with the kinetic energy, total momentum, and center of mass all fixed, the phase space is three dimensional, suitable for analytic study.[7] The ordinary Newtonian constant-energy equations of motion generate an elliptical trajectory in this space because both nonzero normal modes have the same frequency. On the other hand, the solution of the isothermal equations of motion,[4] projected onto a plane described by the displacement coordinates of two of the masses, generates a pattern of precessing figure-eight loops.

The isothermal equations of motion are reversible in the time but do *not* obey Liouville's theorem. This is because the velocity-dependent forces cause the distribution function density to vary with time in the phase space. This variation can be analyzed analytically, with the result

$$\dot{f} = -f \sum \partial \dot{l}/\partial l \equiv -f\dot{E}/kT.$$

Thus the phase space density f varies as $\exp(-\Delta E/kT)$, where ΔE is the energy change induced by the velocity-dependent forces; and a canonical distribution in the phase space is exactly maintained by the isothermal equations of motion.

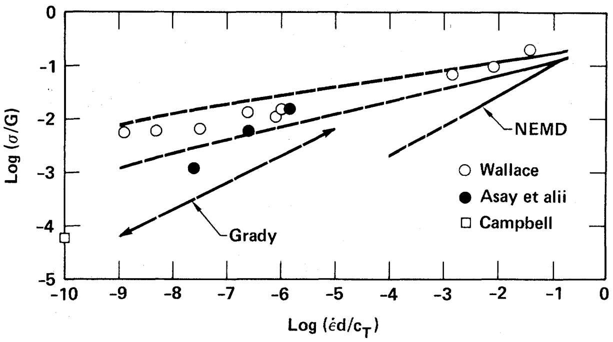

FIG. 1. Strain-rate dependence of the shear stress σ. G is the shear modulus, d the nearest-neighbor spacing in a close-packed lattice, ϵ the strain rate du_x/dy, and c_T the transverse sound velocity. The nonequilibrium molecular dynamics was generated for two-dimensional solids at 1.1 times the stress-free density and temperatures of 0.3 (top full line), 0.6 (middle line), and 0.9 (bottom line) times the melting temperature, using from 64 to 400 particles. The interparticle force used rises linearly to a maximum at 1.15 times the zero-force separation, and then falls linearly, vanishing at 1.30 times the zero-force separation. The beryllium data from Asay *et al.*, Wallace and Grady's estimates for aluminum, and Campbell's older low–strain-rate estimate are shown. The uncertainty in the slope of the lines is a few percent. It should be emphasized that the experimental data are not at the same temperature and density. The effects of the temperature and density variation are relatively small.

Application of these isothermal flow equations to solids is complicated by the number of independent variables: force law, temperature, strain rate, density, and crystal geometry. We have used the simplest possible forces, piecewise-linear forces, in all of our calculations. We have explored the effects of density, dimensionality, and temperature. A comprehensive study of these effects will require considerable time. We believe that the two-dimensional results now available are sufficiently interesting for publication. These data are shown, as solid lines, with a dashed extrapolation to lower rates, in Fig. 1. Each line summarizes about twenty individual steady-state shear calculations, typically proceeding to a strain of ten—the top of our periodic cell would be displaced ten sidelengths, relative to the bottom, during this time—or longer. Three different temperatures are considered here and correspond roughly to 0.3, 0.6, and 0.9 times the melting temperature. These data show, unambiguously, that the stress has a (temperature-dependent) power-law dependence on the strain rate at the rates accessible to our calculation. These rates correspond, in real solids, to strain rates of order 10 GHz to 1 THz. The lower rate corresponds, roughly, to a single dislocation pair in a system of several hundred atoms, the highest rate to a defect density approaching the number density. This highest strain rate could alternatively be described as one at which particles on adjacent glide planes move at a relative velocity equal to the transverse sound velocity.

In order to compare laboratory experiments on beryllium and aluminum with computer experiments, we have used a corresponding-states approach in Fig. 1. The dimensionless ratio, shear stress divided by shear modulus, is displayed as a function of reduced strain rate. Our two-dimensional computer data lie along the heavy lines marked *NEMD*. We have verified that the two- and three-dimensional data are similar and that the slopes are insensitive to density on this scale. It should be noted that the general trend of the computer data, when extrapolated (dashed extension) over the intervening two orders of magnitude in strain rate, is nicely consistent with laboratory measurements. We must emphasize that the laboratory "measurements" do not measure stress directly. The values shown are inferred through the idealized models outlined in Refs. 3 and 8.

We have included Wallace's calculations in the figure, for aluminum at high strain rates.[8] His data represent neither true laboratory experiments nor computer simulations. They are instead a relatively sophisticated educated guess, based on a continuum model, fitted to plastic-wave data and consistent with reasonable thermodynamic bounds on the temperature, stress, and entropy within nonequilibrium shock waves. The discrepancies between Wallace's and Grady's more naive estimates at the lower strain rates reflect the difficulty in estimating shear stress from measured longitudinal data. Asay's estimates for beryllium likewise include some relatively uncertain approximations. The upper bounds for shear stress, computed for aluminum, copper, and iron by Chhabildas and Asay,[3] lie well above our low-temperature calculated line.

We are well aware that the approximate methods used to estimate shear stress in Refs. 3 and 8 are oversimplifications of a complex phenomenon. Nevertheless these estimates represent the best experimental description of the strain-rate dependence of stress available. The semiquantitative agreement of the three kinds of data nevertheless suggests that a common explanation of high-strain-rate data, at rates exceeding about 10 kHz, can be obtained by analyzing the small-system consequences of the nonequilibrium equations of motion. At present there is no x-ray diagnostic capable of providing experimental data on shock fronts at pressures in the megabar range. The data presented here suggest that such shock waves could be successfully described by extrapolation of the stress-versus-strain-rate relation obtained at lower rates.

We thank Mat van Thiel, Duane Wallace, Bill Ashurst, and Dick Grover for helpful discussions detailing the difficulties involved in interpreting experimental data. This work was supported in part by the U. S. Army Research Office and by the U. S. Department of Energy under Contract No. W-7405-Eng-48.

---

[1] *Dislocation Dynamics*, edited by A. R. Rosenfield, G. T. Hahn, A. L. Bement, and R. Jafee (McGraw-Hill, New York, 1968). See also *Shock Waves and High-Strain-Rate Phenomena in Metals*, edited by M. A. Meyers and L. E. Murr (Plenum, New York, 1981). A recent theoretical exposition of dislocation theory appears in R. Bruinsma, B. I. Halperin, and A. Zippelius, Phys. Rev. B 25, 579 (1982).

[2] L. M. Barker, in *Behavior of Dense Media under High Dynamic Pressures* (Gordon and Breach, New York, 1968), p. 483. For a review of earlier work, see J. D. Campbell, Mater. Sci. Eng. 12, 3 (1973).

[3] D. E. Grady, Appl. Phys. Lett. 38, 825 (1981); L. C. Chhabildas and J. R. Asay, J. Appl. Phys. 50, 2749 (1979). See also D. B. Hayes and D. E. Grady, in *Shock Waves in Condensed Matter—1981*, edited by W. J. Nellis, L. Seaman, and R. A. Graham, AIP Conference Proceedings No. 78 (American Institute of Physics, New York, 1982), p. 412; J. R. Asay, L. C. Chhabildas, and J. L. Wise, *ibid.*, pp. 417 and 427.

[4] W. G. Hoover and W. T. Ashurst, Adv. Theor. Chem. 1, 1, (1975); D. J. Evans, Mol. Phys. 37, 1745 (1979); D. M. Heyes, J. J. Kim, C. J. Montrose, and T. H. Litovitz, J. Chem. Phys. 73, 3987 (1980).

[5] W. G. Hoover, D. J. Evans, R. B. Hickman, A. J. C. Ladd, W. T. Ashurst, and B. Moran, Phys. Rev. A 22, 1690 (1980).

[6] This idea was simultaneously and independently developed by Denis J. Evans, private communication.

[7] See, for instance, T. Bountis, H. Segur, and F. Vivaldi, Phys. Rev. A 25, 1257 (1982).

[8] D. C. Wallace, Phys. Rev. B 22, 1477, 1487 (1980), and 24, 5597, 5607 (1981). See also P. W. Bridgman, Rev. Mod. Phys. 22, 56 (1950).