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TITLE MODELING SHOCKWAVE DEFORMATION via MOLECULAR DYNAMICS

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MODELING SHOCKWAVE DEFORMATION via MOLECULAR DYNAMICS

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Molecular dynamics (MD), where the equations of motion of up to thousands of interacting atoms are solved on the computer, has proven to be a powerful tool for investigating a wide variety of nonequilibrium processes from the atomistic viewpoint. Simulations of shock waves in three-dimensional (3D) solids and fluids have shown conclusively that shear-stress relaxation is achieved through atomic rearrangement. In the case of fluids, the transverse motion is viscous, and the constitutive model of Navier-Stokes hydrodynamics has been shown to be accurate - even on the time and distance scales of MD experiments. For strong shocks in solids, the plastic flow that leads to shear-stress relaxation in MD is highly localized near the shock front, involving slippage along close-packed planes. For shocks of intermediate strength, MD calculations exhibit an elastic precursor running out in front of the steady plastic wave, where slippage similar in character to that in the very strong shocks leads to shear-stress relaxation. An interesting correlation between the maximum shear stress and the Hugoniot pressure jump is observed for both 3D solid and fluid shockwave calculations, which may have some utility in modeling applications. At low shock strengths, the MD simulations show only elastic compression, with no permanent transverse atomic strains. This result for perfect 3D crystals is also seen in calculations for 1D chains. We speculate that, if it were practical, a very large MD system containing dislocations could be expected to exhibit more realistic plastic flow for weak shock waves, too.

1. INTRODUCTION

The most successful tool yet developed for studying the collective motion of large numbers of atoms engaged in nonequilibrium flows is the method known as molecular dynamics (MD). Large, fast computers have made it possible to study shock waves in three-dimensional (3D) crystals composed of up to 10,000 atoms interacting with central, pairwise-additive, short-range forces.[1] The principal limitation to these calculations is practical computational size in comparison to the thickness of the shock wave, the approach to a steady-wave profile, and sufficient cross-sectional area. Faster computers with larger memories will expand the microscopic (atomistic) horizons that at present preclude the treatment of extended defects in any serious number in the initial crystal.

In the case of fluids, MD calculations of shock waves showing viscous rearrangement of atoms in the immediate vicinity of the shock front, compared with Navier-Stokes (NS) hydrodynamic solutions have been surprisingly successful.[2] The input for the NS calculations was in fact obtained by atomistic calculations of the equation of state (EOS), with nonequilibrium molecular dynamics (NEMD) calculations of the linear hydrodynamic transport coefficients. In Section 2, we will review the results of the work on fluid shock waves.

In the case of solids, MD shockwave calculations have been carried out,[3-5] but progress beyond identifying the microscopic process of plastic flow[5] has been very slow. In Section 3, we will discuss the three different shock-strength regimes we have observed in MD calculations.[1] Two of the three cases are characterized by shear stress relaxation accompanying atomic rearrangement. On the other hand, the third (weak-shock) regime, where the shear stress provides insufficient impetus to generate a plastic wave, appears to be an artifact of the perfect crystal, at least under the limitations of the MD calculations. We point out some potentially useful correlations for modeling and discuss

some future directions for research on weak shock waves in solids.

2. SHOCK WAVES IN FLUIDS

The techniques for generating shock waves in either solids or fluids via MD, as well as analyzing the results, are well documented in Ref. 2; we briefly recapitulate them here. First of all, a filamental rectangular parallelepiped of atoms is equilibrated at an initial relatively-low density ρ_o and temperature T_o. The length of the parallelepiped in the direction of shock propagation is typically 50-100 face-centered cubic (fcc) unit cells long, or 100-200 planes of atoms in the x-, or <100>-direction. The transverse (y and z) dimensions are usually 3-4 unit cells, or 18-32 atoms per plane. For the fluid shocks, of course, the equilibration process includes time for the initial fcc crystal to melt. Feedback methods have been developed to achieve a desired temperature for the equilibrated initial state [6] A planar shock wave is initiated at time zero by shrinking the x-direction periodic length L_x according to $L_x(t) = L_x(0) - 2u_p t$, while keeping the cross-sectional lengths L_y and L_z fixed; u_p is the piston, or particle velocity. The periodic boundary then behaves very much like the interface of a planar symmetric-impact shockwave experiment. A pair of oppositely-running shock waves move out with shock-front speed u_s from the boundaries toward the middle of the computational cell, leaving behind shocked material at a higher density ρ_1 and temperature T_1, moving along with the interfacial "pistons" at speed u_p.

The shockwave profiles for density, velocity, pressure tensor, temperature, internal energy, and heat flux vector, are obtained by lumping particles and their individual kinetic and potential contributions into bins, in order of their x coordinates, in multiples of the initial number of atoms in a yz cross-sectional plane. These planar Lagrangian mass elements, particularly in the case of solids, lead to smoother profiles than fixed Eulerian boxes. For steady shock waves, time averages of profiles can be gathered for both waves simultaneously by riding along with the shock fronts. Since a steady, planar shock wave has constant mass flux ρu throughout the profile, we can show that the total volumetric strain in the shock is $\epsilon = \rho_o/\rho_1 - 1 = -u_p/u_s$, so that the total strain rate at the shock front ($x = 0$) is $\dot{\epsilon} = \epsilon u_s/\lambda = -u_p/\lambda$, where λ is the shockwave thickness.

In the Navier-Stokes, or linear hydrodynamics view of fluid flow, a steady shock wave is formed when the process of longitudinal compression (leading to steepening of the wave) competes with the dissipative process of viscous flow (spreading of the wave). The NS transport coefficients, the thermal conductivity κ and the longitudinal viscosity, $\eta_L = \eta_V + (4/3)\eta$, where η_V is the volume (bulk) viscosity and η is the shear viscosity, as well as the EOS [pressure $P(\rho,E)$ as a function of density ρ and internal energy E] can be obtained from independent MD calculations. The EOS and the Green-Kubo transport coefficients, which can be related to equilibrium fluctuations of the pressure tensor and heat flux vector for η_L and κ, respectively, can be obtained from equilibrium MD; the nonlinear transport coefficients for finite strain rates and temperature gradients via nonequilibrium MD (NEMD) can be extrapolated to zero rates to obtain the NS transport coefficients. The indirect Green-Kubo calculations are time-consuming because of the statistical errors inherent in fluctuations, while the direct NEMD calculations require extrapolation of several computer experiments. [7] Most of the results to date for transport coefficients are from NEMD.

In Fig. 1 are shown shockwave profiles generated by NEMD, with NS comparisons sketched

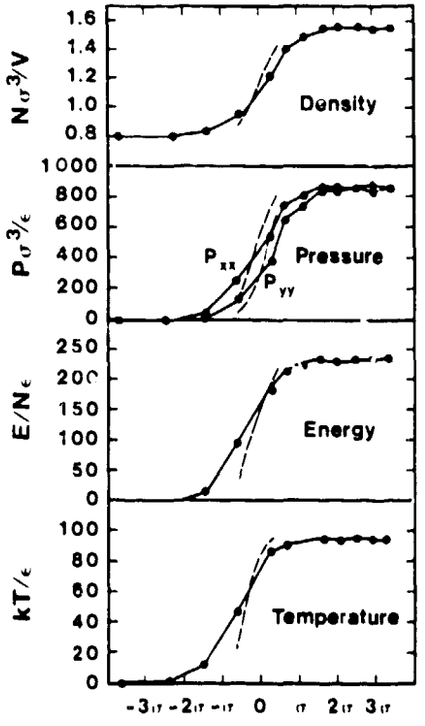

FIGURE 1. Density, pressure, internal energy, and temperature profiles for a strong steady shock [$u_p/\sqrt{(m/\epsilon)} = 22.4$] in a Lennard Jones fluid calculated by nonequilibrium molecular dynamics.[2] Corresponding Navier-Stokes results are shown as dashed lines. (The units for a Lennard-Jones system are: the atomic mass m, the crossing point of the pair potential σ, and the depth of the potential minimum ϵ.)

in as dashed curves.[2] The atoms in this simulation interacted via a Lennard-Jones pair potential (repulsive inverse-12th power of the separation plus attractive inverse-6th power). Using energy and distance parameters in this potential appropriate for argon, the shock strength was such that the final temperature achieved was about 12,000 K, or near the point of ionization. Even so, NS provides a good approximation to the MD results, underestimating the MD viscosity (shock thickness) by only 30-40%. This is the worst case; much better agreement is obtained for weaker shockwaves, where NS and NEMD profiles agree within 4%.

Subsequent to this work, I noticed that even better agreement can be obtained between NS and MD if the temperature component in the direction of propagation of the shock wave, T_{xx}, is used to compute $\eta_L(\rho,T)$, rather than the mean temperature at the shock front, $T = (T_{xx} + T_{yy} + T_{zz})/3$, which can be as much as a factor of two lower than T_{xx}. This nonlinear (non-NS) correction serves to narrow the NS shock thickness at low shock strengths; that is, at lower temperatures, using T_{xx} reduces the apparent viscosity towards the MD value. At the other extreme (strong shock), using T_{xx} rather than T at the shock front enhances the viscosity, as in the dilute gas limit, increasing the thickness to within 10% of the MD result. Attempts to relate frequency and wavelength corrections to the viscosity, in the framework of generalized hydrodynamics, are not so successful. Even less successful is the attempt to include the nonlinear effect on the shear viscosity due to shear-thinning with increased strain-rate. No satisfactory explanation of these observations has yet been proposed.

I have recently reexamined these fluid shockwave results and noted an interesting and potentially useful correlation. The peak shear pressure, $(P_{xx} - P_{yy})/2$, which occurs near the shock front, appears to be a constant fraction (~0.1) of the Hugoniot jump in pressure, $P_1 - P_o$. Hence, for a viscous fluid (the shear pressure for the constant-volume process of compression in the x-direction and expansion in the y- and z-directions is $-\eta\dot{\ell}$), the ratio $2(P_1 - P_o)/(P_{xx} - P_{yy}) = -\rho_o u_s u_p/\eta\dot{\ell} = \rho_o u_s \lambda/\eta$ is a Reynolds number of ~10, essentially independent of shock strength. I have also found that approximately the same ratio holds for plastic shockwave deformation in MD solids, though of course it cannot be associated with a viscous-fluid concept like Reynolds number. Thus, for strong fluid or solid shock waves,

narrow enough to be calculated by MD, it appears that there exists a roughly constant ratio for the balance between compressional steepening of a shock wave and dissipative spreading due to atomic rearrangement.

3. SHOCK WAVES IN SOLIDS

Shock waves in solids display a richer variety of phenomena than steady shocks in fluids. The viscous flow in fluids, which occurs continuously whether or not stress is applied, is relatively simple to model via Navier-Stokes (linear) hydrodynamics, requiring only the total strain rate in the NS constitutive relation, as we have seen in the previous section. Plastic flow in solids, on the other hand, occurs only in response to applied stress, and is not continuous. Moreover, it can be triggered by thermal "defects" (fluctuations) as well as by the presence of crystalline defects, particularly dislocations. The statistical nature of plastic flow is a major stumbling block to atomistic simulation. The constitutive modeling required for solids is inherently more complicated than for fluids, because the strain rate has both elastic and plastic components, corresponding to compressive and dissipative flows, respectively.

Early MD simulations of shock waves in solids by Tsai and coworkers (summarized in Ref. 3) led them to conclude that shock waves are always unsteady. (They have even made that claim for shock waves in liquids.[8] As it turned out, their "fluid" shockwave calculations were plagued by numerical errors in the equations of motion, incorrect formulas for profile averages, and an unfortunate choice of shock strength, which put their final state on the melting line, naturally leading to the possibility of a non-steady, two-wave structure.) We now know that non-steady (supported) elastic 1D waves are typically observed in MD solids for small u_p and T_o, as is shown in Fig. 2. In this recent calculation,[1] the atoms, initially in an fcc crystal, interacted via the truncated (short-range) Lennard-Jones potential,[7] with piston velocity $u_p/c_o = 0.1$ (c_o is the long-wavelength sound speed).

The profile in Fig. 2 shows no shear-stress relaxation, and indeed, there is only uniaxial compression, with no plastic deformation. This result looks identical to shock waves in 1D chains, where there is no mechanism for dissipative motion of the atoms in the direction transverse to the wave propagation. In these 3D simulations, planes of atoms in the x-direction bounce off of each other elastically as though they were 1D "particles." This kind of elastic disturbance grows in thickness linearly with time, and is a phenomenon which can occur in real materials only below the Hugoniot elastic limit.

Following Tsai's early work (before 1970), Dienes and Paskin[4] simulated shock waves in 3D crystals and saw nothing but steady waves, or at best, the transient approach to steady waves,

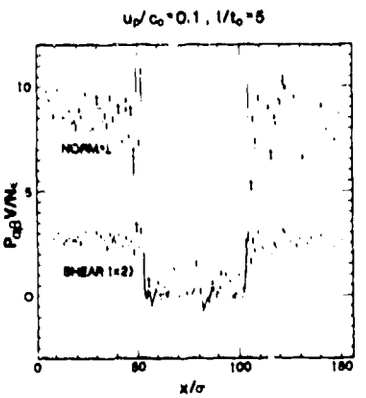

FIGURE 2. Profile of the normal (xx) component of the pressure-volume tensor and twice the shear component [(xx-(yy+zz)/2], for a nonequilibrium molecular dynamics calculation of a shock wave in the Lennard-Jones fcc solid at time $t/t_o = 5$ [$t_o = \sigma\sqrt{(m/\epsilon)}$]; initial conditions: $\rho_o\sigma^3/m = 1.03$, $kT_o/\epsilon = 0.1$, $u_p/c_o = 0.1$ [$c_o = \sqrt{(72\epsilon/m)}$, the nearest-neighbor, zero-temperature, zero-pressure longitudinal sound speed].

primarily because they were looking mostly at strong shock waves. There appeared to be no way to reconcile these very disparate results.

In 1979, we resolved this controversy over the 1D waves by discovering that they are an artifact of perfect crystals in MD: by setting the initial temperature low enough (such as zero), they can be obtained for large u_p, where otherwise, at finite initial temperature (such as $kT_o/\epsilon = 0.1$) a strong, steady shock wave (overdriven plastic wave) would be observed.[5] This zero-temperature 1D elastic wave is very unstable to perturbations, however. If, after propagating such an artificially-1D wave for some time, the coordinates and velocities are instantaneously rounded off from 14-figure accuracy to 7 figures, then the profile begins to collapse rather suddenly toward the overdriven, steady plastic-wave result for finite T_o!

We also identified a possible deformation mechanism which leads to shear-stress relaxation for strong shocks in solids, namely, slippage of one part of the crystal over the other, in the vicinity of the plastic wavefront, parallel to one of the four independent close-packed planes. We observed that the regions of slip are quite localized:

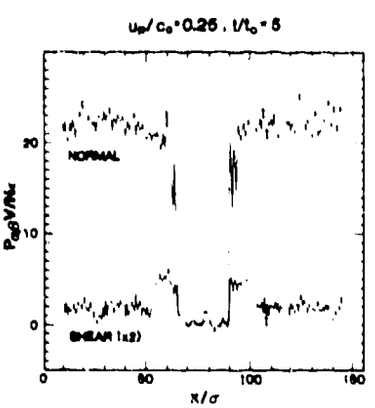

FIGURE 3. Normal and shear (×2) components of the pressure-volume tensor (see Fig. 2 for key); $u_p/c_o = 0.25$; $t/t_o = 5$. Note the width of the elastic disturbance (see Fig. 5).

individually, the atoms move less than one interatomic spacing. The choice of slip plane is apparently statistical, being selected at random according to local thermal fluctuations. The overall pattern of slippage is therefore incoherent and heterogeneous, albeit on a very fine scale of a few lattice spacings.

Recent calculations[1] for a series of shock strengths show three distinct regimes for shock waves in 3D solids via MD: Fig. 2 shows an elastic unsteady wave, a regime that extends up to $u_p/c_o \gtrsim 0.2$; Fig. 3 shows clearly the emergence of an unsteady elastic precursor, followed by a steady plastic wave; Fig. 4 shows an overdriven, steady plastic wave. (At $u_p/c_o \sim 1$, the final state is very near the melting line.)

The transition from purely elastic response to elastic-plastic waves, which occurs in MD calculations at $u_p/c_o \sim 0.25$, is especially interesting. At this shock strength, the shear pressure should be equal to the theoretical strength of a perfect crystal,[9] which is approximately 1/10th the shear modulus for slippage of close-packed planes over each other. We observe from Figs. 3 and 4 that, as in fluids, the Hugoniot pressure rise is about

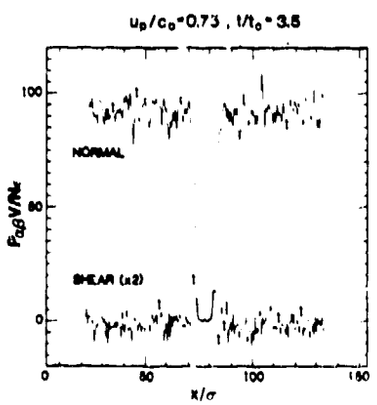

FIGURE 4. Normal and shear (×2) components of the pressure-volume tensor (see Fig. 2 for key); $u_p/c_o = 0.75$; $t/t_o = 3.5$. Note that the plastic wave has overtaken the elastic wave.

10 times the maximum shear pressure independent of shock strength. Consequently, the threshold for plastic flow in MD should occur when the Hugoniot pressure is roughly equal to the shear modulus, as is confirmed in Fig. 3.

For $u_p/c_o = 0.25$, a series of snapshots of twice the shear component of the pressure-volume tensor is presented in Fig. 5, showing the growth of the elastic region in front of the plastic wave, which is accompanied by relaxation of the shear stress to a quasi-hydrostatic state. Several years ago, in unpublished work,[10] we made a computer-generated movie of deformation in a shock of this strength. A frame from the movie is shown in Fig. 6, where chunks of crystal have slipped as the plastic wave passes by. The pattern of plastic deformation in this particular calculation is the most coherent yet seen. Other MD calculations near the onset of shock-induced plastic flow reveal a sensitivity to initial conditions, including cross-sectional area. For shocks near the elastic-plastic transition, then, the presence of initial dislocations ought to lower the theoretical-strength barrier, as in real solids, where the Hugoniot elastic limit is lowered considerably

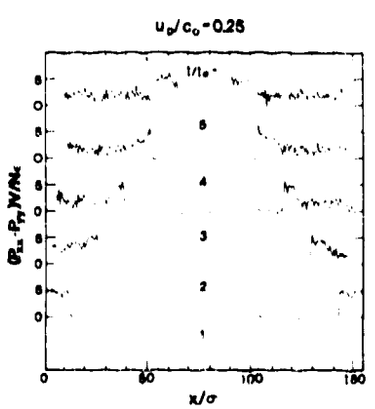

FIGURE 5. Shear (×2) component of the pressure-volume tensor for $u_p/c_o = 0.25$ at times t/t_o = 1, 2, 3, 4, and 5. Note the growth of the elastic region in front of the plastic wave, where the shear stress returns almost to zero.

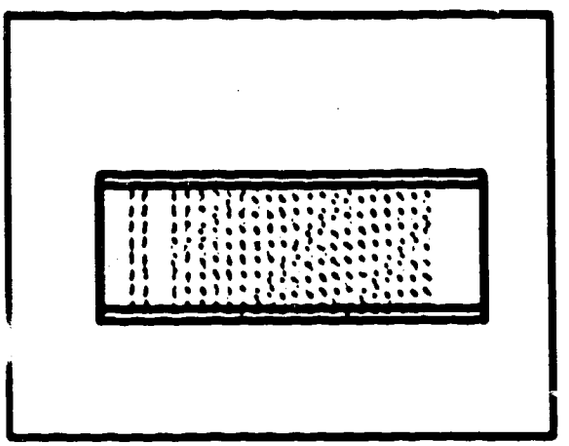

FIGURE 6. Snapshot from MD movie of chunks of slipped fcc crystal (along <111>-type planes) for a shock wave in the <100>-direction at $u_p/c_o = 0.25$.

due to dislocations. Stronger shocks show much less sensitivity to initial conditions. From these MD results, we conclude that even a perfect crystal exhibits plastic flow at sufficient shock strength, so that the presence of initial defects becomes secondary. There is a counterpart in real materials in the transition from weak-shock, heterogeneous shear bands to homogeneous deformation (or at least very small heterogeneity) at higher shock strengths.[11]

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