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Molecular Dynamics of Shock Waves in Three-Dimensional Solids: Transition from Nonsteady to Steady Waves in Perfect Crystals and Implications for the Rankine-Hugoniot Conditions

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Molecular-dynamics calculations of shock waves in perfect three-dimensional solids at nonzero initial temperatures reveal a transition in the nature of the asymptotic shock-wave structure as a function of shock strength. The key to this transition from nonsteady to steady waves where the Rankine-Hugoniot relations are obeyed is the partial relaxation of compressive shear stress behind the shock front which accompanies small, but permanent, transverse strains in atomic positions.

Molecular dynamics (MD) has been used as a tool to study the nature of shock waves for many years. An early three-dimensional (3D) MD calculation of a shock wave in a perfect crystal carried out by Tsai and Beckett[1] showed nonsteady-wave behavior. They concluded that the Rankine-Hugoniot (RH) jump conditions could not be used to analyze data from planar impact experiments. The RH relations between initial and final states in a shock wave depend on the existence of a steady wave in addition to the conservation of mass, momentum, and energy.[2] The equations of motion solved in MD explicitly obey the conservation laws, so that the test of the validity of the RH relations in MD shock calculations centers only on the question: Is the wave steady? In contrast to Tsai and Beckett's discovery of nonsteady waves, Paskin and Dienes[3] reported a series of MD calculations of shock waves in perfect Lennard-Jones 6-12 potential (LJ 6-12) crystals at nonzero initial temperature, where only steady waves were observed (and therefore, no significant deviations from the RH relations). A satisfactory resolution of these disparate findings has not yet been published.

In this paper we report the results of MD calculations of shock waves in perfect 3D LJ 6-12 crystals. As shock strength is increased, we observe a transition from linear growth of the shock-wave thickness (self-similar wave) to a finite shock width (steady wave) when the initial temperature T_0 is nonzero. A convenient measure of shock strength is the product αv, where α is the cubic anharmonicity coefficient for the pair potential (10.5 for LJ 6-12) and v is the piston velocity normalized by the long-wavelength sound speed. If $T_0 = 0$, we always observe self-similar waves, just as in the (1D) nonlinear chains.[4] We conclude that the transition from nonsteady to steady waves in perfect 3D $T_0 > 0$ crystals, as shock strength passes a critical value, is due principally to the increase in coupling between vibrational excitations normal and transverse to the direction of shock-wave propagation.[5] For strong shocks, the coupling between vibrational modes is strong and, along with the observation of steady shock waves, we see nearly complete compressive shear-stress relaxation behind the shock front accompanying small, but permanent, transverse strains in the atomic positions. The time and distance scales that are feasible for MD calculations may be far too restrictive to trace all the details of plastic flow behind a shock wave, especially where processes that depend upon the presence of defects may dominate. Thus, the observation of nonsteady waves for

weak shocks in MD experiments should not be used as a basis for attacking the RH relations. We find then that previous calculations reporting linear growth of the shock thickness[1] are in the 1D regime (weak shock strengths and low initial temperatures) and, therefore, not characteristic of a 3D solid, while others who have investigated LJ 6-12 solids[3] studied only the strong-shock or steady-wave regime.

We have performed MD caluclations of a 3D face-centered-cubic crystal of particles interacting with a pairwise LJ 6-12 central potential. Periodic boundary conditions were used in the x and y directions and the shock waves were generated by shrinking periodic boundary conditions in the z direction.[5] The initial and final thermodynamic states were both in the solid crystalline phase. Figures 1 and 2 give the results for two particular calculations: The first is for an initial temperature $T_0 = 0$ and is characteristic of the systems that exhibit one-dimensional behavior; the second is for $T_0 > 0$, corresponding to

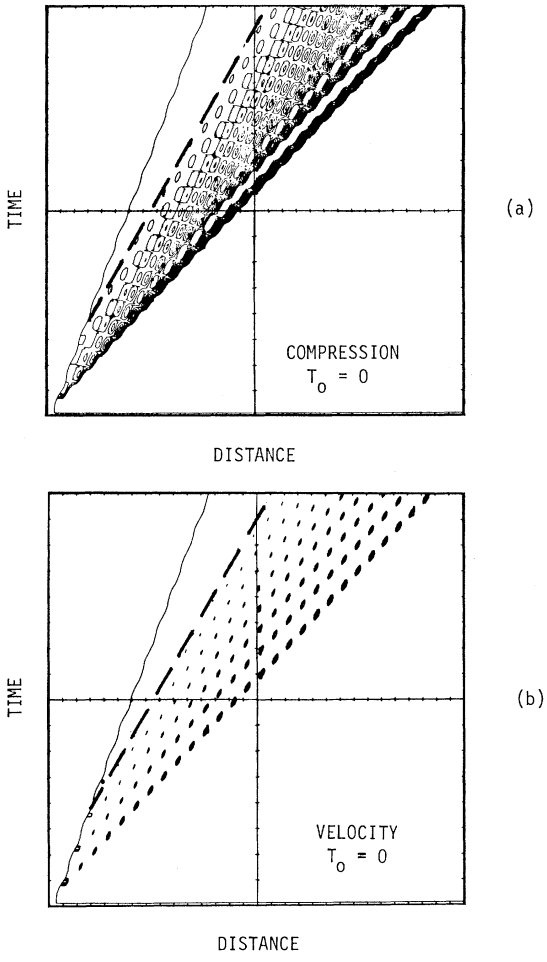

FIG. 1. Strong-shock wave in a $T_0 = 0$ Lennard-Jones system interacting with nearest neighbors. Distance-time contours plots of (a) the compression η, and (b) the z component of the particle velocity, v_z. The highest plotted contour is at the peak value while the lowest contour is at one e-fold decay down from the peak to the final value. The dashed lines are drawn to indicate the position of the lowest contour behind the shock front. Since the dashed lines are straight, but at an angle to the shock front, the wave is nonsteady and its thickness grows linearly with time.

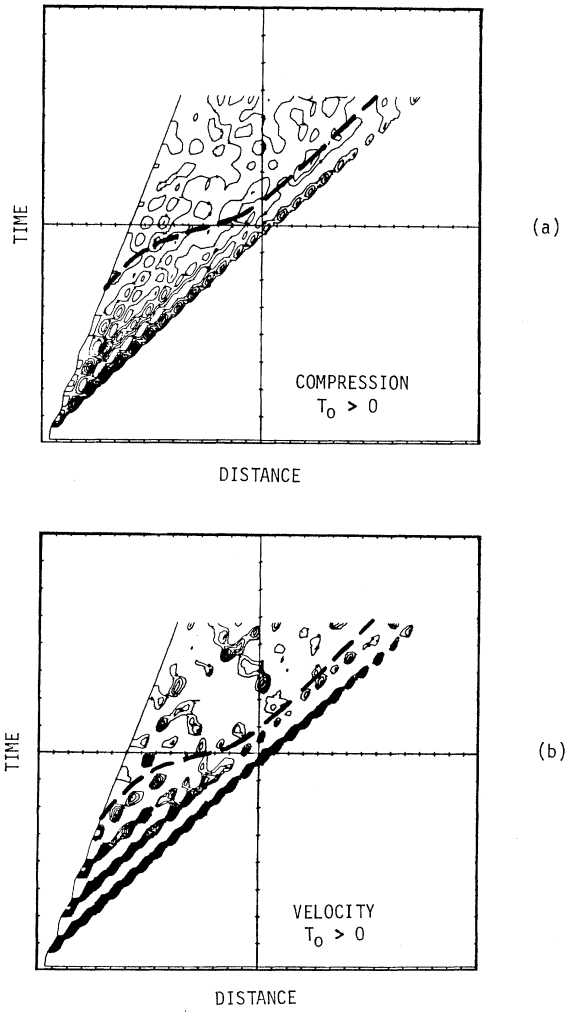

FIG. 2. Strong-shock wave in a $T_0 > 0$ Lennard-Jones system interacting with three shells of nearest neighbors. Distance-time contour plots of (a) the compression η, and (b) the z component of the particle velocity, v_z. Contours are determined in the same manner as in Fig. 1. The dashed lines are drawn at the rear of the shock where the final equilibrium thermodynamic state is achieved.

about one-tenth of the LJ 6-12 well depth, and shows steady-wave behavior. For both calculations the shock-strength parameter is given by $\alpha v = 10.5$ and is, therefore, considered to be a strong shock.[4] The $T_0 = 0$ system contained 1600 particles arranged in 200 planes with eight atoms per plane (2×2 unit-cell cross section). The $T_0 > 0$ system contained 1800 particles arranged in 100 planes with 18 atoms per plane (3×3 unit-cell cross section). In all cases, the initial density is such that nearest neighbors sit at the minimum of the potential well.

The $T_0 = 0$ calculation was purposefully chosen to be one dimensional in nature. The range of the potential was limited to first-nearest neighbors. Without any initial random motion of the particles, the shock generated in the z direction has no chance to transfer energy to vibrational modes in the x and y directions. The same qualitative behavior (self-similar wave) shown in the $T_0 = 0$ calculation was also observed in a $T_0 > 0$, $\alpha v = 0.525$, weak-shock calculation. In Fig. 1 we show distance-time contour plots of the z component of the particle velocity, v_z, and the compression η. The highest contour plotted corresponds to peak values and the lowest contours are at one e-fold decay down from the peak to the final value. The $T_0 = 0$ calculation shows no stress relaxation and the approach of the temperature to its final value is significantly slower than in calculations showing some stress relaxation. The kurtosis, or fourth-order cumulant, of the velocity distribution far behind the shock front is nonzero, implying a non-Maxwellian distribution.[6] The width of the shock wave grows linearly as indicated in the distance-time plots. For the weak shock $T_0 > 0$ calculation the width also grows linearly, so that the behavior is essentially one dimensional.

In Fig. 2 we show the v_z and η contour plots for a strong shock with $T_0 > 0$. The range of the potential is limited to a sphere containing third-nearest neighbors at the initial density. Stress relaxation of components normal and transverse to the direction of the shock propagation is observed along with small, but permanent, transverse strains in atomic positions.[7] The temperatures calculated from velocity components in the normal and transverse directions quickly equilibrate and the kurtosis of the velocity distribution goes to zero far behind the shock front, indicating a Maxwellian distribution. As indicated in Fig. 2, the shock-wave structure becomes steady with a finite width; consequently, the RH conditions are appropriate for describing the MD results. We have observed similar qualitative behavior for strong shocks in solid systems using other pair potentials. In MD calculations starting with a fluid as an initial state, we also see steady-wave behavior with finite shock thickness.

Steady-wave behavior is obtained by an appropriate combination of initial temperature and shock strength. For $T_0 = 0$ the shock is nonsteady and one dimensional for all values of αv. For $T_0 > 0$, we have found that the wave is nonsteady (self-similar) for small αv, but steady for large αv. As αv increases for a finite $T_0 > 0$ the anharmonic coupling increases until the vibrational modes are strongly coupled. It is possible that, by increasing T_0, steady-wave behavior will begin at a smaller αv, although we have not yet quantitatively determined the values for T_0 and αv where the transition from nonsteady to steady-wave behavior occurs. It is likely that this transition is an artifact of the perfect crystal, and that nonsteady-shock-wave behavior is unobservable in real crystals because of additional plastic flow mechanisms.

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