MOLECULAR DYNAMICS SIMULATIONS OF DEFORMATIONS OF TWO-DIMENSIONAL LENNARD-JONES CRYSTAL UNDER SHOCK COMPRESSION

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Résumé

Des simulations de dynamique moléculaire d'ondes de chocs dans un cristal bi-dimensionnel de Lennard-Jones sont présentées.
De telles simulations incluent automatiquement l'essentiel de la création et le mouvement des défauts qui ne peuvent pas être obtenus par une voie fondamentale à partir d'un modèle macroscopique.
Les représentations des configurations atomiques du cristal durant une compression par choc sont tracées par l'ordinateur. A partir de ces figures les processus de déformation du cristal ont été mis en évidence. La contrainte et la déformation dans un état intermédiaire au front de choc ont été calculées par dynamique moléculaire. Il a été observé que sous des ondes de choc suffisamment fortes l'état des contraintes en arrière du front d'onde devenait hydrostatique.

Abstract- Molecular dynamics simulations of shock wave in two-dimensional Lennard-Jones crystal are reported. Such simulations automatically include the essentials of defect creation and motion, which are not obtainable in a fundamental way from a macroscopic continuum model. Figures of atomic configurations of the crystal during shock compression are drawn by computer. From these figures, the processes of deformations of crystal can be watched. The stress and strain in intermediate state at the shock front are calculated by MD. It has been observed that under sufficiently strong shock waves, the state of stress behind the shock front became hydrostatic.

INTRODUCTION

Many articles have been published on the behaviour of solid subjected to dynamic loads which produce large inelastic deformations. The microscopic behaviour of solid under shock compression is only now beginning to be understood. One can simulate solid deformation on three different levels. The three levels refer to different scales of size and time. The macroscopic scale is the continuum field theory of heterogeneous plastic flow; the intermediate scale is dislocation dynamics, where moving and interacting dislocations are studied; and the finest scale is the atomic scale, where the motions of individual atoms are studied. The final scale is just the molecular dynamics simulation.

The procedure in molecular dynamics (MD) is to place N particles in a computational cell, specify the potentials of interaction among the particles, and calculate directly the motion of the particles by numerically intergrating the classical equations of motion (Newton's law). As MD calculations are usually limited at time intervals of the order of 100-1000 vibrational periods, it is best suited to events that take place quickly. According to this, molecular dynamics simulation techniques are of particular value in studying shock wave problems. A number

of MD simulations have been carried out to study shock wave problems/1-3/. In these early calculations, the main questions that have been studied are concerned about: (i) the shock wave profile and its stability; (ii) the validity of Hugoniot relations for an atomic solid; (iii) the linear behaviour of shock wave velocity with particle velocity. In this paper, we simulate the processes of shock compression of a two-dimensional Lennard-Jones crystal. We invetigate the mechanisms of deformation. We find that under sufficiently strong shock waves, the creation and motion of defects induced by shock may exert considerable influence on deformation development.

MODEL

The MD calculations are performed for a two-dimensional triangular lattice. We will assume that the atoms in the lattice interact through a Lennard-Jones potential:

$$V(r)=\varepsilon\left[(r_0/r)^{12}-2(r_0/r)^{6}\right]$$

In this expression V is the potential energy, r is the seperation of a pair of atoms, r_0 is the seperation at the minimum of the potential, and ε is the dissociation energy of the pair.

Before the lattice can be subjected to shock compression, the initial displacements and velocities of the atoms in the primary lattice must be specified. We assume the atoms are at their equilibrium lattice sites, and the lattice is in thermal equilibrium at temperature T, so velocities of the atoms may be distributed according to Maxwellian distribution.

When an appropriate set of initial conditions has been generated, the shock compression is applied by having the atoms at the surface layer, x=0, move continuously with a constant velocity U_0 along the x axis. The shock wave is then allowed to progress through the lattice in the x direction. The transverse surfaces to the wave motion are eliminated by using periodic boundary conditions in these directions.

Once the equations of motion have been solved to determine the positions and velocities for each atoms in the lattice, the results can be used to calculate macroscopic thermodynamic quantities of interest in the lattice. R.J.Hardy/4/ has derived formulas for determining local properties in molecular dynamics simulations. Using these formulas we can calculate macroscopic quantities such as the mass density ρ, local velocity u, energy density $\mathcal{E}$, and stress tensor $\vec{\sigma}$.

RESULTS

Using the laws of conservation of mass, momentum, and energy, one obtains the Hugoniot relations for a steady plane shock wave:

$$P_0 D = P_1 (D-u)$$

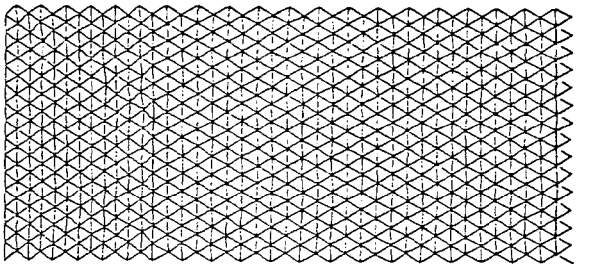
$$P_1 - P_0 = P_0 D u$$

$$E_1 - E_0 = \tfrac{1}{2}(P_1 + P_0)\left(\frac{1}{\rho_0} - \frac{1}{\rho_1}\right)$$

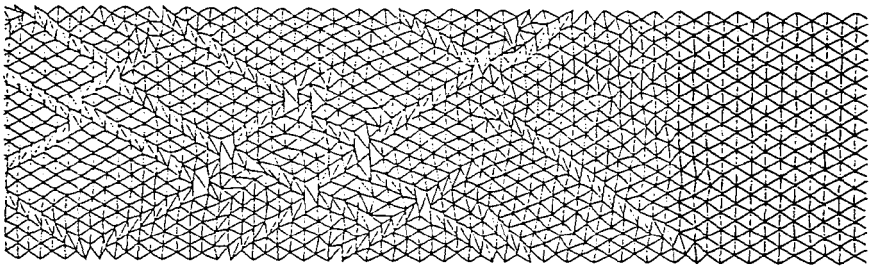
Here ρ is density, P is stress in the direction of wave propagation, i.e. σ_x, E is energy density, D is shock wave velocity, u is mass velocity behind the shock front, and indices '0' and '1' refer to the original and compressed states respectively.

In our computer simulations we calculate directly ρ , P , D and u and thus we can appraise the validity of the Hugoniot relations. We find that our results are in agreement with Hugoniot relations within about 5%. This is similar to the Paskin's calculations/1/.

In this paper we are more interested in deformations of the lattice under shock compression. We drew figures of atomic configurations of the lattice during the shock compression. From the change of the atomic configurations, we watched the processes of deformations. See Fig.1



(a)



(b)

Fig.1- Atomic configurations of the lattice under shock compression. (a) for a weak shock, $U_p=2.0(\sqrt{\varepsilon/m})$, m is the mass of an atom. (b) for a strong shock, $U_p=6.0(\sqrt{\varepsilon/m})$.

In Fig.1a, the lattice has been subjected to uniaxial compressive strain 12%. We can see a reduction in the lattice vector component along the axis of applied strain. In the vertical direction , the lattice vector component do not change, and the atoms still display sixfold coordination. In Fig.1b, the lattice has been subjected to larger uniaxial compressive strain 25%. In this case dislocations appeared. Because of the motions of dislocations, the rearrangement of the lattice took place, and the lattice displayed plastic behaviour obviously. After great plastic deformations, the conditions behind the shock front are almost hydrostatic. The consequences are similar to Smith's model/5/.

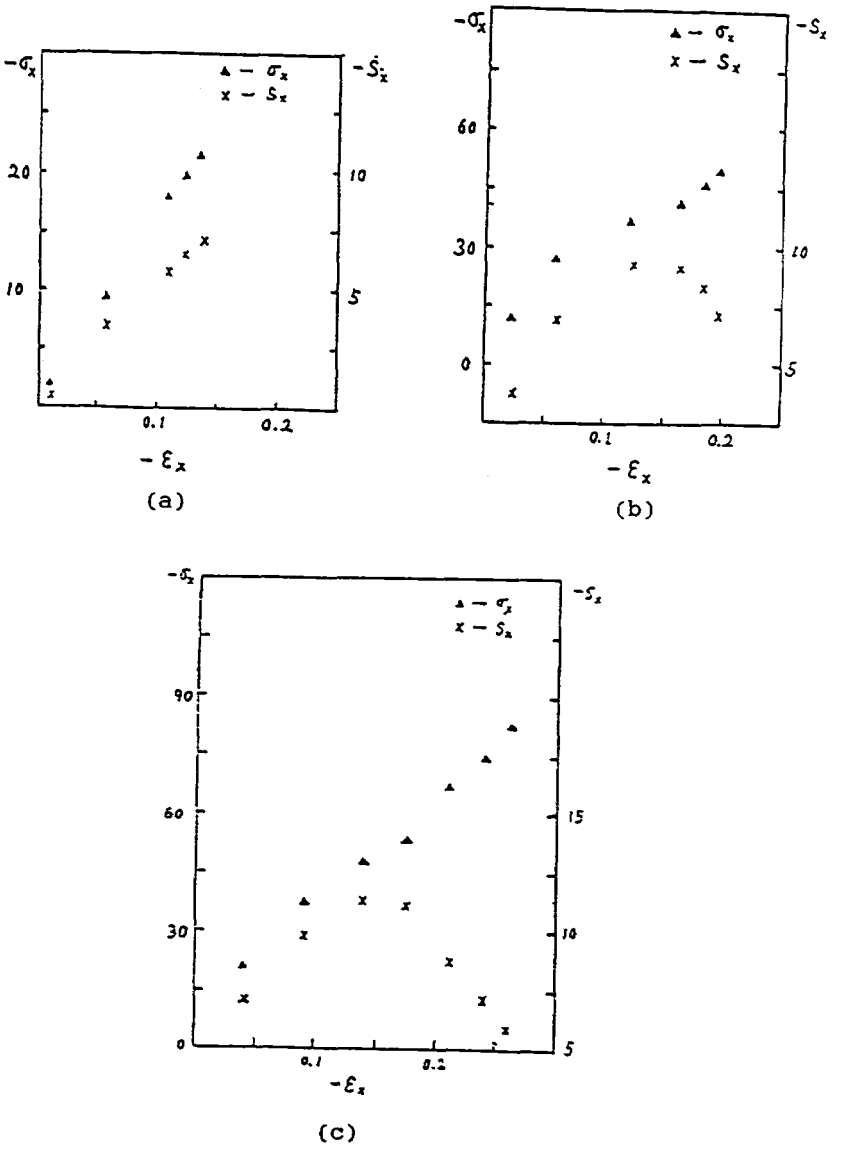


Fig.2- Stress state at the shock front. (a) for U_0=2.0($\sqrt{\varepsilon/m}$); (b) for U_0=4.0($\sqrt{\varepsilon/m}$); (c) for U_0=6.0($\sqrt{\varepsilon/m}$). The unit of stress σ_x and S_x is ($2\varepsilon/r_0^2$).

Fig.2 shows data calculated for the stress component σ_x and deviator stress component S_x in intermediate states at the shock front as function of strain ε_x in the direction of propagation of the wave for vairous shock compression intensities. Where the deviator stress $\hat{S}$ is defined by

$$S_{ij} = \sigma_{ij} - \sigma_m \delta_{ij}$$

Here σ_m is hydrostatic pressure $\sigma_m = (\sigma_x + \sigma_y + \sigma_z)/3$
The uniaxial strain ε_x is defined by

$$\varepsilon_x = (P_0 - P)/P$$

S_x is related to the maximum shear stress τ_{max} by

$$S_x = \frac{4}{3}\tau_{max}$$

Shear stress τ_{max} is very important for an analysis of the development of plastic deformations.

From Fig.2, we noticed the following characteristics of the stressed state:

1. When shock wave is weak, as shown in Fig.2a, stress σ_x and deviator stress S_x increased monotonicly with an increase of strain ε_x in the shock front, which corresponding to the situation of Fig.1a.

2. As shock wave intensity increased, as shown in Figs.2b and 2c, $\sigma_x - \varepsilon_x$ function was still monotonic, but $S_x - \varepsilon_x$ function became nonmonotonic. After S_x reached a peak value, it began to decrease with increases of ε_x. This phenomenon demonstrated that the shear stress relaxation by plastic flow occured in the shock wave front.

3. It can be seen from Figs.2b and 2c that the stronger shock wave, the higher peak value of S_x is. It is possible for the shear stress to exceed the theoretical strength. The corresponding state is called "supercritical shear".

Some of the above mentioned characteristics have been observed in experiments. Nevertheless, it is inaccessible to measure more details of the stress state at the shock wave front by experiments.

CONCLUSIONS

In this paper we have summarized a program of work aimed at providing a understanding of mechanism of deformations of crystals under shock loading. The molecular dynamics results can be at least semi-quantitatively reproduced by a model which involves the creation and motion of defects. Future studies will focus on the determinations of the relations between shear stress and motions of dislocations induced by shock. We will also study the effects of density and velocity of dislocations on plastic deformations.

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