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A molecular dynamics study of the shock-induced defect microstructure in single crystal Cu

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ABSTRACT

Molecular dynamics simulations of shock compression are carried out over a range of pressures (from 22 GPa to 75 GPa) to investigate the shock-induced defect microstructure in single crystal Cu. The results show that under increasing shock pressure, we can detect three distinct phases of the defect regimes for single crystal Cu: dislocations → stacking faults → twins. We show the evolution processes of different defect microstructures. According to the analyses of these evolution processes, the formation mechanisms of various defect microstructures are studied. When the shock pressure is less than 30 GPa, the motion of dislocations is a significant mechanism in single crystal Cu under the shock compression. The motion between various dislocations and loops widely exists on the (1 1 1) close-placed plane. The interesting dislocation loops are obtained at a relatively low pressure, and a new mechanism of nucleation and development of the dislocation loop is proposed. When the shock pressure is greater than 30 GPa, a large number of intersecting stacking faults are formed. On the (0 0 1) surface, stacking faults align along the [2 2 0] and [$\bar{2}$ 2 0] directions at exactly 90 degrees, and they are present roughly in the same proportion. The stacking fault spacing decreases with the increase of shock pressure, and shock-induced plasticity increases as a function of shock strength. The structure of the simulation, based on the topology, matches extremely well with that found in recent transmission electron microscopy studies of single crystal Cu recovered from laser shock experiments. At a relatively high pressure (61 GPa), we find that the stacking faults and twins exist together in single crystal Cu. It is shown that two types of stacking faults with vertical directions are the competitive mechanism. When one of them dominates, twins will be formed from this type of stacking fault. Thus, the directions of twins are randomly distributed in the initial stage. Rotation and combination of twins are significant mechanisms, and these mechanisms lead to the final formation of twins. At 75 GPa, twins elongate along [1 $\bar{2}$ 1] and [$\bar{1}$ $\bar{2}$ $\bar{1}$] directions on the ($\bar{1}$ 0 1) surface. The configuration and direction of the twins are in agreement with experimental results.

1. Introduction

The dynamic mechanical behavior of materials is crucial for detonation physics, solid mechanics, condensed matter physics and materials science. As basic research, it is important to national defense technology, manufacturing and production safety, and so on. The response of materials to an extreme load and the mechanism of the evolution of the microstructure have been topics of great interest for decades [1]. Laser quasi-isentropic compression and laser shock with single crystal Cu experiments have attained pressures of tens of GPa and strain rates greater than 10^7 [2–6]. The defect structures and deformation mechanism of metal Cu change with increasing shock pressure. At relatively low shock pressures, it was found [2] that the structural defect of single crystal Cu is a dislocation cell; moreover, a large number of dislocation loops exist in the dislocation cell. A significant number of stacking faults were observed [2] in single crystal Cu when it was subjected to intermediate pressures. Furthermore, when the shock pressure was higher than 50 GPa, twins became the dominant defect substructures. Experimental studies [2–5] illustrated that the defect regimes of single crystal Cu under increasing shock pressure followed the following pattern of structural change:

dislocation cells → stacking faults → twins

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As a complementary method to laser shock compression experiments, molecular dynamics (MD) simulations are an effective tool for studying the microstructural evolution of metal materials because of the similar time and length scales. Using MD simulations, Holian and Lomdahl [7] investigated the plasticity induced by shock waves in face-centered cubic crystals. Shock-induced plasticity was proposed to quantitatively analyze the plasticity. Bringa et al. [8] presented MD simulations of the Hugoniot relationship for Cu, for pressures in the range of 2–800 GPa, and large anisotropies were found for shock propagation along ⟨1 0 0⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩. Davila et al. [9] studied the shock-induced void collapse in Cu. In 2002, Kadau et al. [10] examined the monocrystalline Fe undergoing shock wave loading by using two different embedded atom methods (EAM) [11] potentials. The shock-induced phase transformation (bcc → hcp) of solid iron was investigated, and a split two-wave shock structure was observed above a critical shock pressure. Kadau et al. [12] further studied the propagation of shock waves through polycrystalline Fe. The simulated shock Hugoniot relationship compared well with the experimental results. Herbert et al. [13] investigated the interplay of plasticity and phase transformation in shock wave propagation in nanocrystalline iron. They showed that plasticity was mostly given by the deformation of dislocation loops, which crossed the grains and left behind screw dislocations. With the c axis analysis technique and lattice tracking algorithm, Wang et al. discussed different phase transition mechanisms in monocrystalline [14] and polycrystalline iron [15] under shock loading conditions. The shock compression of monocrystalline and nanocrystalline Ni was simulated by Jarmakani et al. [16]. Contributions to the strain from the different mechanisms of plastic deformation, such as partial dislocation, perfect dislocations and twins were quantified in nanocrystalline Ni. Cao et al. [17] studied the structures of monocrystalline Cu under shock compression on [0 0 1] and [2 2 1]. The topology of these structures compared extremely well with that observed in transmission electron microscopy (TEM) studies of shock-induced plasticity in samples recovered from laser shock experiments. Murphy et al. [18] used X-ray diffraction to measure shear strains in single crystal copper shocked at pressures above 100 GPa, and the results showed that the compressions deduced from the diffraction data are in agreement with MD. Milathianaki et al. [19] also reported femtosecond X-ray diffraction measurements unveiling the response of copper to a laser shock-compression of ~73 GPa and strain rates of 10^9 per second. The results provided a direct comparison with multimillion-atom MD simulations. Because of the close resemblance of the resulting stress state with that one behind a shock front, Dupont and Germann [20] studied the dependencies of the strain rate and crystal orientation on the strength of single crystal copper under uniaxial strain compression at various temperatures. Kattoura and Shehadeh [21] utilized multiscale dislocation dynamics plasticity (MDDP) simulations to study the mechanical response of single crystal copper undergoing shock loading at high strain rates. The review article of Meyers et al. [22] contributed to a comprehensive understanding of metals under shock compression. The defect microstructure of single crystal Cu under different shock pressures and strain rates were described in shock compression experiments. However, the evolution of defects, which were difficult to observe by experimentation, can be obtained in MD simulations, and some important deformation details can be obtained from MD results.

In this study, we use MD simulations to study the propagation of shock waves through single crystal Cu samples along the [0 0 1] direction over a range of shock pressures (from 23 GPa to 76 GPa). By observing dislocation loops, shock-induced plasticity, directions of stacking fault traces, sizes and directions of twins, and so on, the defect microstructure of single crystal Cu under different shock pressures is analyzed in detail. Moreover, the MD results are compared to results obtained from laser-shock experiments. In particularly, we examine the motion between various dislocations and loops at a relatively low shock pressure, and a new mechanism of nucleation and development of a dislocation loop is proposed.

2. Computational methods

The simulations are performed with the open-source LAMMPS code [23]. Cu atoms interact via the EAM potential developed by Mishin et al. [24], which was used in previous studies for shock waves in single crystal Cu [25]. This potential is fitted to provide a stacking-fault energy (SFE) of 45 mJ/m^2. The [0 0 1] single crystal Cu sample contains 2 million atoms, has a length of 72.3 nm in the direction of the shock (z direction) and has an edge length of 18.075 nm perpendicular to it (x and y direction). It is therefore deemed large enough to study the stages of shock-induced plasticity and the defect microstructure. The initial samples are perfect fcc single crystal copper and there is no defect in the simulation domain. The advantage of the ideal perfect fcc sample is that it can eliminate the influence of other factors (initial dislocations, vacancies, interstitials, etc.). The samples are first equilibrated to achieve a minimum energy state. An initial low temperature of 5 K is set. This low temperature is chosen to minimize thermal noise and thus to facilitate the analysis of defect formation. Shock waves in the MD simulations are produced by the piston driven algorithm [7]. A thin slab (three lattice constant thicknesses of atomic planes of Cu) of the simulation volume is treated as the piston in the simulation. The atoms of the piston are assigned a piston velocity U_p in the z direction and zero velocity transverse to it. In this study, the piston velocities U_p vary from 500 m/s to 1400 m/s. To minimize edge effects, periodic boundary conditions are imposed on the lateral surfaces, and the shock waves propagation direction is set as a free boundary.

To analyze the results, we divide the sample into small slabs with a thickness of 0.723 nm along the z direction, and the results of each slab are determined as the average value of that slab. We monitor the stress in the z direction, P_{zz}, and the shear stress P_{shear}. The shear stress P_{shear} is defined as:

$$P_{shear} = \frac{1}{2}\left[P_{zz} - \frac{1}{2}(P_{xx} + P_{yy})\right] \quad (1)$$

where P_{xx} and P_{yy} are transverse normal stresses. The shock pressure is also obtained by the Hugoniot relation [26]:

$$P = \rho_0 U_s U_p \quad (2)$$

where ρ_0 is the density of Cu. The velocity of the shock wave, U_s, can be calculated from the propagating front at different times in our samples. The shock pressure can be calculated both from our MD simulations (P_{zz}) and the Hugoniot relationship (Eq. (2)) once U_s and U_p are known. Finally, we analyze the defect microstructure using adaptive common-neighbor analysis (CNA) [27]. The Dislocation Extraction Algorithm (DXA) [28] is utilized to visualize the dislocation motion by OVITO [29].

3. Results and discussion

Fig. 1 shows P_{zz} and P_{shear} along the z direction of different piston velocities at 6 ps. The Hugoniot Elastic Limit (HEL) [30] of Cu is identified by the dashed line. Bringa et al. [8] found that the HEL of single crystal Cu is 32 ± 2 GPa from MD simulation. When the piston velocity is above 650 m/s, the shock pressure is above HEL. The shear stress is approximately 4.5 GPa at a shock pressure of 30 GPa. At shock pressures above the HEL, shock waves traveling along the [0 0 1] orientation leads to the emission of intersecting Shockley