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Investigations of shock-induced deformation and dislocation mechanism by a multiscale discrete dislocation plasticity model

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ABSTRACT

There are many theoretical and computational investigations devoted to the dislocation mechanism based crystal plasticity under static or quasi-static conditions. However, the dislocation behavior, specifically the nucleation and multiplication of dislocations, remains unclear in crystal under shock loading. In this paper, the dislocation mechanism in single crystalline copper under shock loading is investigated through a multiscale numerical model, which couples discrete dislocation dynamics (DDD) with explicit finite element (FE) analyses. Firstly, since the homogeneous nucleation (HN) of dislocations is considered as the dominant dislocation generation mechanism at extremely high strain rates, the typical parameters of HN are obtained by systematic molecular dynamics (MD) simulations, which include critical shear stress, saturation time, stable density, etc. Then, these parameters are implemented into DDD-FE model by a coarse grained method. It can remarkably improve the computational efficiency without loss of typical dislocation characters. The interactions between shock wave and dislocations are studied in detail. Band-like dislocation walls and their shielding effect on other dislocations are observed during the shock wave propagation. The simulation results are in good agreement with experimental observations. It is also found that both fast HN and avalanche-like dislocation multiplication get involved and lead to the softening of shear stress. Finally, by comparing the dynamic behavior under different impact speeds, a threshold speed around 1000 m/s for the dislocation dominant mechanism is proposed from the computations in this work. Beyond this speed, the effect of other defects such as stacking fault and twinning would be prominent.

1. Introduction

The mechanical response of material under shock loading has been a topic of interest for more than a century. The exploration of material dynamic deformation is valuable and has a wide range of applications, such as explosive forming, shale oil and gas horizontal well perforation and shock synthesis. Various experiments [1–3] have been carried out to investigate the dynamic mechanical behavior of materials, especially the equation of state (EOS) and the strength of materials under shock loading. A uniaxial strain state of deformation is achieved in the material under shock conditions, and a high-pressure wave propagates along the loading direction. With the increase of impact strength, plastic deformation happens when the applied pressure exceeds the Hugoniot elastic limit, accompanying an amount of dislocation nucleation and multiplication.

In the case of high strain rate loading, dislocation plays an important role in determining the material behavior. Many researchers contribute their talents to explore the connection between microscopic dislocation structures and dynamic mechanical behavior of material through a series of experiments [4–6]. Simultaneous shock compression and X-ray diffraction experiments were introduced by Johnson et al. [7], who offered an attractive method of observing distortions in the lattice as it was being compressed. By the laser-induced shock compression of monocrystalline copper, Meyers et al. [8] found that the number of dislocation loops was much larger than that observed in undeformed copper. They suggested that the loop nucleation was an essential event of laser-induced shock compression at pressures of 12 and 20 GPa. Chang et al. [9] revealed that there was a close relationship between the laser shock processing induced nanocrystallization and dislocation generation. In general, the dislocation microstructures observed in the recovered samples consist of dislocation

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cells, shear bands and deformation twins [10,11]. It is also found that there is a threshold pressure at which the deformation mechanism changes from dislocation glide to twinning [12], and the transition pressure is dependent on the crystal orientation. These studies provide significant understandings on the evolution of microstructures under shock loading. However, to our best knowledge, a higher resolution observation of the simultaneous evolution of dislocations is still lacking since much of what we know is inferred from the recovery experiments or analysis of wave profiles.

Various simulations are carried out to investigate how the simultaneous microstructures affect the dynamic mechanical behavior of material [13–16], especially the shock-induced dislocation plasticity. Cao et al. [17] analyzed the dislocation structure under shock loading by molecular dynamics (MD) simulations. The density of microstructures in the simulations was extremely larger than that in the experiments and they attributed the difference to the recovery process and the much longer stress rise time ($\sim$1 ns) in flyer-plate shock experiments. In order to eliminate the space-time gap between MD simulation and experiment, multiscale DDD simulations [18] were conducted to investigate the dislocation structure and stress distribution in silicon crystal during the laser shock process. The homogeneous and heterogeneous nucleations of dislocations in copper single crystals were investigated by the same model [19], the results suggested that the homogeneous nucleation (HN) of dislocations would be dominant as shock rise time decreases. This conclusion is consistent with the simulation results obtained by Benat et al. [20]. The HN would become the dominant dislocation generation mechanism when the strain rates exceeded $5 \times 10^7\ s^{-1}$. It is because that the Frank-Read sources were unable to operate before HN relaxed elastic stresses. In these studies, the HN of dislocation was generally introduced at the position where critical shear stress exceeded a specific value. The density of nucleated dislocation sources was always artificially defined and lack of discussion [19,21]. However, the density of dislocation sources has a significant effect on the dynamic mechanical behavior of materials, especially the stress relaxation at the front of shock wave. How to properly introduce the HN processes, i.e. dislocation shape, location and nucleation density, is still lack of critically tested.

In this paper, the dynamic mechanical behavior of single crystalline copper pillar and the corresponding dislocation microstructure are investigated by coupling discrete dislocation dynamics (DDD) with explicit finite element (FE) analyses. Dislocation motion and discrete plasticity are determined by DDD modeling. The basic laws of continuum mechanics including the momentum balance and the conservation of energy equation are solved by FE method. The HN of dislocation is introduced into the DDD-FE calculation by a coarse grained model developed from systematic MD simulations. The coupling procedures are described in detail in Section 2. Then the shock-induced plasticity and dynamic mechanical behavior of single crystalline copper pillars are investigated in Section 3. The typical dislocation microstructures and their connection with dynamic mechanical responses are analyzed. The results are compared with the experimental findings available in the literature. Finally, some discussions and conclusions are given in the last two sections.

2. Methodology

DDD-FE simulation merges discrete and continuum modeling and is used to establish the connections between dislocation microstructures and macroscopic mechanical behavior. The goal of this section is to present new features in our DDD-FE model for shock simulation, which is compared with existing multiscale discrete dislocation plasticity model. Particularly, a coarse grained description of HN is proposed to bridge the space-time gap between MD and DDD-FE simulations, it avoids the artificial introduction of dislocation sources [19].

2.1. Dynamic multiscale discrete dislocation plasticity model

Multiscale discrete dislocation plasticity model that links discrete and continuum analysis has achieved various remarkable research results [22–24]. In the framework, DDD method has been presented in detail in our previous work [25–27]. Dislocation curves are discretized into straight segments. At each time step, the forces acting on all dislocation segments are evaluated and the dislocation velocities are calculated by solving the equations of motion. Then, the dislocation positions are updated for the next time step.

To investigate impact problems, the DDD-FE coupling procedure is quite different from those static issues [24,28]. Firstly, under shock loading, a large amount of plastic work is generated in a very short time as a result of dislocation motion. The plastic work can be converted to thermal energy and lead to significant local temperature rise. The conservation of energy equation is expressed as

$$\rho c\dot{T} = \lambda_t \nabla^2 T + \gamma \cdot (\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^{\boldsymbol{p}}), \tag{1}$$

where ρ is the mass density, T is the temperature, c and λ_t are specific heat and thermal conductivity. γ is a thermal scaling factor representing the transformation from plastic work to thermal energy. $\boldsymbol{\sigma}$ is the stress tensor and $\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{p}}$ is the plastic strain rate due to dislocation motion.

Then, the thermo-elastic response of metal materials can be expressed using the rate form of Hooke's law for large deformation such that:

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{C}^{\boldsymbol{e}} : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{p}) + \beta_t \dot{T} \cdot \boldsymbol{I}. \tag{2}$$

Here, $\dot{\boldsymbol{\sigma}}$ is the co-rotational stress rate and $\boldsymbol{C}^e$ is the elastic stiffness tensor, $\dot{\boldsymbol{\varepsilon}}$ and $\dot{\boldsymbol{\varepsilon}}^p$ are total strain rate tensor and plastic strain rate tensor. $\beta_t = -\frac{E}{1-2\nu} \cdot \alpha$, in which E, ν and α are Young's modulus, Poisson ratio and line expansion coefficient, respectively. $\dot{T}$ is the temperature change rate and $\boldsymbol{I}$ is a unit matrix.

The momentum equation is solved using the dynamic FE method such that:

$$\boldsymbol{M}\ddot{\boldsymbol{U}} + \boldsymbol{C}\dot{\boldsymbol{U}} + \boldsymbol{K}\boldsymbol{U} = \boldsymbol{F}, \tag{3}$$

where $\boldsymbol{M}$, $\boldsymbol{C}$ and $\boldsymbol{K}$ are mass matrix, damping matrix and stiffness matrix, respectively. $\boldsymbol{U}$ is the nodal displacement. $\boldsymbol{F}$ is the force vector which includes the external nodal force and the thermal force due to temperature change. The coupled thermal-stress analysis is implemented by the commercial software ABAQUS, an explicit integration scheme is used to solve the displacement vector. The determination of the time step in FE procedure is related to two processes, i.e. the stable time increment of solid deformation and the stability limit for thermal diffusion.

As a summary, the DDD-FE coupling procedure is illustrated as shown in Fig. 1 and mainly contains the following information-transfer processes: (1) Calculate the plastic strain $\boldsymbol{\varepsilon}^{\boldsymbol{p}}$ generated by dislocation slip in DDD simulation. Then the discrete plastic strain is localized to continuum material points by a new regularization method proposed by Cui et al. [29]. (2) Solve the heat conduction equation by taking the plastic work as inner heat source. The dynamic stress field associated with the thermal effect is calculated by FE method under a specific boundary condition. The stress field $\boldsymbol{\sigma}$ is then transferred to DDD and serves as the applied force to drive dislocation motion. (3) The displacement field U of FEM cell is