Study of dynamical mechanical properties and dislocation dynamics of copper single crystals by discrete dislocation dynamics simulation

S L He\(^1\), W T Jiang\(^{1,3}\), J S Bai\(^2\), M Y Zhang\(^2\) and H D Fan\(^{1,3}\)

\(^1\)Department of Mechanics, Sichuan University, Chengdu 610065, China
\(^2\)Institute of Fluid Physics, CAEP, Mianyang 621999, China

E-mail: scubme@aliyun.com(W T Jiang); hfan85@scu.edu.cn (H D Fan)

Abstract. In this work, the dynamical mechanical properties and dislocation evolution of copper single crystals were studied using the discrete dislocation dynamics (DDD) method coupled with dynamical finite element method. The influence of strain rate, dislocation density and crystalline orientation were investigated. Strong strain rate effect was observed in DDD simulations, namely, the yield stress increases with the increasing strain rate. In addition, the dislocation density shows an unexpected influence on the yield stress, i.e., the yield stress decreased with dislocation density. The crystalline orientation was also studied and discussed.

1. Introduction

With the rapid development of science and technology, more and more attentions were paid to the dynamical mechanical properties of metallic materials in the fields of defense weapons, vehicles and aerospace. The deformation mechanisms and mechanical responses of metallic materials under dynamical loadings are fundamentally different from those under static loadings. Due to the short duration of dynamical loadings, the material properties show strong strain rate effects, shock wave effects and temperature effects [1]. Because of the high temperature and high pressure environment caused by high speed or impact loadings, dislocation loops, dislocation cells, phase transformation and deformation twins may occur, which are difficult to occur under static loadings. The failure modes also show significant differences, such as thermoplastic shear bands, dynamic fracture, spalling [2]. It is significant to study the dynamical properties of metallic materials and reveal their relationship with the microstructure.

Dislocation slip is a general plastic deformation mode and the collective dislocation behavior plays an important role in the dynamical responses of metallic materials. Therefore, discrete dislocation dynamics (DDD) simulation is an effective method to study the dynamical property of metallic materials. In DDD method, dislocations are treated as line defects in an elastic medium. Various dislocation mechanisms are considered, such as long-range interaction, dislocation junction, dislocation cross slip, dislocation glide [3-8]. Shehadeh et al. introduced shock wave loading in DDD software multiscale dislocation dynamics plasticity (MDDP). Results show that dislocation density increases with the increase of peak pressure and duration time of shock wave loading, and especially irregular dislocation cells were observed [9, 10]. They also studied dislocation homogeneous nucleation and heterogeneous nucleation, and pointed out that the stress of homogeneous nucleation is about 20 GPa [11]. Furthermore, Zbib and Hamid developed a continuum dislocation dynamics (CDD) plasticity model based on DDD
simulations to analyze the mechanical behavior of polycrystalline materials under unidirectional tensile test [12, 13]. Liu et al. and Hu et al. used the DDD method coupled with the finite element method to simulate the dynamical mechanical properties of copper. Numerous dynamical mechanisms were revealed, including strain rate hardening effect, dislocation uniform nucleation, banded dislocation wall, and critical impact velocity of dislocations [14, 15]. Cheng and Shehadeh conducted DDD simulations of laser shock peening and found that laser shock peening processing conditions are strongly relied on dislocation density, dislocation multiplication rate, and dislocation microstructure [16]. Shehadeh employed MDDP to investigate shock-induced deformation in monocrystalline copper and showed that the effect of resident dislocations on the strain rate effect can be ignored when a homogeneous nucleation mechanism is considered [17]. Gurrutxaga-Lerma et al. found that the nucleation strength of dislocation sources increases with the increase of strain rate, but when the strain rate is higher than 5×10⁷/s, dislocations can be nucleated uniformly [18].

During the plastic deformation mediated by dislocation slip, the dislocation density plays an important role. Zhao et al. pointed out that a large fraction of equilibrium high-angle grain boundaries and a low dislocation density improve the toughness and uniform elongation of ultrafine grained materials [19]. Yellakara and Wang revealed that for low dislocation density, the relationship between yield stress and dislocation density is not as definite as the linear relationship in crystal plasticity theory. The plastic flow is very sensitive to the initial distribution of dislocations in material systems with low dislocations [20]. However, Young showed that the yield stress is determined by the stress necessary to break the gliding dislocations through impurity atom barriers in the crystal, which is weakly related to the initial dislocation density [21]. It can be seen that the influence of dislocation density on the material strength under dynamical loading is not clear.

As aforementioned, the mechanical properties of metallic materials are strongly dependent on the evolution of dislocation microstructure. Especially strain rate, dislocation density and crystalline orientation have a strong influence on the material strength, but the dislocation density was not understood fully. DDD method is an effective tool to study the dynamical property of metallic materials. Aiming at this, DDD simulations were performed towards revealing the dynamical mechanical property and dislocation evolution of copper single crystals.

![Simulation cell with Frank-Read dislocation sources.](image)

**Figure 1.** Simulation cell with Frank-Read dislocation sources.

### 2. Simulation method

The coupling algorithm of DDD and finite element method (FEM) is used here to study the relationship between dislocation evolution and macroscopic mechanical properties [22]. FEM is performed by
ANSYS, where the inertial effect of material is considered. The simulation cell has a size of $X-4000b*Y-4000b*Z-40000b$, where the magnitude of Burgers vector $b$ is 0.25 nm. Elastic modulus is 101.38 GPa. Frank-Read dislocation sources are generated in the simulation cell. A simulation cell with Frank-Read dislocation sources is shown in figure 1. The dislocation source length is 4000 b. Dislocation mobility coefficient is $10^{-4}$ Pa∙s. A strain-controlling loading is applied in the Z direction of the simulation cell, as shown in figure 1. Free surface boundary conditions are used in the Z direction, and periodic boundary conditions are used in the X and Y directions. In this paper, three cases were studied, where the strain rate was changed from 10 to 1000 s$^{-1}$, dislocation density from $10^{11}$ to $10^{13}$ m$^{-2}$ and crystalline orientation angle $\theta$ from 0° to 90° ($\theta$ is the angle between loading direction and [001] direction). In order to avoid contingency, in each case, three simulations were performed with same dislocation density but different random distributions of initial dislocations.

3. Simulation results

First, the strain rate effects were studied in copper single crystals. Three strain rates were selected here, namely 10$^1$, 100$^1$, and 1000 s$^{-1}$. The initial dislocation density is $10^{12}$ m$^{-2}$, and the orientation angle is 0°, i.e. [001]. The calculated stress-strain curves with different strain rates are shown in figure 2(a). It can be seen that the three curves in each case show no significant difference, indicating that the random distributions have minor influence on the current predictions. The crystal under strain rate of 1000 s$^{-1}$ was observed to have the shortest elastic stage and lowest yield stress. When the strain reaches 0.6%, the crystal yields at a stress of 590 MPa. In the case of 100 s$^{-1}$, the crystal yields at the strain of 0.09% and stress of 90 MPa. In the case of 10 s$^{-1}$, the crystal yields when the strain reaches 0.03% and stress reaches 30 MPa. It could be seen that the strain rate has a strong influence on the material strength. In order to see the strain rate effects, the yield stress at plastic strain of 0.2% is plotted in figure 2(b) as a function of strain rate. Clearly, the yield stress increases exponentially with the increasing strain rate. In previous experiments of Al-Mg-Sc alloys by Pereira et al. [23], the strength exhibited an exponential relationship with strain rate, which was in good agreement with the current simulations.

![Figure 2](image-url) (a) Stress-strain curves of copper single crystals under different strain rates. (b) The yield stress versus strain rate.

The stress-strain curves of copper single crystals of different dislocation densities ($10^{11}$ m$^{-2}$, $10^{12}$ m$^{-2}$, $10^{13}$ m$^{-2}$) are shown in figure 3(a). It could be seen that the stress levels in the flow stage decrease remarkably as the dislocation density increases, i.e. ~350 MPa at density of $10^{11}$ m$^{-2}$, ~200 MPa at $10^{12}$ m$^{-2}$, 100 MPa at $10^{13}$ m$^{-2}$. In figure 3(b), the yield stress is plotted as a function of initial dislocation...
density. It can be seen that the yield stress has an inverse exponential relationship with the dislocation density. As is well-known, the yield stress increases with the increasing dislocation density under quasi-static loading, namely, the famous Taylor formula, \( \sigma \propto \sqrt{\rho} \). Here the material strength under dynamical loading is different from that under quasi-static loading. Previously, Yellakara and Wang observed that the yield stress of copper single crystal does not increase with the increase of dislocation density before density of \( 10^{12} \text{ m}^{-2} \). They pointed out that for low dislocation density or small number of dislocations, the relationship between yield stress and dislocation density is not as deterministic as the linear relationship in crystal plasticity theory [20]. The relationship between yield stress of materials and low dislocation density will be further explored in our future work.

Aiming at the effects of orientation angle on the dynamical property of copper single crystals, six crystals are investigated here which have different orientation angles including 0, 15, 30, 45, 60, 75, and 90°. The initial dislocation density is \( 10^{12} \text{ m}^{-2} \), and strain rate is 100 s\(^{-1}\). The stress-strain curves are shown in figure 4(a), and the yield stress is shown in figure 4(b) as a function of the orientation angle. It could be seen that the orientation has a strong influence on the dynamical property. As the orientation angle increases from 0° to 15°, the yield stress decreases, then rises before 45°, and finally drops again.

**Figure 3.** (a) Stress-strain curves of different initial dislocation densities. (b) The yield stress as a function of the initial dislocation density.

**Figure 4.** (a) Stress-strain curves of copper single crystals of different orientation angles. (b) The yield stress as a function of orientation angle.
4. Summary
The dynamical mechanical property of copper single crystals was studied in this paper. Especially, the influence of dislocation density, strain rate and crystalline orientation was studied on the yield stress of copper single crystals. It was found that the yield stress increases exponentially with strain rate. When strain rate grows from $10$ to $1000$ s$^{-1}$, the yield stress rises from $36$ to $1055$ MPa. The yield stress increases with the decrease of dislocation density. When dislocation density drops from $10^{13}$ to $10^{11}$ m$^{-2}$, the yield stress rises from $114$ to $338$ MPa. As the loading axis deviates from the [001] axis, the yield stress first decreases, then increases, and finally drops again. When the orientation angle is $45^\circ$, the yield stress reaches the peak value of $296$ MPa.

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