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## On the rate sensitivity in discrete dislocation plasticity

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## ABSTRACT

Discrete dislocation dynamics simulations are carried out to systematically investigate the rate dependent deformation behaviour of polycrystalline bulk copper by varying the loading rate in the range of 100–25,000 s<sup>-1</sup> under tension. The underlying material model not only incorporates the realistic definition of nucleation time but also put emphasis on the role of obstacle density and their strength on dislocation motion. In the simulations, plasticity arises from the collective motion of discrete dislocations of edge character. Their dynamics is incorporated through constitutive rules for nucleation, glide, pinning and annihilation. The numerical results show that the rate sensitivity of yield stress in bulk polycrystals is controlled by the density of Frank-Read sources, obstacles and their strength.

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## 1. Introduction

The plastic deformation of materials as a function of the applied loading rate has long been the subject of extensive research (e.g., Follansbee et al., 1984; Klopp et al., 1985; Clifton, 1990; Tong et al., 1992; Armstrong and Walley, 2008). The understanding of dynamic plastic behaviour of metals is important in many engineering applications including high speed machining, impact loading etc. Numerous experiments have demonstrated that the mechanical properties of materials such as yield stress and strength depend on the applied loading rate (Follansbee et al., 1984; Klopp et al., 1985; Rittel et al., 2002; Vural et al., 2003). It is generally observed that the flow stress slowly rises with strain rate at low rates, and increases more rapidly at strain rates  $\dot{\epsilon} > 10^3$  s<sup>-1</sup> (Follansbee et al., 1984; Clifton, 1990; Tong et al., 1992). Based on the experimental findings of flow behaviour of aluminium and copper, Kumar et al. (1968), Kumar and Kumble (1969) have attributed this increase in flow stress to the different deformation mechanisms at low and high strain rates. In a similar study on copper, Follansbee et al. (1984) and Regazzoni et al.

(1987) concluded that the deformation is controlled by thermal activation in low strain rate region ( $\dot{\epsilon} \leq 10^3$  s<sup>-1</sup>). In the high strain rate regime ( $\dot{\epsilon} \geq 10^4$  s<sup>-1</sup>), viscous drag was identified as the rate limiting mechanism. In another study, Fruttschy and Clifton (1998) have shown that at high loading rates, the viscous resistance to dislocation motion not only governs the response of OFHC copper at room temperature but is important at elevated temperatures too.

Rate sensitivity is strongly material dependent and has been studied most intensively at the macroscopic scale within the context of superplasticity. Along with the identification of the mechanisms behind rate sensitivity, there has been much interest in constitutive models that include rate dependence. More recently, it has been found that the rate sensitivity depends on the grain size of the material, with values increasing for decreasing grain size (Hallberg et al., 2010). At these small grain sizes, there are size effects that cannot be captured by classical continuum plasticity models, as they lack a material length scale.

Discrete dislocation plasticity (DDP) is a modelling framework that is endowed with several length scales and has been shown to be able to quantitatively predict small-grain size plasticity of copper thin films (Shishvan and Van der Giessen, 2010). However, it has not been used

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yet, to study the complex rate dependent response of materials. In the context of probing the rate sensitivity of plastic flow, it is important to note that this DDP framework has two intrinsic time scales: one being the dislocation nucleation time  $t_{\text{nuc}}$  and the other given by the ratio of elastic modulus  $E$  and viscous drag  $B$ . This raises the question to what extent these two are capable of capturing the experimentally observed trends.

In order to answer this question, we perform DDP simulations of the tensile response of polycrystalline copper (Cu) as a function of strain rate. The effect of various parameters, such as viscous drag  $B$ , nucleation source density  $\rho_{\text{nuc}}$ , obstacle density  $\rho_{\text{obs}}$  and obstacle strength  $\tau_{\text{obs}}$ , on the hardening behaviour of Cu is also investigated. The results are compared with experimental data from the literature.

## 2. DDP model

A polycrystalline bulk material under tension is modelled as a two-dimensional array of rectangular grains with height  $h$  and width  $d$ , as shown in Fig. 1. Each grain has three slip systems oriented  $60^\circ$  relative to each other, see Fig. 1(b). The orientation of each grain  $\phi$  is different and is determined by random selection from a uniform distribution. Consistent with the plane strain conditions perpendicular to the plane of observation, only edge dislocations having Burgers vector  $b$  are used as carriers of plasticity. All grain boundaries (GBs) are assumed to be impenetrable for dislocations. Periodic boundary conditions are used across the simulation cell to prescribe the tensile strain  $\varepsilon$ . The top and bottom surface of the bulk are assumed to be traction free. The boundary conditions are imposed through the superposition method of Van der Giessen and Needleman (1995).

The analysis of the deformation process is performed in an incremental manner. After every update of the dislocation structure, the new driving force for the evolution of the structure is computed. This so-called Peach–Koehler force is determined by the applied stress and the long-range

interactions of dislocations, which are accounted for by modelling them as line defects in a linear elastic solid. The driving force for the change in position of any dislocation is computed from superposition of the singular stress field of all other dislocations as if they were in infinite space and an image field that corrects for the actual boundary conditions, see Van der Giessen and Needleman (1995). The glide component of this force,  $f^l$ , controls the glide velocity  $v^l$  of dislocation  $l$  through the drag law  $v^{(l)} = f^l/B$ , where  $B$  is the drag coefficient.

While long-range interactions are taken into account by the elastic fields, a set of constitutive rules is used to incorporate the short ranged dislocation mechanisms that govern nucleation, annihilation and pinning of dislocations at obstacles. The Peach–Koehler force also controls the nucleation of dislocations through a two-dimensional (2d) version of the Frank–Read source, as proposed in Van der Giessen and Needleman (1995). According to this model, a dislocation dipole is generated when the resolved shear stress at a source exceeds its strength  $\tau_{\text{nuc}}$  for a time span of  $t_{\text{nuc}}$ . The sign of the dipole is determined by the direction of the Peach–Koehler force. Following the source model of Shishvan and Van der Giessen (2010), the nucleation strength  $\tau_{\text{nuc}}$  of the Frank–Read source contains two contributions,

$$\tau_{\text{nuc}} = \tau_{\text{nuc}}^{\text{LN}} + \tau_{\text{nuc}}^0. \quad (1)$$

The first term is a random value from a log-normal distribution that is determined by the grain size and the theoretical strength of the material. The second term,  $\tau_{\text{nuc}}^0$ , is a material dependent parameter that accounts for the fact that a Frank–Read segment cannot always bow-out freely, but may interact with various types of obstacles such as small precipitates and forest dislocations. The mean effect of these size and position dependent obstacles to dislocation motion is incorporated by an offset value  $\tau_{\text{nuc}}^0$ . It is considered a fit parameter to be obtained from comparison of simulation and experiments, as explained in the subsequent section.

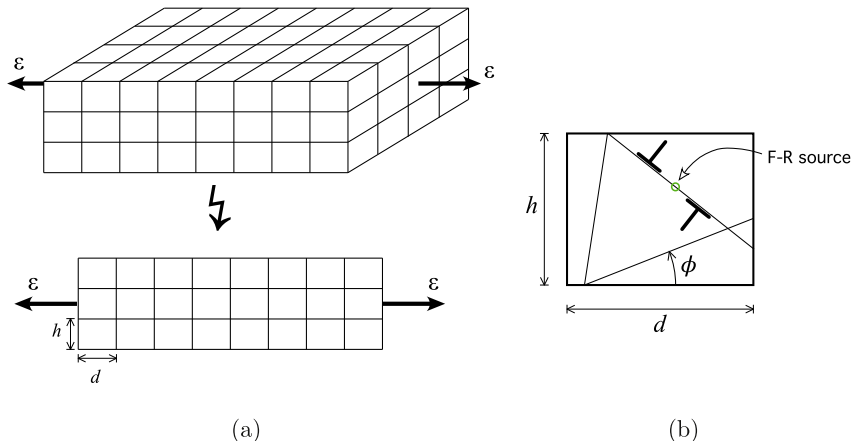


Fig. 1. (a) Two-dimensional representation of a polycrystal under tension and (b) plane strain model of single grain with slip systems and a source with dislocation dipole.

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