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Dislocation-precipitate interaction map

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ABSTRACT

The present research is the first attempt to systematically quantify the dislocation-precipitate interaction in terms of the applied shear stress, precipitate resistance, and required time to reach the critical state of dislocation-precipitate interaction when a dislocation line is about to pass through precipitates. A modified line dislocation dynamics is adopted to model the dislocation-precipitate interaction. In the present modeling approach utilizing three-dimensional dislocation dynamics simulations, thousands of data points on Cu are obtained accounting for various precipitate resistances, applied shear stresses, and precipitate spacing. A universal equation is found based on simulations to quantify dislocation-precipitate interactions in terms of the applied shear stress, precipitate resistance scale, and dislocation-precipitate interaction time. The dislocation-precipitate interaction time versus precipitate resistance and stress, referred to as "dislocation-precipitate interaction map," determines the "pass" or "no-pass" state of the interaction. Using this map, we incorporate the dislocation-precipitate interaction time in a two-dimensional dislocation dynamics approach (DD) coupled with the finite element method (FEM). This framework, FEM-DD, is applied to model mechanical behavior of a free-standing copper thin film. Simulation results show a dual effect of the dislocation-precipitate interaction time on hardening behavior.

1. Introduction

Precipitation hardening has been utilized to design alloys with the desired ductility and strength; however, this phenomenon was not well-understood until the 20th century as the development of transmission electron microscopy made it possible to observe dislocations. Precipitates restrict the motion of dislocations, resulting in a higher strength as the movement of each dislocation contributes to the total macroscopic plastic deformation. In order to provide a comprehensive understanding of precipitation hardening phenomenon, the physics of dislocation motions and their interactions with obstacles should be quantified more effectively.

Computational approaches have been widely adopted to study dislocation-precipitate interactions. Early computational attempts are basically focused on the movement of a dislocation line through a random array of precipitates and the geometrical deformation of the dislocation line [1,2]. Generally, precipitates are considered dimensionless and modeled as obstacles against dislocation motions. Geometrical approaches successfully capture the critical resolved shear stress (CRSS). For more details on the development and limitations of the geometrical approaches, see a review by Ardell [3].

The development of the dislocation dynamics approach (DD) [4–7], a computational methodology for modeling dislocation motions and their interactions at the micron scale, and the coupling of DD with continuum modeling such as FEM [8–12], BEM [13], and recently XFEM [14] provide the capability of solving more complex physical and realistic models. Several studies have addressed physical issues of dislocation-precipitate interactions by applying dislocation dynamics such as precipitate shearing by a dislocation [15], the role of the matrix-precipitate shear modulus difference [13], and misfit stresses at the boundary of a precipitate [16]. In addition to early geometrical approaches and dislocation dynamics, studies have also adopted molecular dynamics (MD) [17,18] and multiscale approaches [19–22] to investigate dislocation-precipitate interactions.

The dislocation-precipitate interaction results from several factors: (1) the matrix-precipitate shear modulus difference, (2) misfit strains caused by thermal effects, (3) misfit dislocations at the boundary of precipitates due to the matrix/precipitate different crystalline structures, (4) the change in dislocation core energy as the dislocation passes through precipitates, etc. [23]. Since micro-scale computational approaches for modeling dislocation-precipitate interactions are not capable of treating all mentioned

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factors, most micro-scale studies are limited to the first factor [10,13,15,24–29]. Monnet defined precipitates as friction stress opposed to the dislocation movement [30]. Mohles conducted pioneer research studies to model lattice mismatches [31–33] and imperfect matrix-precipitate interfaces [34]. Duesbery and Sadananda modeled the motion of edge and screw dislocations through an array of spherical coherent obstacles for various obstacle sizes, array dimensions, and misfit values, via molecular dynamic simulations [35]. Keyhani et al. [36] developed an efficient computational technique which implicitly accounts for majority of the mentioned factors by introducing the precipitate resistance scale. In addition, the geometrical arrangement of precipitates plays a role and adds further complexities to the simulation of dislocation-precipitate interactions. Because of all complexities of this interaction and the diversity of determining factors, most studies only focus on the role of a few factors, resulting in a limited understanding of the interaction. Furthermore, the relation between the precipitate resistance and the required time to reach the critical state of the dislocation-precipitate interaction has not been addressed so far.

A key parameter analyzed in this study is the required time to reach the critical state of the dislocation-precipitate interaction. This is the time difference between when a dislocation line initially starts to deform under the influence of precipitates and when a dislocation line goes on the verge of passing the precipitate, briefly called the critical time here. As the applied shear stress level increases, the dislocation-precipitate interaction undergoes a transition, which may affect the interaction time. The critical time at which a dislocation-precipitate interaction occurs depends mostly on the applied shear stress and precipitate properties. At high homologous temperatures precipitates can be also overcome by thermal activations such as climb. The present study, however, does not account for thermally activated processes controlling the critical time at high homologous temperatures (creep conditions) [37]. The temperature dependence of obstacle-dislocation interactions in solid solution hardening alloys are discussed in a review article by Kocks [38]. Other studies analyzed the strain rate sensitivity (SRS) in terms of obstacle strength and distributions, temperature, and applied shear stress [39,40]. For further details on modeling interactions of precipitates with dislocations see [23]. The adopted dislocation-precipitate interaction model is fundamentally developed here for short-range interactions and long range interactions due to the difference in elastic modulus of matrix and precipitate or lattice parameters are not taken into account.

The aim of the present research is to open a new window to understanding the dislocation-precipitate interaction. In order to accomplish this, extensive computational simulations are performed to find one of the fundamental relations for the dislocation-precipitate interaction in terms of the applied shear stress, precipitate resistance, and critical time named as "dislocation-precipitate interaction map". The dislocation-precipitate interaction map is constructed for copper (Cu) with various precipitate resistances and spacing. I addition, the concept of precipitate-dislocation interaction time has been used to model plastic deformation of a copper thin film with various precipitate densities.

2. Framework of the analysis

2.1. Computational scheme

The interaction between dislocation lines and arrays of equally spaced precipitates has been modeled by Keyhani et al. [36] through a recent developed methodology based on the standard line dislocation dynamics (DD) simulation code, DDLab. We use the DD procedure to discretize a dislocation line into straight segments defined by two end nodes; the dislocation drag governs mobility relating the nodal forces to the nodal velocities [41]. The usual overdriven dynamics of DD assumes that the drag coefficient is a constant. Since the dislocation-phonon interactions, which lead to a drag force, vary with short-range dislocation-precipitate interactions, this approach is an approximation. In addition, we assume that the simulations are based on elastic isotropy.

In the adopted approach, when a dislocation line encounters a precipitate, the corresponding nodes of the dislocation closer than a specific distance to the precipitate are locked. Consequently, the free part of the dislocation line bends, so the related shear stress, which the dislocation exerts on the precipitate, increases. If the resulting shear stress from the dislocation curvature reaches the precipitate resistance, the locked nodes get unlocked; therefore, the dislocation begins to pass through the precipitate by shearing mechanism. If the resulting shear stress from bending the dislocation line does not reach the precipitate resistance, the dislocation line forms a loop to pass the precipitate.

The precipitate resistance scale, R, is originally introduced and quantified in the authors' former research [36],

$$R = \frac{\tau_p}{\tau_{max}} \tag{1}$$

where τ_p is the shear stress against the dislocation movement in the vicinity of precipitates and $\tau_{max} = \mu b/D_1$ is the maximum possible shear stress exerted to the precipitate by a dislocation when the radius of dislocation curvature is equal to the radius of the first Orowan loop, D_1. μ is the shear modulus of the matrix and b is the magnitude of the Burgers vector. The resistance scale, R, is equal to unity for non-shearable precipitates, representing the Orowan mechanism, and less than unity for shearable precipitates. The adopted methodology is not capable of modeling prismatic loops, known as the Hirsch mechanism, which may form in FCC crystals as well as Orowan loops [42,43].

2.2. Simulation setup

The critical time for the interaction of a straight edge dislocation line with an array of collinear equally spaced precipitates with similar resistance and diameter is calculated, Fig. 1. According to the adopted computational methodology, the critical time is the time difference between when the first node of a dislocation line is locked as it reaches to the distance from the precipitate equals to the diameter of the corresponding Orowan loop and when the dislocation line starts to pass the precipitate either by forming Orowan loops or by cutting through the precipitate.

The critical time of the dislocation line interacting with precipitates is calculated for thousands of interactions by varying the applied stress, precipitate resistance, and ratio of L/D for a Cu crystal. The applied shear stress, τ_{app}, is considered to be a fraction of the critical shear stress for non-shearable precipitates ($\tau_c^{R=1}$) [44],

$$\tau_c^{R=1} = \frac{\mu b}{2\pi L} \ln\left(\frac{\bar{D}}{r_0}\right) \tag{2}$$

where L is the internal spacing of precipitates, $\bar{D} = (D^{-1} + L^{-1})^{-1}$ in which D is the precipitate diameter considered to be 100 nm for all simulations, and r_0 is the dislocation core radius. Similar to the Frank-Read mechanism, the time for dislocation-precipitate interaction at the critical state goes to infinity if the applied shear stress is equal to the critical stress, $\tau_c^{R=1}$; therefore, we introduce $\tau_c' = 1.05\tau_c^{R=1}$ and t_c' is the corresponding time at the critical state for τ_c'. We perform simulations for Cu, an FCC crystal, applying three