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An efficient computational technique for modeling dislocation–precipitate interactions within dislocation dynamics

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ABSTRACT

A new computational technique for modeling dislocation interactions with shearable and non-shearable precipitates within the line dislocation dynamics framework is presented. While shearable precipitates are modeled by defining a resistance function, non-shearable ones are modeled by drawing a comparison between the two well-known Orowan and Frank–Read mechanisms. The precipitates are modeled directly within the dislocation dynamics analysis without the need for any additional numerical methods. Due to low computational cost the method is appropriate for simulation of a high dislocation density interacting with large number of precipitates considering different types and various sizes and resistances. It is also efficient for coupling dislocation dynamics with finite element method in multi-scale frameworks since it does not require the mesh to be consistent with the precipitates geometry.

1. Introduction

Computational approaches to study dislocation–precipitate interaction, commenced from 60s, have provided more insight in understanding plasticity of metals and alloys [1]. A comprehensive review of classical simulation methods can be found in [2]. Since the advent of the dislocation dynamics (DD), which is a computational framework to analyze dislocation motions and their related phenomena at micron scale [3–7], some attempts have been made to study dislocation interactions with precipitates and boundaries within the dislocation dynamics analysis [8–10]. For a comprehensive review of advances in dislocation dynamics modeling, see [11].

Modeling precipitates in dislocation dynamics analysis was generally limited to specific assumptions for the stress fields arising from precipitates. In some studies, precipitates were introduced as spherical stress fields [12–18], while some others evaluated the stress field due to matrix and precipitate shear modulus difference by applying the superposition principle, in which the problem was disintegrated into two problems: an infinite domain containing dislocations and a correction problem for considering the elastic field of precipitate and treating the boundary conditions. As a result, an extra numerical method, such as FEM or BEM, was required for analysis of the second part [19–21]. The stress fields due to lattice misfit at internal boundaries were taken into account in a few studies or by coupling DD with FEM [12,22] or with the fast Fourier transform (FFT) [23].

The abovementioned approaches suffer from one or several flaws in terms of physics or disadvantages with reference to computational cost or both. First, the effect of misfit dislocations was not considered in some methodologies, though it had a significant role in dislocation–precipitate interaction. For instance, a dislocation could pass a precipitate with the similar shear modulus of matrix without any interactions. This was in contrast with real problems where dislocations might stop behind the precipitate or hardly pass through it because of misfit dislocations at the coherent precipitate–metal matrix interface. Second, due to the high stress gradient near precipitates, considerable time was required to obtain a converged solution for the dislocation motion near precipitates. Third, even after forming the Orowan loops, the associated nodes still remained in the mobility equations, increasing the computational effort required to solve the mobility equations at each time step. Finally, an extra numerical method such as FEM, BEM or FFT was required to analyze the stress field of a precipitate. In a number of studies [12–18], the extra numerical method was avoided by defining precipitates as spherical stress fields; however, the first three disadvantages remained unsolved.

In the present study, a computational technique is proposed to model precipitates with various sizes and resistances within the line dislocation dynamics analysis which eliminates the mentioned drawbacks. The developed method is also efficient for modeling

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precipitates in a combined FEM-DD framework to address plastic deformations in small scales. Implementation of this technique in FEM-DD framework allows for the independency of mesh generation from the precipitates geometry, which simplifies the solution of large systems with random distribution of precipitates by adopting very simple mesh generations, less degrees of freedom (DOFs) and low computational costs.

2. Modeling approach

In this study, a modified version of line dislocation dynamics (DD) simulation code, DDLab, is adopted to model dislocation motions [24]. In dislocation dynamics simulations, a dislocation curve is discretized into straight segments defined by two end nodes. The mobility function **M** relates the vector of nodal forces $\mathbf{f}_i$ to the nodal velocities $\mathbf{v}_i$,

$$\mathbf{v}_i = \mathbf{M}(\mathbf{f}_i) \quad (1)$$

The velocity of the node i, $\mathbf{v}_i$, also relies on the forces acting on the other nodes. The dislocation segment orientation and material properties are the main influential factors on the mobility function. In the dislocation dynamics procedure, the nodal velocity is calculated by solving the mobility equations and the dislocation motion is computed via topological considerations [25].

When a dislocation encounters a precipitate, it bends so the related shear stress which the dislocation exerts on a precipitate increases. If this stress reaches a critical value, the dislocation goes on the verge of passing the precipitate. At this point, the dislocation can pass the precipitate by two mechanisms relying on the precipitate resistance, τ_{obs}, which is defined as the minimum required shear stress to cut a precipitate. First, the dislocation rounds the precipitate (the Orowan mechanism) unless the arising stress from the dislocation bending overcomes the precipitate resistance. Second, the dislocation cuts through the precipitates if the precipitate resistance is lower than the induced stress due to the dislocation bending. It is worth emphasizing that the applied stress to the dislocation must be large enough to bend the dislocation to a critical state in order to pass a precipitate.

To model the first mechanism (non-shearable precipitates), it is considered that a dislocation node which locates closer than a specific distance to a precipitate gets locked, as depicted in Fig. 1. By this approach, the main problem of dislocation–precipitate interaction is transformed into the Frank–Read mechanism, since the dislocation line pinned between two precipitates behaves similar to a Frank–Read source. The critical resolved shear stress (CRSS) obtained from the Frank–Read and the Orowan mechanisms depends on the maximum dislocation line curvature and the material properties. Therefore, for an identical material, the two mechanisms predict the equal CRSS for a given dislocation line curvature. Assuming a constant curvature along the bowing dislocation line results in $\tau_{nuc} = \mu b/L_f$, where μ is the shear modulus, b is the magnitude of the Burgers vector and L_f is the length of the initial dislocation line. If the anisotropic line tension is considered, the dislocation line at the critical state will have an oval shape [26]. The critical stress is expressed in a general form $\tau_{nuc} = \beta\mu b/L_f$ by adopting the concept of self-stress [27] to investigate the bowing of dislocation line [28]. The constant β depends on the Poisson's ratio, the dislocation core radius and the dislocation line properties.

For the critical stress of two mechanisms to be equal, it is assumed that a dislocation rounds a precipitate with a modeling diameter D_1, which is not equal to the precipitate diameter D. Having equivalent Frank–Read nucleation stress and Orowan stress $\tau_{Orowan} = \mu b \ln(\bar{D}/r_0)/(2\pi L)$, the modeling diameter of a precipitate can now be determined (see Fig. 1):

$$L_f = L + D - D_1 \quad (2)$$

$$D_1 = L + D - 2\pi L\beta\left[\ln\left(\bar{D}/r_0\right)\right]^{-1} \quad (3)$$

where L is the internal distance between the two precipitates, r_0 is the core radius of dislocation and $\bar{D} = \left(D^{-1} + L^{-1}\right)^{-1}$.

The maximum stress that a dislocation can exert on a precipitate occurs when the dislocation radius of curvature equals the modeling radius, $\tau_{max} = \mu b/D_1$. Whenever the precipitate resistance reaches to this magnitude (i.e. $\tau_{obs} = \tau_{max}$), the dislocation stops behind the precipitate completely, representing the Orowan regime. If the precipitate resistance is lower than the maximum stress (i.e. $\tau_{obs} < \tau_{max}$), the dislocation can pass the precipitate by exerting a lower level of stress to the precipitate, which generates a radius of curvature larger than the modeling radius.

To keep up with the second mechanism (i.e. shearable precipitates), the precipitate resistance scale, $R = \tau_{obs}/\tau_{max}$, is defined; which is set to 1 for a non-shearable precipitate and 0 when no precipitate exists. When the distance of a node from the center of a precipitate is less than the modeling radius, the node gets locked in the dislocation dynamics procedure. At each step, the local shear stress, which is related to the local curvature at this point, is compared with the precipitate resistance. If the related local shear stress exceeds the precipitate resistance, the node is released.

The precipitate resistance arises from several factors including the matrix and precipitate shear modulus difference, misfit dislocations and strains and the dislocation core energy change due to the difference between crystalline structures of matrix and precipitates. While the first factor is usually considered in modeling precipitates in dislocation dynamics, the second and third ones have a controlling effect. Small scale analyses are required to determine the precipitate resistance in a matrix. Some attempts have been made to introduce the critical resolved shear stress, τ_c, as a function of shear modulus difference between the

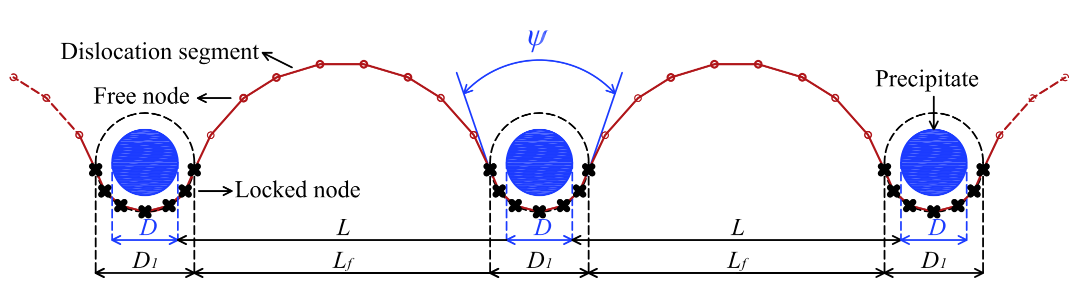

Fig. 1. Nodes which are positioned closer than a specific distance to the precipitate get locked. The circles and crosses represent the free and locked nodes, respectively. A dislocation line between two precipitates with the internal distance L acts as a Frank–Read source with length L_f. ψ is the angle between the dislocation tangents at both sides of the precipitate.