レベルセット転位動力学法を用いたプリズマティック転位ループのモデリング

Prismatic Dislocation Loop Formation by Level Set Dislocation Dynamics

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The whole process of a prismatic dislocation loop (PDL) formation around a misfitting spherical inclusion embedded in a homogeneous isotropic matrix is studied using level set dislocation dynamics. Two small half loops are first punched out around a spherical particle on a specific cylindrical surface along which the magnitude of the misfit shear stress reaches the maximum among all the homocentric cylinder surfaces. The edge dislocation segments glide away from the inclusion-matrix interface under the influence of the shear stress, while the screw components cross slip around the cylindrical surface. When two ends with opposite orientations of the top and bottom half dislocation loops intersect, the screw segments annihilate and a PDL is finally produced.

Key Words: *Prismatic Dislocation Loop, Misfitting Spherical Inclusion, Level Set Method, Dislocation Dynamics, Cross slip*

1. Introduction

The punching of coaxial prismatic dislocation loops (PDLs) in crystalline materials at precipitate-matrix interfaces without long-range applied stress is often observed by experiments and it can be exploited as the improvement of material strength. Precipitates employed in strengthening technique of quench-aging process generate misfit strain in the vicinity and constitute nucleation sites for PDLs. These misfit stresses associated with internal stresses from PDLs can be the barriers for mobile dislocations in matrix phase and thus they are the reasons for precipitation hardening.

Level set method (LSM)^{(1),(2)} associated with fast marching method (FMM) does not track individual dislocation line segments directly and thus can demonstrate such topological changes of dislocations observed in two or three dimensions naturally^{(3),(4)}. Spatial internal stress distributions in the region containing complex topological dislocation configurations can be easily calculated by the elastic field equations with dislocations in the infinite body. The internal stress field can be solved efficiently using FFT, assuming a periodic boundary condition. In the present paper, we study the mechanism of PDL formation around a misfitting spherical particle and discuss the elastic strain energy variation during the whole process based on level set dislocation dynamics.

2. Level Set Dislocation Dynamics

A curve can be represented by the intersection of the zero level sets of two level set functions ϕ and ψ , where the two functions satisfy $\phi(x,y,z) = \psi(x,y,z) = 0$. One should be noted that, the set of segments satisfying $\phi = C_1$ and $\psi = C_2$ (C_1 and C_2 are constants) are also curves in $\mathbf{R}^3$ ^{(1),(2)}.

Moving the curves in $\mathbf{R}^3$ is, in fact, moving the level set functions ϕ and ψ in space. First, the velocity vector $\mathbf{v}$ of a curve under some specific conditions is investigated, and then ϕ evolves under the partial differential equation of,

$$\phi_t + \mathbf{v} \cdot \nabla \phi = 0, \quad (1)$$

where ϕ_t is the partial derivative of ϕ with respect to time and $\nabla \phi$ is

the partial derivative with respect to position vector $\mathbf{x}$ in Cartesian coordinate system, respectively. All the level sets of ϕ are moved according to $\mathbf{v}$. Similarly, for the level set function ψ , all the level sets of ψ are moved according to the same $\mathbf{v}$ as follows.

$$\psi_t + \mathbf{v} \cdot \nabla \psi = 0. \quad (2)$$

Therefore, the system of partial differential equations (Eqs. (1) and (2)) moves the intersections of any level sets of ϕ and ψ according to $\mathbf{v}$, especially the intersection of the zero level sets which we intend to deal with.

3. Mechanism of Prismatic Dislocation Loop Formation

In this section, we present the formation of PDL using level set dislocation dynamics. The simulations were performed using the simulation cell which one side l has plus and minus units normalized by the real length of 250b (b denotes the magnitude of Burgers vector, 0.286 nm). The cell box is divided into $64 \times 64 \times 64$ grid points. The shear modulus μ_M and μ_P are set to be 161 GPa and 80 GPa, respectively, and Poisson ratio ν is set to be 1/3. For all the calculations, the stresses are scaled by $3\mu_M b(1-\nu)/(2l(1+\nu))$ and time is scaled by $2l/(\mu_M m_g)$ (that is, $t^* = t/(2l/\mu_M m_g)$) where m_g is the mobility constant for dislocation glide and is set to be 1.0 in the present calculations.

During the simulations, the fifth order weighted essentially non-oscillatory (WENO) is used for spatial differentiation and the third order total variation diminishing Runge-Kutta (TVD-RK) is used for temporal differentiation. Reinitializations for keeping the level set functions be signed distance function (SDF) are performed after each time step of solving the evolution equations (1) and (2) to reduce the numerical errors. We do not present climb mobility if not specified and the periodic boundary condition is assumed in x , y and z directions.

3-1 Misfit Stress Field

Consider a homogeneous linear elastic solid D with a spherical sub-domain Ω which undergoes a uniform permanent deformation (such as phase transformation, precipitate and recrystallization). The stress fields generated by the dilatational misfitting spherical inclusion are written by linear elasticity. The

stress at a point outside a particle of radius R locating at the origin coordinate $(0, 0, 0)$ in an isotropic elastic matrix ($r > R$) is

$$\sigma = \frac{2\mu_M \bar{\epsilon} R^3}{r^5} \begin{pmatrix} r^2 - 3x^2 & -3xy & -3xz \\ -3xy & r^2 - 3y^2 & -3yz \\ -3xz & -3yz & r^2 - 3z^2 \end{pmatrix}, \quad \bar{\epsilon} = \frac{1-\nu}{3(1+\nu)} \epsilon_0, \quad (3)$$

where $r^2 = x^2 + y^2 + z^2$, μ_M is shear modulus of matrix, ϵ_0 is a dilatational misfit strain and ν is Poisson ratio. Meanwhile, the stress tensor inside the particle ($r < R$) is

$$\sigma = -4\mu_p \bar{\epsilon} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (4)$$

where μ_p is shear modulus of precipitate. It is easy to see the maximal magnitude of shear stress (MSS) at the inclusion-matrix interface is on the cylinder surface of radius $R/\sqrt{2}$, where MSS meets the critical shear stress for dislocation nucleation and, as a result, small half loops are punched out (see Fig. 1).

Fig. 1 A misfitting spherical inclusion and the cylindrical surface with maximum resolved shear stress in x direction.

3-2 Simulation Results

In this simulation, we specify a misfitting spherical particle of radius $R = 50b$ with the dilatational misfit strain $\bar{\epsilon} = 0.01$ and the normalized Burgers vector $\mathbf{b}^* = [1 \ 0 \ 0]$ defined on both inclusion and matrix. During the whole calculation, this spherical particle keeps invariable and produces a misfit stress field according to Eq. (3) in a homogeneous isotropic matrix ($r > R$) and the stress tensor according to Eq. (4) inside the inclusion ($r < R$), respectively. As indicated in section 3-1, the magnitude of the misfit stress field reaches the maximum on the cylindrical surface of the radius $R/\sqrt{2}$ with the axis paralleling to the Burgers vector (see the light green cylinder of Fig. 2(a)). When the MSS exceeds the critical stress for nucleation of dislocation loops of radius equal to $15b$, two small half dislocation loops are injected of which the half loop on top has the clockwise orientation and the bottom one has the anticlockwise orientation (according to top-down view as Fig. 2(a)). Thus, the farthest segments of the two half loops are edge dislocations and the segments on the inclusion-matrix interface are screw dislocations. The velocity vector of the dislocation evolution is projected onto the cross-slip plane (light green cylinder) to make sure that the dislocations always receive the MSS from the inclusion among all the slip planes.

Under the shear stress generated by the inclusion, the forward edge components glide away from the inclusion-matrix interface by repel force and the screw components paralleling to the axis of the glide cylinder experience a force causing them to cross slip around the circular surface of the cylinder (see Fig. 2(b)). As the half loops are expanding on the cylinder, the two screw components with opposite orientations of the two half loops approach to each other (see Fig. 2(b)), and annihilate when two

half dislocation loops merge. Finally, they become one dislocation loop (see Fig. 2(c)). The middle mixed dislocation segments experience more intense shear stress than top and bottom edge dislocation segments and also internal stress of dislocation acting like line tension of the loop. Therefore, the middle-bended dislocation loop preferably becomes a prismatic dislocation loop with all the segments perpendicular to the Burger vector (see Fig. 2(d)). This PDL glides along the cylinder surface away from the inclusion-matrix interface (as seen in Fig. 2(e)), the loop can only glide on the cylinder because any other motions need climb mobility). Since the influence of the stress decreases as the distance from inclusion to dislocation increases (see Eq. (3)), the driving force on the PDL gradually weakens. At last, the motion ceases at the position where the driving force is no larger than friction stress by Peierls potential (5MPa).

Fig. 2 Formation of a PDL under the shear stress generated by a misfitting spherical inclusion.

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