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Simulation of dislocation cross-slip

By

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Abstract

This contribution deals with the numerical simulation of dislocation dynamics, their interaction, merging and changes in the dislocation topology. The glide dislocations are represented by parametrically described curves moving in slip planes. We focus on the simulation of the cross-slip of two dislocation curves where each curve evolves in a different slip plane. The dislocations evolve, under their mutual interaction and under some external force, towards each other and at a certain time their evolution continues outside slip planes. During this evolution the dislocations merge by the cross-slip occurs. As a result, there will be two dislocations evolving in three planes - two planes and one plane where cross-slip occurred. The goal of our work is to simulate the motion of the dislocations and to determine the distance of slip planes which is necessary for the cross-slip to occur. The simulation of the dislocation evolution and merging is performed by improved parametric approach and numerical stability is enhanced by the tangential redistribution of the discretization points.

§ 1. The model

Dislocation cross-slip is one of key processes of crystal plasticity. The most important cross-slip models are reviewed in [1]. The present simulation is focused on the annihilation of screw dislocation parts by cross-slip as an important factor in the generation and dynamics of persistent slip bands. In the bands screw parts of glide dislocations moving in channels of low dislocation density mutually annihilate when the distance between their respective slip planes falls below a critical limit. The remaining edge parts are stored in multipolar walls. The

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annihilation by cross-slip is governed by the line tension, the applied stress in the channels and the interaction force between dislocations. In the present simulation a dissociation of the glide dislocations both in their slip planes and the cross-slip plane is neglected. In discrete dislocation dynamics modeling dislocations as "zig-zag" lines jumping on a discrete network cross-slip is a standard ingredient [2]. This article describes the incorporation of the annihilation by cross-slip into the discrete dislocation dynamics by considering dislocations as moving smooth curves. This approach is a mathematically challenging alternative.

The interaction of dislocations can be approximately described using the curvature flow. We consider perfect dislocation curves with the Burgers vector $\vec{b} = (0, 0, b)$ oriented in the x-direction of the x,y,z coordinate system. The discloation curve motion Γ is located in a slip plane, identified as xz-plane. The glide of dislocation is governed by the relaxation law in the form of the mean curvature flow equation in the direction of the normal vector to the dislocation

$$Bv = L\kappa + b(\tau_{app} + \tau_{int}), \tag{1.1}$$

where B is a drag coefficient, and $v(\vec{x}, t)$ is the normal velocity of a dislocation at $\vec{x} \in \Gamma$ and time t. The term $L\kappa$ represents self-force expressed in the line tension approximation as the product of the line tension L and local curvature $\kappa(x, t)$. The term τ_{app} represents the local shear stress acting on the dislocation segment produced by the bulk elastic field. The term τ_{int} represents interaction force between dislocations. In our simulations, we consider the "stress controlled regime" where the applied stress in the channel is kept uniform. In the slip plane, the applied stress τ_{app} is the same at each point of the line and for numerical computations we use $\tau_{app} = const$. The "strain controlled regime" analyzed in [3] could be an alternative.

§ 2. Parametric description

The motion law (1.1) in the case of dislocation dynamics is treated by parametrization where the planar curve $\Gamma(t)$ is described by a smooth time-dependent vector function $\vec{X} : S \times I \to \mathbb{R}^2$, where $S = [0, 1]$ is a fixed interval for the curve parameter and $I = [0, T]$ is the time interval. The curve $\Gamma(t)$ is then given as the set $\Gamma(t) = \{\vec{X}(u, t) = (X^1(u, t), X^2(u, t)), u \in S\}$.

The evolution law (1.1) is transformed into the parametric form as follows. The unit tangential vector $\vec{T}$ is defined as $\vec{T} = \partial_u \vec{X}/|\partial_u \vec{X}|$. The unit normal vector $\vec{N}$ is perpendicular to the tangential vector and $\vec{N} \cdot \vec{T} = 0$ holds. The curvature κ is defined as

$$\kappa = \frac{\partial_u \vec{X}^{\perp}}{|\partial_u \vec{X}|} \cdot \frac{\partial_{uu} \vec{X}}{|\partial_u \vec{X}|^2} = \vec{N} \cdot \frac{\partial_{uu} \vec{X}}{|\partial_u \vec{X}|^2},$$

where $\vec{X}^{\perp}$ is a vector perpendicular to $\vec{X}$. The normal velocity v is defined as the time derivative of $\vec{X}$ projected into the normal direction, $v = \partial_t \vec{X} \cdot \partial_u \vec{X}^{\perp}/|\partial_u \vec{X}|$. The equation (1.1) can be written as

$$B\partial_t \vec{X} = L \frac{\partial_{uu} \vec{X}}{|\partial_u \vec{X}|^2} + b(\tau_{app} + \tau_{int}) \frac{\partial_u \vec{X}^{\perp}}{|\partial_u \vec{X}|}. \tag{2.1}$$

This equation is accompanied by the periodic boundary conditions for closed curves, or by the fixed-end boundary condition for open curves, and by the initial condition. These conditions are considered similarly as in [4]. For long time computations with time and space variable force, the algorithm for curvature adjusted tangential velocity is used. To incorporate a tangential

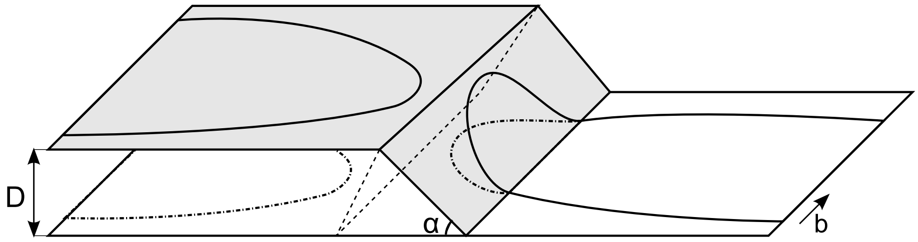

Figure 1: Geometry of the model

redistribution, a tangential term α has to be added to equation (2.1). The term α depends on the curvature κ of the dislocation and controls the distance between discretization points, i.e., either keeps the same distance of the discretization points along the whole curve, or accumulates the points in areas with higher curvatures to improve accuracy. Details are described in [5]. Complete equation reads as

$$B\partial_t\vec{X} = L\frac{\partial_{uu}\vec{X}}{|\partial_u\vec{X}|^2} + L\alpha\frac{\partial_u\vec{X}}{|\partial_u\vec{X}|} + b(\tau_{app} + \tau_{int})\frac{\partial_u\vec{X}^\perp}{|\partial_u\vec{X}|}. \tag{2.2}$$

For numerical approximation we consider a regularized form of (2.2),

$$\partial_t\vec{X} = \frac{\partial_{uu}\vec{X}}{Q(\partial_u\vec{X})^2} - \alpha\frac{\partial_u\vec{X}}{Q(\partial_u\vec{X})} + F(X,t)\frac{\partial_u\vec{X}^\perp}{Q(\partial_u\vec{X})}, \tag{2.3}$$

where $Q(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + \varepsilon^2}$ with ε being a small parameter. The equation is then solved by means of matrix factorization. Since there are two components of $\vec{X}$, two linear systems are solved in each timestep.

In case of the single dislocation dynamics, the mathematical model of curve evolution is 2D only. However, the cross-slip phenomenon requires a 3D configuration to be considered (two slip planes and one cross-slip plane). Our idea is to perform a linear mapping from a virtual plane to 3D according to Fig. 1. The curve motion is computed in the virtual plane and then mapped to the real physical configuration of the slip and cross-slip planes. The angle β is $\pi/4$ according to the features of the crystalline lattice.

Since the parametric approach cannot handle topological changes, a modified algorithm is used (see [6]). Every timestep, the distance of dislocation curves is determined and if the distance is lower than a given threshold (in our case 5 nm), a new curve is created, discretization points from both curves are copied in a correct order into the new one (points where minimal distance was reached are omitted), and the computaion continues only with the new curve.

The interaction force between dislocations is computed by Devince's formula [8] for a straight dislocation segment. Stress fields of two half-line dislocations τ_{int}^A and τ_{int}^B, where τ_{int}^A is a stress field from half line A to infinity; τ_{int}^B is a stress field from half line B to infinity, are subtracted (see Fig. 2). The resulting stress from each segment of the dislocation curve in the point X is computed as follows:

$$\tau_{int} = \tau_{int}^A - \tau_{int}^B.$$

Using Peach-Koehler formula $\vec{F} = (\tau_{int} \cdot \vec{b}) \times \vec{T}$, interaction force is computed from the stress field. Here $\vec{T} = (T_1, T_2, T_3)^T$ is a tangetial vector of the dislocation, $\vec{b}$ is a Burgers vector, τ_{int}

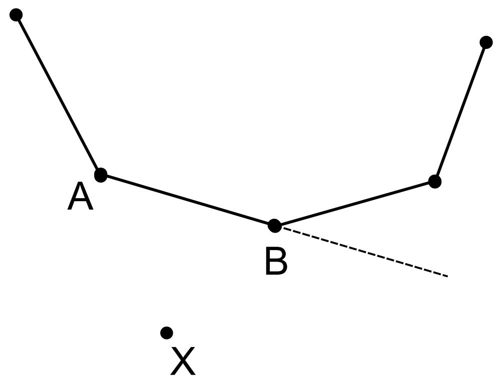

Figure 2: Devincre's formula for straight dislocation segment.

is a stress tensor. Taking into account the geometry of the model, the forcing term has the following form

$$\vec{F} = b(\tau_{21}T_3 - \tau_{31}T_2, \tau_{11}T_3 - \tau_{31}T_1, \tau_{11}T_2 - \tau_{21}T_1)^T.$$

The magnitude of the force on dislocation in normal direction is

$$F = \vec{F} \cdot \vec{N},$$

where $\vec{N}$ is a normal vector of the dislocation which the force field is applied to.

§ 3. Numerical simulation

The numerical simulations were performed for copper under the following set of parameters:

Burgers vector magnitude	$b = 0.25$ nm
Line tension	$L = 2$ nN
Drag coefficient	$B = 1.0 \cdot 10^{-5}$ Pa $\cdot$ s
Applied stress	$\tau_{app} = 15$ MPa
Plain distance	$D = 30 - 45$ nm
Cross-slip plane angle	$\beta = \pi/4$
Channel width	1000 nm
Discretization points per curve	$M = 175$

During the simulation, the dislocation curves have fixed ends at the channel edges and their initial distance is 1100 nm. The number of discretization points does not have a big influence on the simulation result. Less number causes worse detection of topological changes but speeds the computation up. Accodring to our experience, $M = 175$ is a good compromise between speed and accuracy.

We performed a set of numerical simulations of dislocation cross-slip to determine the critical slip plane distance for which the cross-slip occurs. In our model, each dislocation carries its own cross-slip plane with itself and when the two planes coincide, the condition for cross-slip is evaluated. The condition is defined as follows: when the interaction force between dislocations acting in the cross-slip plane is higher than the applied stress acting in the usual

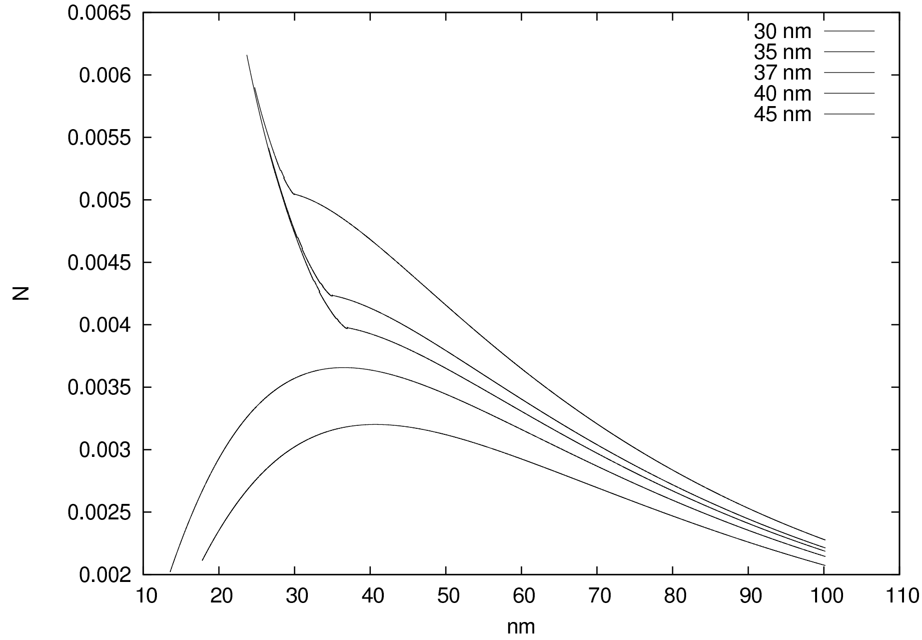

Figure 3: The interaction force between dislocations; slip plane distance (from top to bottom): 30 nm, 35 nm, 37 nm, 40 nm, 45 nm. Discretization nodes $M = 175$.

slip plane, the cross-slip occurs. Otherwise, the dislocations continue to move in their slip planes.

Computations in this article are done for $\tau_{app} = 15$ MPa. For such value of applied stress and under parameters stated above, the simulation provided the critical cross-slip distance approximately 37 nm. Figure 3 shows the graph of the interaction force for several slip plane distances. Simulation was performed for 30 nm, 35 nm, 37 nm,40 nm, and 45 nm (from top to bottom). The sharp point in the graph corresponds to the moment of cross-slip. In this point, the force acting on the dislocation changes and with the decreasing distance both dislocations are attracted more and more. When the dislocations touch, annihilation by cross-slip occurs.

The example in Fig. 4 shows the simulation of the actual annihilation by cross-slip. Initially the dislocations move towards each other under the external stress $\tau_{app} = 15$ MPa. When they approach each other the interaction force rises and they are pulled together into the cross-slip plane. Finally they annihilate by cross-slip and stick to the channel walls. In reality this mechanism is hindered by dissociation of dislocation core but the presented approximation does not consider such phenomenon yet.

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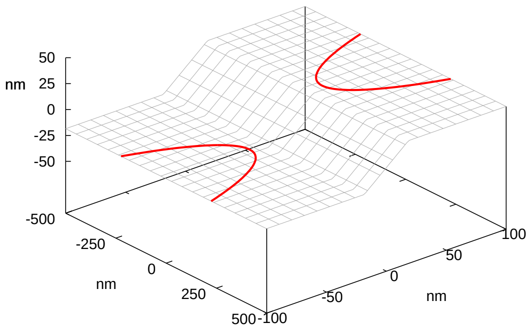
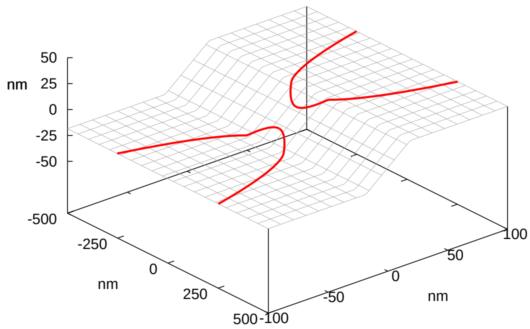
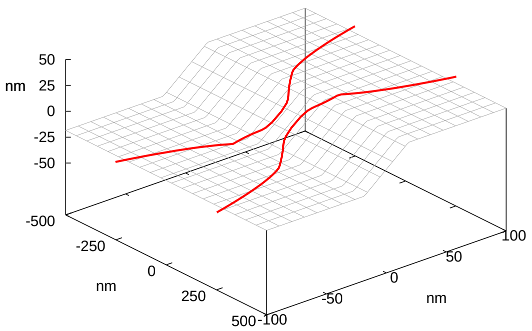


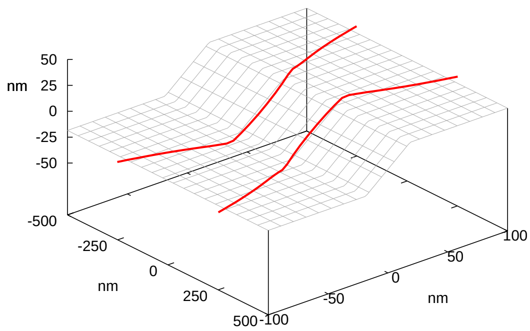
(a) $t = 0.14$ s



(b) $t = 0.314$ s



(c) $t = 0.318$ s



(d) $t = 0.324$ s

Figure 4: Visualization of dislocation motion during annihilation by cross-slip, $\tau_{app} =$ 15 MPa, $t \in (0, 0.324)$, plane distance $D = 37$ nm, each dislocation curve discretized by $M = 175$ nodes. This representes one simulation from Fig. 3.

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