# *Numerical simulation of dislocation dynamics*

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## 1 Introduction

The dislocations are defined as irregularities or errors in crystal structure of the material. The presence of dislocations strongly influences many of material properties. Plastic deformation in crystalline solids is carried by dislocations. Dislocation is a line defect of the crystalline lattice. Along the dislocation curve the regularity of the crystallographic arrangement of atoms is disturbed. The dislocation can be represented by a curve closed inside the crystal or by a curve ending on the surface of the crystal. At low homologous temperatures the dislocations can move only along crystallographic planes (gliding planes) with the highest density of atoms. The motion results in mutual slipping of neighboring parts of the crystal along the gliding planes.

## 2 Motion and evolution law

**Motion law** The mathematical model is based on the evolution of dislocation curve $\Gamma^t$ driven by mean curvature according to the law

$$v = \kappa + F(x,t)$$

in the direction of normal vector. There $\kappa$ is (mean) curvature, $v$ is a normal velocity, and $F = F(x,t)$ sum of all forces acting on $\Gamma^t$.

**Parametrization** $\Gamma^t$ is parametrized on the fixed interval $\langle 0,1\rangle$, and depending on time in $\langle 0,T\rangle$:

$$X : \langle 0,1\rangle \times \langle 0,T\rangle \to \mathbb{R}^2, X = X(u,t).$$

Here $X^\perp$ is a vector perpendicular to $X$, $v = \frac{\partial_t X}{|\partial_u X|}\frac{\partial_u X^\perp}{|\partial_u X|}$, $\kappa = \frac{\partial_{uu} X}{|\partial_u X|^2}\frac{\partial_u X^\perp}{|\partial_u X|}$ (Deckelnick).

**Evolution law** Parametrization $X$ is required to satisfy

$$\partial_t X = \frac{\partial_{uu} X}{|\partial_u X|^2} + F\frac{\partial_u X^\perp}{|\partial_u X|}.$$

The equation is accopanied with initial condition $X(\cdot,0)$ and **periodic** or **fixed ends** boundary conditions. Long-time computations and topological changes are required $\rightarrow$ redistribution of discretization points is needed.

$$\partial_t X = \frac{\partial_{uu} X}{|\partial_u X|^2} + \alpha\frac{\partial_u X}{|\partial_u X|} + F(x,t)\frac{\partial_u X^\perp}{|\partial_u X|}.$$

The red term represents the tangential force.
The value of $\alpha$ depends on the curvature [8].

## 3 Numerical scheme

For numerical approximation we consider a regularized form of the previous equation which reads as

$$B\partial_t X = L\frac{\partial_{uu} X}{Q(\partial_u X)^2} + L\alpha\frac{\partial_u X}{Q(\partial_u X)} + b\tau_{app},\frac{\partial_u X^\perp}{Q(\partial_u X)},$$

where $Q(x_1,x_2) = \sqrt{x_1^2 + x_2^2 + \varepsilon^2}$ is a regularization term and $\varepsilon$ a small parameter. We use the backward Euler semi-implicit scheme for numerical solution of the differential equation. The approximation of the first derivative is denoted as $X_{\bar{u},j}$ and the second derivative as $X_{\bar{u}u,j}$.

The semi-implicit scheme for equation has the following form

$$BX_j^{k+1} - Lt\frac{X^{k+1}_{\bar{u}u,j}}{Q^2(X^k_{\bar{u},j})} - Lt\alpha_j\frac{X^{k+1}_{\bar{u},ej}}{Q(X^k_{\bar{u},j})} = BX_j^k + tb\tau_{app}\frac{X^{\perp k}_{\bar{u},j}}{Q(X^k_{\bar{u},j})},$$
$$j = 1,\cdots,m-1, k = 0,\cdots,N_T - 1,$$

where $Q(x_1,x_2)$ is a regularization term, $X^\perp_{\bar{u},j}$ is a vector perpendicular to $X_{\bar{u},j}$, and $\alpha_j$ is redistribution coefficient. The term $\varepsilon$ serves as a regularization to avoid singularities when the curvature tends to infinity. $X_j^k \approx X(jh,kt)$, $t$ is a time step and $N_T$ is the number of time steps. The matrix of the system for one component of $X^{k+1}$ has the following tridiagonal structure:

$$\begin{pmatrix} B + \frac{2tL}{h^2Q^2} - \frac{tL\alpha}{hQ} & \frac{-tL}{h^2Q^2} & 0 & \cdots \\ \frac{-tL}{h^2Q^2} + \frac{tL\alpha}{hQ} & \ddots & \ddots & \ddots \\ 0 & \ddots & & \\ \vdots & \ddots & & \end{pmatrix}.$$

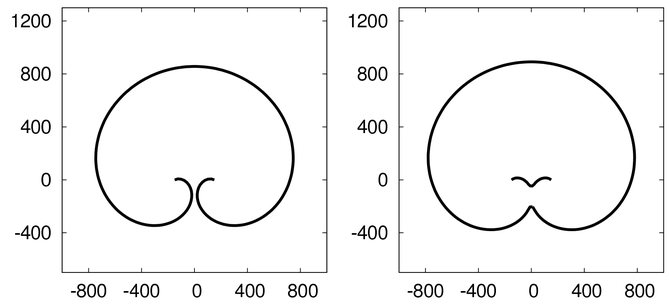
The scheme is solved for each $k$ by means of matrix factorization. Since there are two components of $X$, two linear systems are solved in each timestep.

## 4 Numerical results

Dislocation curves as defects in material evolve in time. The dislocation evolution history contains shape changes of open curves, closing of open dislocation curves up to collision of dipolar loops (see [1, 2]). Interaction of dislocation curves and dipolar loops has been studied, e.g., in [3–7]. Our numerical simulations were performed 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 | $\tau_{app} = 40$ MPa |

### 4.1 Strong obstacle



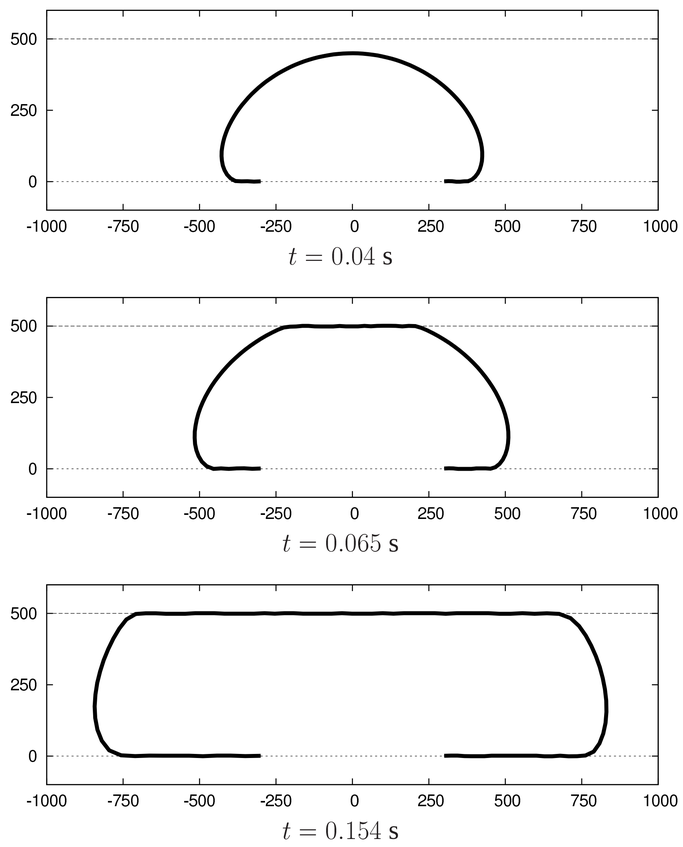

Evolution through a strong obstacle, $F_O = 0.01$ nN, $\tau_{app} = 40$ MPa, $t \in (0, 0.088)$, curve discretized by $M = 200$ nodes.

### 4.2 Frank-Read mechanism



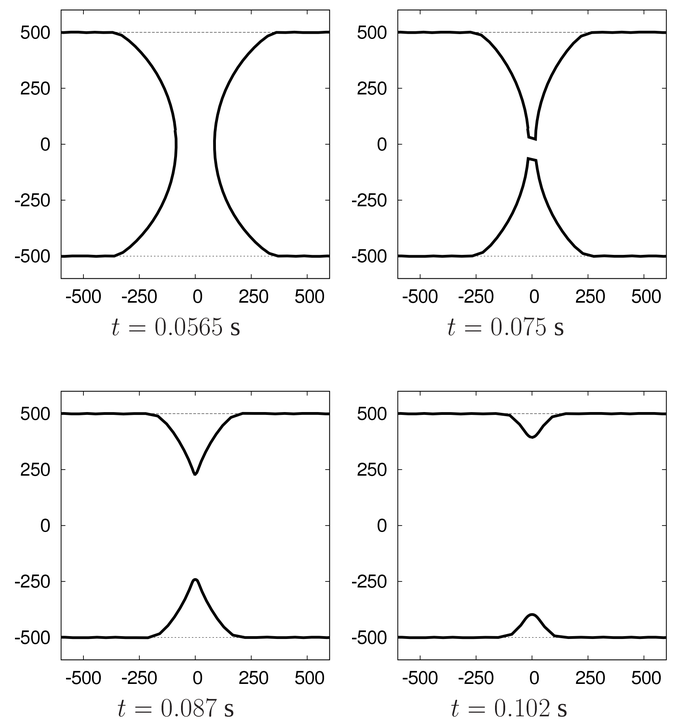

Frank-Read source, $\tau_{app} = 40$ MPa, $t \in (0, 0.29)$, curve discretized by $M = 400$ nodes.

### 4.3 Infinite channel




Single dislocation in an infinite channel, $\tau_{app} = 40$ MPa, $t \in (0, 0.154)$, curve discretized by $M = 200$ nodes.

### 4.4 Cross-slip




Merging two dislocations in a channel, $\tau_{app} = 40$ MPa, $F_C = 0.01$ N for $z < -500$ nm and $z > 500$ nm, $t \in (0, 0.102)$, each curve discretized by $M = 100$ nodes.

## 5 Conclusion

The simulation of dislocation dynamics is important in practice as dislocations affect many material properties. Dislocation dynamics can be mathematically modelled by the mean curvature flow. We presented a method based on a parametric approach. We applied the model to situations similar to the real context including a mechanism of creating new dislocations (i.e., Frank-Read source, cross-slip, etc.). The scheme had to be improved by an algorithm for tangential redistribution of points and by an algorithm for topological changes for parametric model.

## 6 Acknowledgement

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Mathematical Modelling Group

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