Friedrich-Alexander-Universität
Faculty of Engineering

Department Materials Science

WW8: Materials Simulation

Practical: Discrete Dislocation Dynamics simulation

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Supervision:

Contents

1 Introduction

The topic of this practical is to get an introduction into *discrete dislocation dynamic* (DDD) simulations. In the course of the following exercises the open-source software *microMegas* (mM) is utilized [1].

1.1 General Aspects of Dislocation Dynamics

As it is common for DDD simulation, three steps are carried out to model the dynamics of the dislocations:

1. calculate the stress field
2. calculate the Forces acting on the dislocation line segments (according to eq. 1 - the Peach-Köhler equation)
3. moving the line segments accordingly - the velocities are calculated according to eq. 2a and are moved following forward Euler (eq. 2b)

$$F = (\sigma_{ext} + \sigma_{int})\mathbf{b}l \tag{1}$$

The Peach-Köhler Equation (eq. 1) takes into account internal- σ_{int} and external stresses σ_{ext} acting on dislocation segments of vector l with a burgers vector of $\mathbf{b}$. In mM (and similar frameworks) σ_{ext} is imposed on the system as a parameter.

$$v = M(F) \tag{2a}$$

$$r(t + \Delta t) = r(t) + v(t)\Delta t \tag{2b}$$

The velocities of the segments are a functional of the mobility function $M(F)$ depending on the individual forces, the material and the orientation of the segment. The segments positions are calculated as a result of the the application of the forward Euler scheme - eq. 2b. The new position $r(t + \Delta t)$ after a time step of Δt is calculated as the position $r(t)$ being moved according to its velocity $v(t)$. For forward Euler being applicable we assume quasi-static deformation.

As a result of the forces imposed on a dislocation, the dislocation might curve. In mM this is achieved by cutting the curved line into several segments. These segments are discretized as depicted in fig. 1.1. The choice to include 8 slip systems in mM was made as trade-off - balancing the increasing complexity with the best representation of the curved dislocation [1].

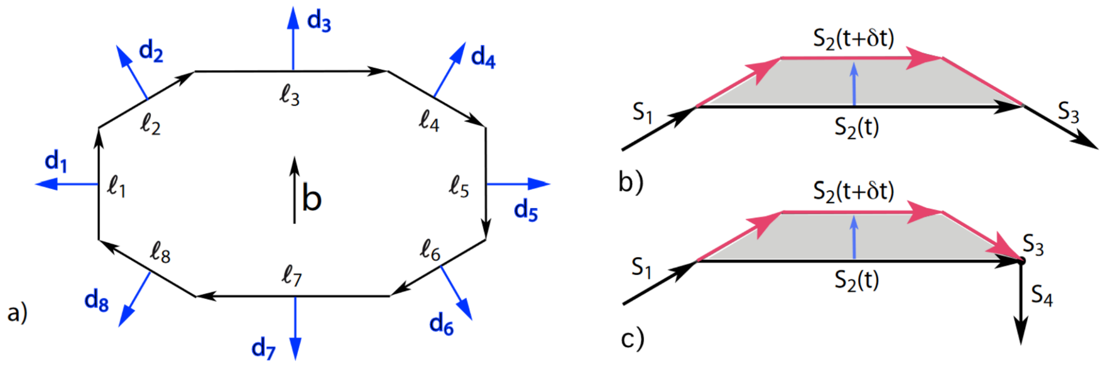

Figure 1: a) Schematic representation of the elementary vectors used per slip system to discretize dislocation lines in mMs. The vectors l_{1-8}(in black), are used for the definition of the segments directions and the vectors $\mathbf{d}_{1-8}$(in blue) for the corresponding displacement directions. b) and c) Geometrical procedures for the displacement of a segment and its length variation. b) The trapezoidal area swept by segment S2 during a time step Δt(in grey) produces and increment of plastic shear.This procedure accounts for the direction of the two neighbouring segments. c) Before the displacement, a local rule for connections imposes the presence of a "pivotal segment" S_3 (segment of zero length) between segments S_2 and S_4 reproduced from [1].

1.2 Frank-Read Source

The Frank-Read source is going to be in the main focus of these exercises. A Frank-Read source is a dislocation segment that is pinned at two points. The force acting on it is generally the Peach-Köhler equation (eq. 1), where the resolved shear stress τ is acting on the segment:

$$F = \cdot\tau\mathbf{b}l \tag{3}$$

Above a certain critical shear stress τ_{crit} the dislocation segment is becoming an infinite source for dislocation loops (see fig. 1.2)

The bow out stress given by Hirth ([3], P. 752):

$$b\tau_{crit} = \frac{\mu b^2}{4\pi r(1-\nu)}\left\{\left[\ 1 - \frac{\nu}{2}(3 - 4\cos^2\beta)\right]\ \ln\frac{L}{\rho} - 1 + \frac{\nu}{2}\right\} \tag{4}$$

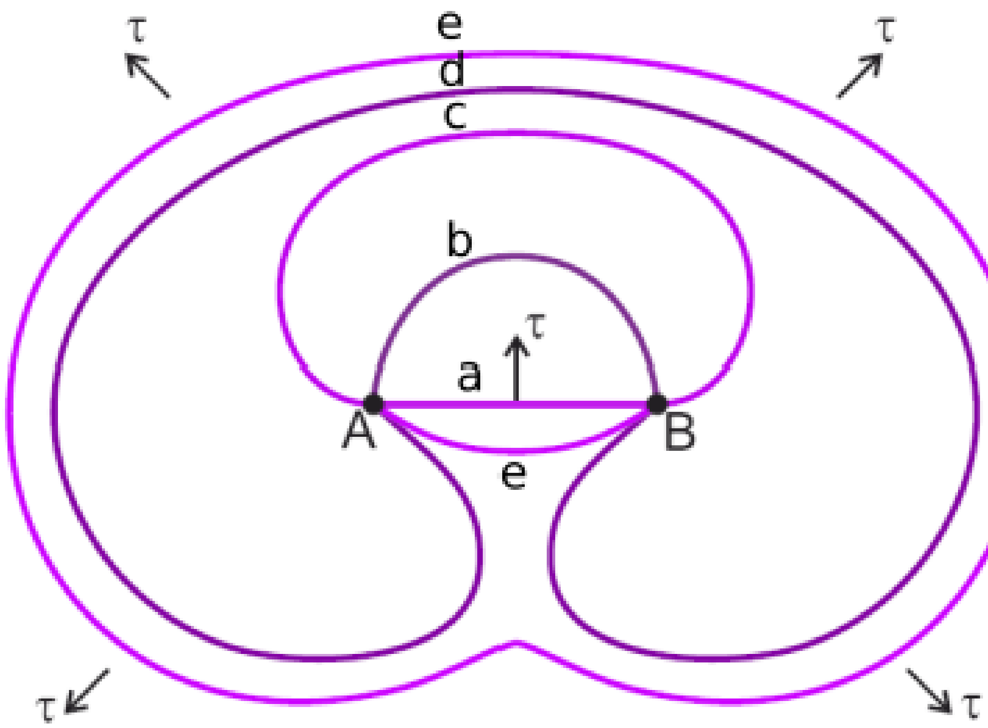

Figure 2: Activation of a Frank-Read source: Dislocation segment (a) is pinned at point A and B. Under the applied shear stress τ it starts to bow out (b) till it reaches its critical configuration (c), and then expands through its unstable state (d) till self-anihilates to a dislocation loop and a new FR segment (e) reproduced from [2].

References

1. Devincre, B., Madec, R., Queyreau, S. & Kubin, L. Modeling Crystal Plasticity with Dislocation Dynamcis Simulations : The MICROMEGAS Code. (Jan. 1, 2011).
2. Zaiser, M. *Discrete Dislocation Dynamics Simulation - Problem Statement*
3. Anderson, P. M., Hirth, J. P. & Lothe, J. *Theory of Dislocations* 721 pp. ISBN: 978-0-521-86436-7. Google Books: LK7DDQAAQBAJ (Cambridge University Press, Jan. 16, 2017).