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].

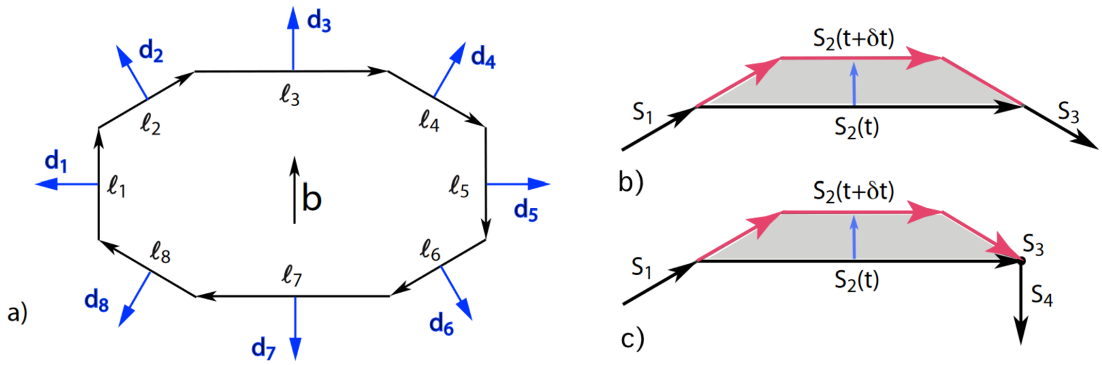

Figure 1: a) Schematic representation of the elementary vectors used per slip system to discretize dislocation lines in mMs. The vectors l_{1-8}(in black), are used for the definition of the segments directions and the vectors $\mathbf{d}_{1-8}$(in blue) for the corresponding displacement directions. 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. 2). The two folders

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

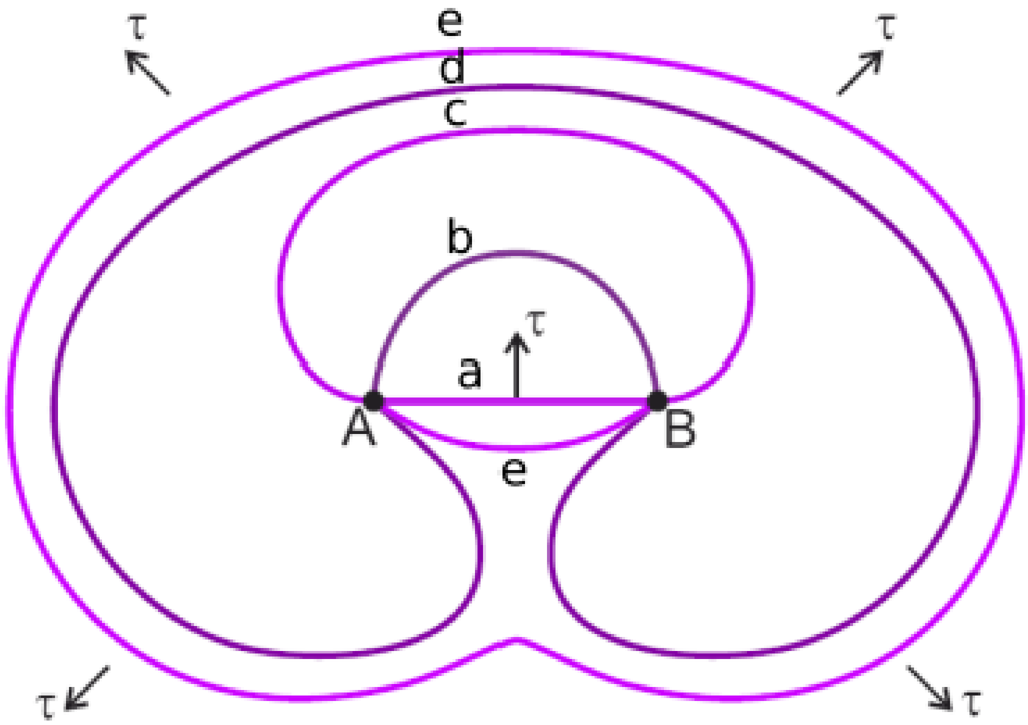

Figure 2: Activation of a Frank-Read source: Dislocation segment (a) is pinned at point A and B. Under the applied shear stress τ it starts to bow out (b) till it reaches its critical configuration (c), and then expands through its unstable state (d) till self-anihilates to a dislocation loop and a new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

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

for the common case of $L = 1000\rho$ is simplified to:

$$\tau_{crit} = \alpha\frac{\mu b}{L} \tag{5}$$

with α being 0.5 for pure edge dislocations and 1.5 for pure screw dislocations [2].

2 Simulation Setup (Task 1)

The first Task deals with setting up a simulation of a pinned edge dislocation in mM. It acts as both an introduction the the software and an initial state for the following tasks.

2.1 Installing and Getting to Know The Software (Task 1.1 - 1.3)

In the first Task the required software is installed from the microMegas Homepage. The folder in which most work are done are `\in` and `\out`

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).