



Friedrich-Alexander-Universität
Faculty of Engineering

Department Materials Science

WW8: Materials Simulation

Practical: Discrete Dislocation Dynamics simulation

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Supervision:

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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)

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

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.

$$v = M(F) \quad (2a)$$

$$r(t + \Delta t) = r(t) + v(t)\Delta t \quad (2b)$$

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].

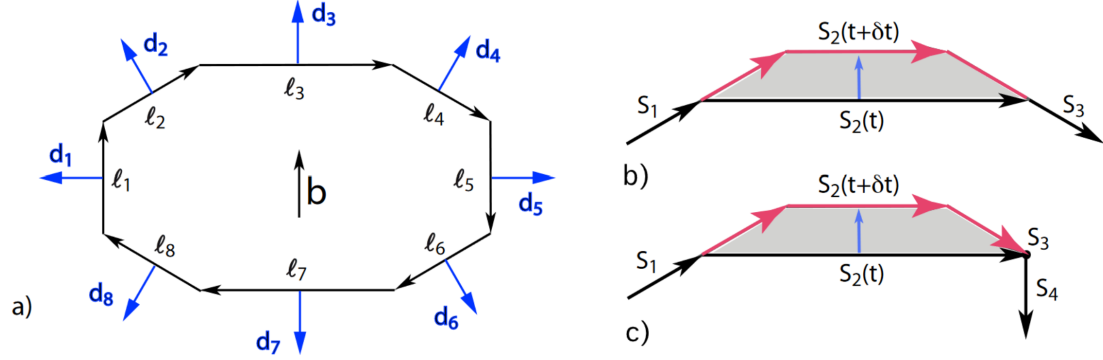


Figure 1: a) Schematic representation of the elementary vectors used per slip system to discretize dislocation lines in mM. The vectors l_{1-8} (in black), are used for the definition of the segments directions and the vectors d_{1-8} (in blue) for the corresponding displacement directions. b) and c) Geometrical procedures for the displacement of a segment and its length variation. b) The trapezoidal area swept by segment S_2 during a time step Δt (in grey) produces an 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:

$$F = \tau b l \quad (3)$$

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):

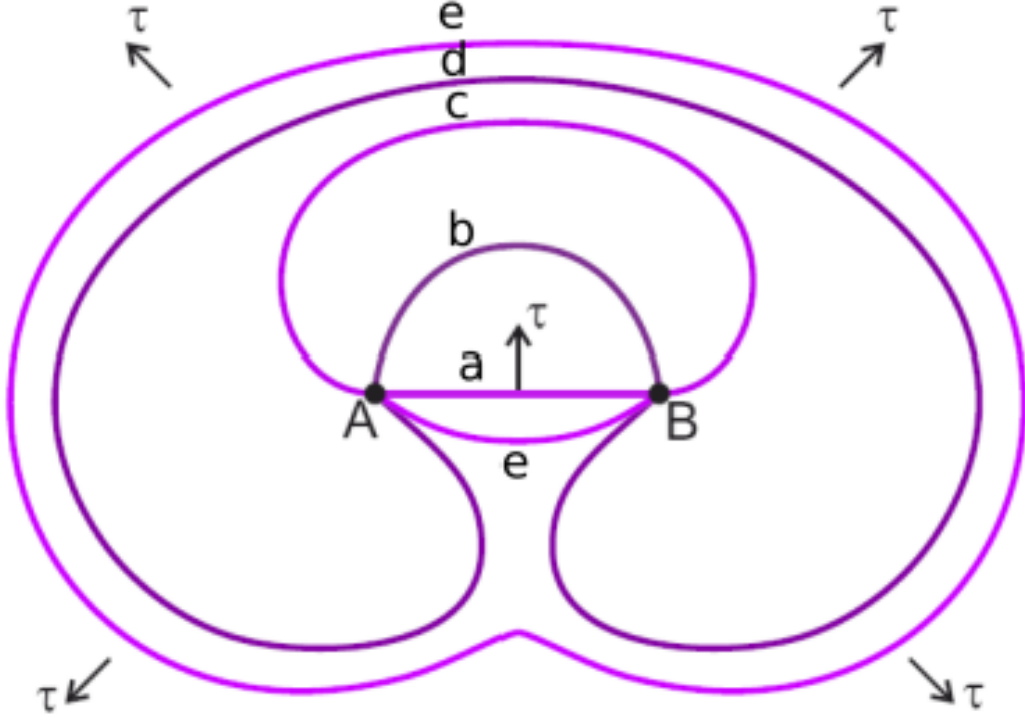


Figure 2: Activation of a Frank-Read source: Dislocation segment (a) is pinned at point A and B. Under the applied shear stress τ it starts to bow out (b) till it reaches its critical configuration (c), and then expands through its unstable state (d) till self-annihilates to a dislocation loop and a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

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

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

$$\tau_{crit} = \alpha \frac{\mu b}{L} \quad (5)$$

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 to 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. When running on a linux machine, virtual machine or WSL one can go to the `\bin` folder and run `make all` to compile the source files. The folder in which most work are done are `\in` and `\out`. Under `\in` the input files are defined in `input.dd`:

1. material specific data (e.g. Shear Modulus, Burgers Vector Norm, slip planes, slip directions)
2. simulation specific data (e.g. initial stress, stress increment, time step, echelle - size of elementary screw vector)
3. data defining the dislocation segments (position, composition, pinning)

To run the simulation we run `.bin\gmm` (for interactive mode with graphical interface - see fig. 3). The output can be visualized in the `\out` folder using plotting the data saved to the `graph.txt` file.

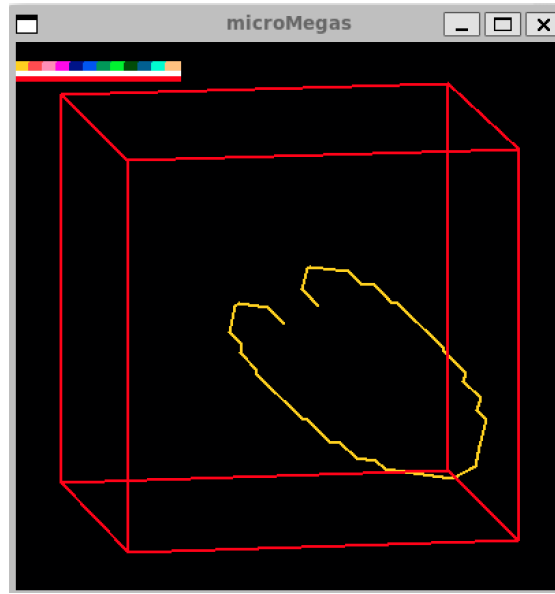


Figure 3: GUI of mM

References

1. Devincre, B., Madec, R., Queyreau, S. & Kubin, L. Modeling Crystal Plasticity with Dislocation Dynamics Simulations : The MICROMEAS 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).