FAU

Friedrich-Alexander-Universität
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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].
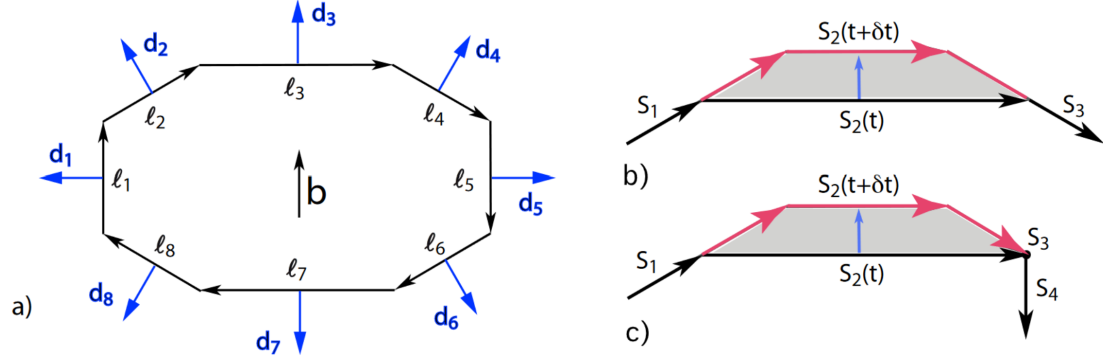

Figure 1: a) Schematic representation of the elementary vectors used per slip system to discretize dislocation lines in mMs. The vectors l_{1-8}(in black), are used for the definition of the segments directions and the vectors $\mathbf{d}_{1-8}$(in blue) for the corresponding displacement directions.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

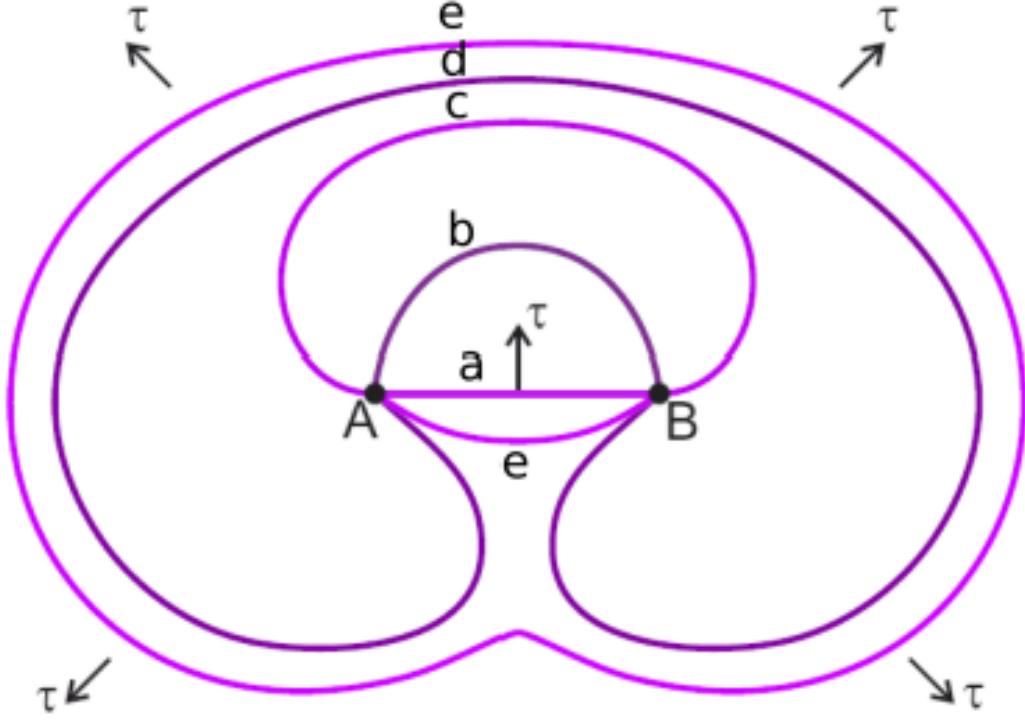The bow out stress given by Hirth ([3], P. 752):

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].

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

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

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

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 - 1.4)

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 ron `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.

2.2 Defining the Simulation Box (Task 1.5)

Since the documentation of mM is not very clear on how the input is interpreted, it has to be deduced which input has an effect on the output. The `echelle` value in the `CuSeg` file seems to have an effect on the reference scale of the simulation as depicted in the `BVD.CFC` file. If we leave the initial value of `echelle` at 13.5 the reference scale is $1.2183007689602674'10^{-9}$. Following the notes given in the respective README files and assuming that this value is given in units of meter, we can derive, that in the file defining our dislocation segments, we need to use a value of 2464 to have approximately 3 $\mu m5$as the box dimensions.
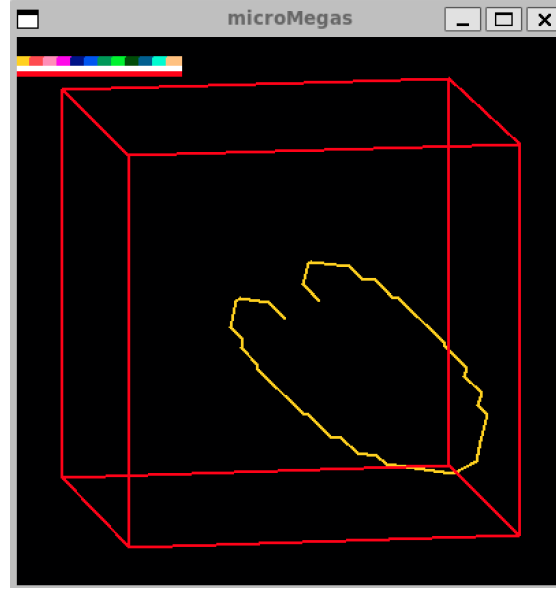
Figure 3: GUI of mM

2.3 Defining the Pinned Edge Dislocation (Task 1.6)

For the pinned edge dislocation we define an input file `Seg_Pinned_Edge` as follows:

```
1 1 1 1 1 1 1 1 1 1 1 1 1
1
2464 2464 2464
1 1200 1200 1200 80 3 0 0 0 0 F 0 0
```

The first line defines which slip-systems are active (here all), the second is the number of dislocation segments the third defines the box size as a multiple of BVD units. The third line defines the dislocation as follows: column 1 - The segment index, column 2 - x coordinate of the segment origin, column 3 - y coordinate of the segment origin, column 4 - y coordinate of the segment origin, column 5 - length of the segment in BVD vector unit, column 6 - index of the BVD vector parallel to the segment direction, column 7 - first neighbor segment at the origin of the segment (zero for pining point), column 8 - first non zero length neighbor segment at the origin (idem), column 9 - first neighbor segment at the extremity side (idem), column 10 - first non zero length neighbor segment at the extremity side (idem), column 11 - Flag for junction segment, column 12 - index of the binome segment use to form a junction, column 13- Flag for screw segment in cross-slip state (blocked at the intersection of different glide planes). This is stated as a

comment in an initial file, although it is not explicitly stated, what "idem" means. When running the simulation without an applied stress the `graph.txt` output shows a value for the dislocation density that is 4 times the expected value. For these reasons the number of segments previously chosen in section 2.3 is readjusted to be 20 instead of 80. This now leads to a dislocation density of $\rho = 0.44127 * 10^{10} \; \frac{1}{m^2}$ that is a segment length of $L \approx 119 \; nm$.

2.4 Estimation of Critical Activation Stress (Task 1.7)

The critical shear stress τ_{crit} can be estimated using 4. With $\alpha = 0.5$, $\mu = 25.0 \; MPa$, $b = 2.5525$ Å and a length of $L \approx 119 \; nm$. Resulting in an estimate value of $\tau_{crit} = 45.0 \; MPa$.

2.5 Calculating the Critical Activation Stress (Task 1.8)

To calculate the critical activation stress we start a Simulation at with an initial shear stress of 45 GPa and increase the stress by a value of $3 * 10^9 \; \frac{MPa}{s}$ where the time step set to $0.125 * 10^{-11} \; s$. Plotting the dislocation density ρ with increasing τ (see fig. 4)) allows us to find the point at which the density starts to increase - meaning: the source has been activated. Using a python script implemented with the elbow method the point at which ρ starts to deviate (τ_{crit}) can be reproduced. Here it is 73.5 MPA.
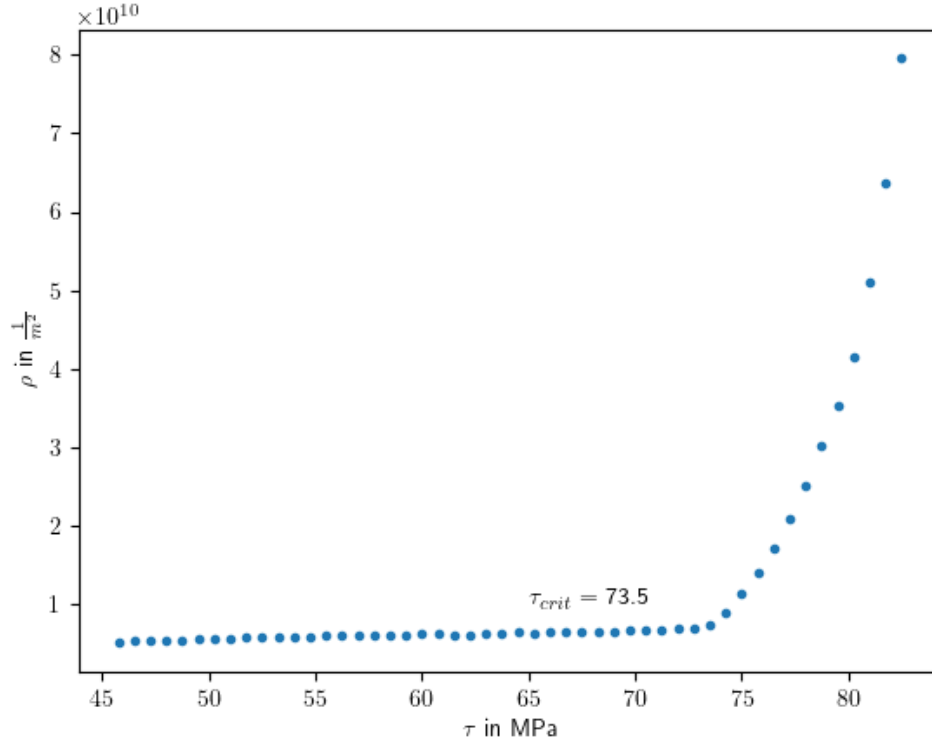
Figure 4: Dislocation density ρ with increasing shear stress τ. τ_{crit} is reached at 73.5 MPa.

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).