



Friedrich-Alexander-Universität
Faculty of Engineering

Department Materials Science

WW8: Materials Simulation

Practical: Discrete Dislocation Dynamics simulation

Leon Pyka (22030137)

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].

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.

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

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

$$(2c)$$

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. 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].

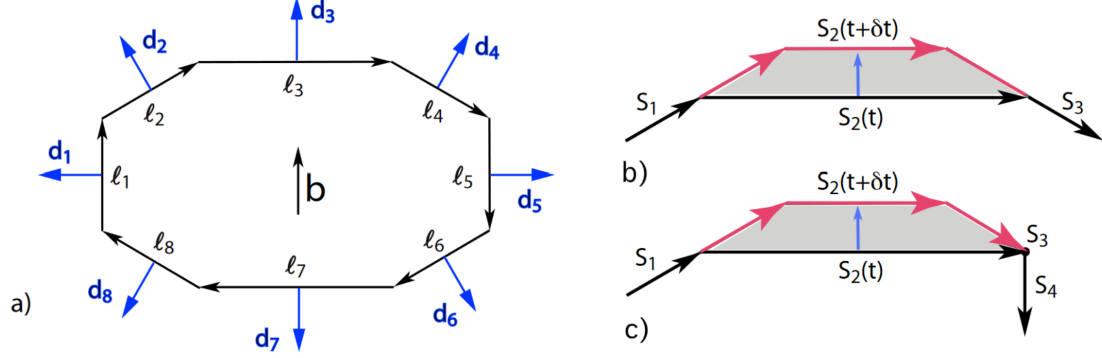


Figure 1: a) Schematic representation of the elementary vectors used per slip system to discretize dislocation lines in mMs. The vectors l_{1-8} (in black), are used for the definition of the segments directions and the vectors d_{1-8} (in blue) for the corresponding displacement directions. b) and c)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

References

1. Devincere, B., Madec, R., Queyreau, S. & Kubin, L. Modeling Crystal Plasticity with Dislocation Dynamics Simulations : The MICROMEGAS Code. (Jan. 1, 2011).