(Discrete) Dislocation Dynamics Simulations

Mesoscopic simulations of dislocations collective properties and plastic deformation

riccardo.gatti@cnrs.fr

LEM, CNRS-ONERA, 29 av. de la Division Leclerc
92322 Cedex, Chatillon, FRANCE

école d'été "Modélisation des Matériaux" 2024

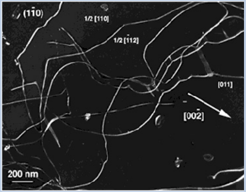
Plan

1. Introduction
2. Discrete Dislocation Dynamics Simulations (DD)
3. Main ingredients in DD simulations
4. DD : Boundary conditions
5. Simple examples

The different scales of crystal plasticity

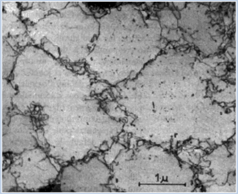
Nano-Micro

Dislocation properties



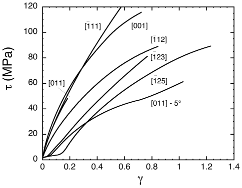
Meso

Collective properties



Macro

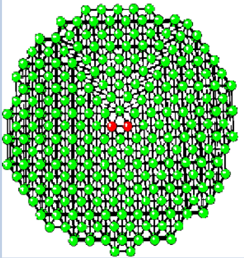
Mechanical properties



Simulations of plastic deformation

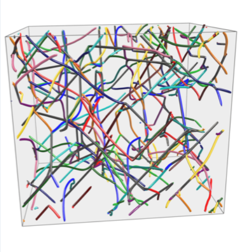
Atomistic modeling

nm and 10^{-15} s



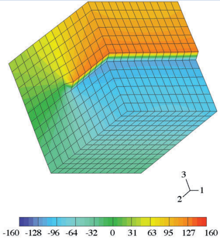
DD and Phase field

μm and $10^{-10} - 10^{-5}$ s



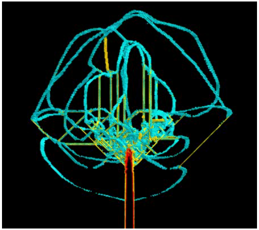
FEM, BEM, etc..

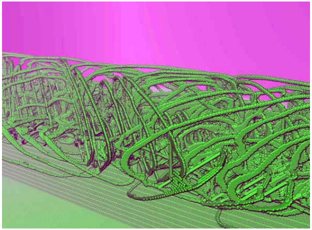
mm - km and s - y



Modeling in 'material sciences' and 'mechanical engineering' is today a strategic activity of many businesses.

Atomistic simulations of plasticity





Atomistic simulations can today accounts for more than 10^{10} atoms.

Nevertheless such simulations will always be restricted to the modeling of volumes as small as a few nanometers per side.

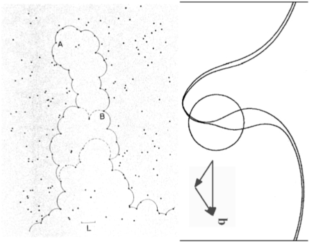
DD simulations

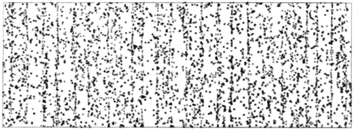
At beginning - 2D simulations

1966 — 2D in plane: Brown, Bacon, Foreman ..

1986-87 — 2D end on: Lépinoux & LK, Ghoniem & Amodeo

→ many others in 2D





- **Line tension, obstacle pinning** but planar slip in a single plane
- **Patterning: (1/ r) interactions** but no curvature and line tension

Real plasticity is a combination of both

Three dimensions DD simulations

3D DD - microMegas (1992)

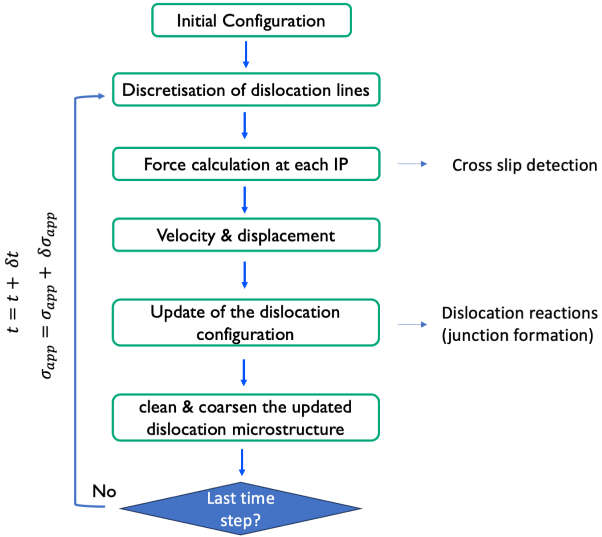
Elastic Properties
Local rules
Periodic boundary conditions ...

What are DD simulations good for?

- Expand the dislocation theory predictions
  - To Explain and to model complex plastic behaviors
  - To simulate single crystal, polycrystals and multiphased materials with a unique formalism.
- Do the link between discrete and continuous modeling
  - Identify, test and validate new physically justified material laws.
  - Measure model parameters for large scale simulations (coarse graining).

1. Introduction
2. Discrete Dislocation Dynamics Simulations (DD)
3. **Main ingredients in DD simulations**
4. DD : Boundary conditions
5. Simple examples

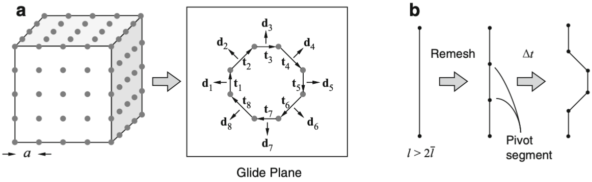
DD flowchart



Discretization of the dislocation lines

Lattuce simulations

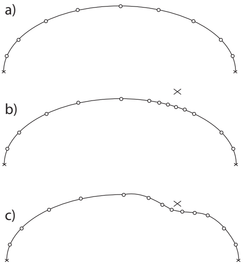
Dislocation lines are describe with "chains" of straight segments including one or few integration points (IP) to compute forces.



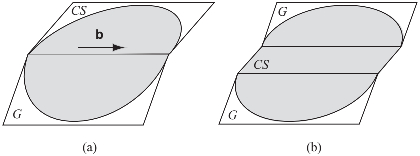
- Crystal symmetry
- Coding simplicity

Remarks on line discretization

- The number of integration point is imposed by the stress gradient



Dislocation cross-slip



Cross-slip, like other stochastic processes taking place during dislocation dynamics can be simulated with a "Monte-Carlo" algorithm, if one can define the corresponding probability function.

$$P(l) = \beta \frac{l}{l_0} \frac{\Delta t}{\Delta t_0} \exp\left(\frac{|\tau| - \tau_{\mathrm{III}}}{kT}\right)$$

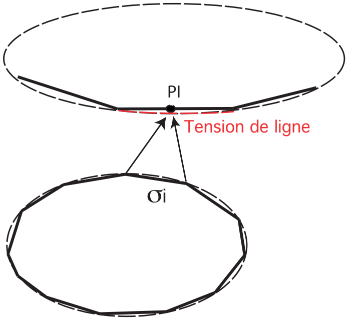
Forces in infinite crystals

- Dislocation segment stress field, σ_i.
- Peach-Koehler force

$$\frac{\mathbf{F_j}}{\mathbf{L_j}} = (\sum_i \sigma_i + \sigma_{app}).\mathbf{b_j}) \times \boldsymbol{\ell}_j$$

- Line tension correction

$$\Gamma \approx \frac{\mu b^2}{4\pi R} \ln(\frac{R}{r_0})$$



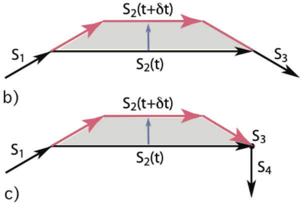
Computation of forces at the IP is the most CPU extensive part of DD simulations ($\approx 90\%$).

Dynamics and time integration

For many problems, dislocations can be considered as classical objects with a very low mass and high energy. Hence, Newton law equations can be integrated without considering inertial effects.

$$\mathbf{r}(t+\delta t) = \mathbf{r}(t) + \delta t.\mathbf{v}(t)$$

$$\mathbf{v}(t) = \frac{\tau^*(t).\mathbf{b}}{B(T)}$$



B is a viscous coefficient accounting mainly for dislocation-phonon interactions. It is material and temperature dependent.

Optimizations of the forces computation

1. Multi-poles algorithm
2. Parallelization
3. Multi time steps integrations

- Today, free (and open source) codes exist and can be download on the web.
  - microMegas - http://zig.onera.fr/mm_home_page
  - Paradis - http://paradis.stanford.edu
  - Model - https://bitbucket.org/model/model/wiki/Home
  - etc ...

Deformation and rotation fields

A plastic shear increment on glide system "s" is induced by each displacement of the dislocations in their glide planes.

$$\gamma^{(s)} = \sum_{i=1}^{N} \frac{|b_i|\, A_i^{(s)}}{V}$$

At each time step, increments of the deformation and the rotation tensor are calculated for the total simulated volume (or in sub-volumes)

$$\mathrm{d}\varepsilon_{ij}^{p} = \sum_{s=1}^{n} \gamma^{(s)} \mathrm{d}\epsilon^{(s)} \qquad \text{et} \qquad \mathrm{d}\Omega_{ij}^{p} = \sum_{s=1}^{n} \gamma^{(s)} \mathrm{d}\omega^{(s)}$$

with

$$\mathrm{d}\epsilon^{(s)} = \frac{1}{2}(\mathbf{m}^{(s)} \otimes \mathbf{n}^{(s)} + \mathbf{n}^{(s)} \otimes \mathbf{m}^{(s)})$$

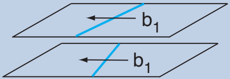
$$\mathrm{d}\omega^{(s)} = \frac{1}{2}(\mathbf{m}^{(s)} \otimes \mathbf{n}^{(s)} - \mathbf{n}^{(s)} \otimes \mathbf{m}^{(s)})$$

m=shear direction

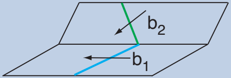
n=glide plane normal

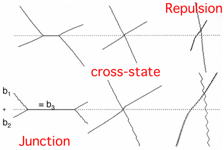
Dislocation-dislocation reactions

Dipole

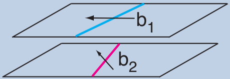


Junctions

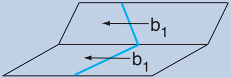




Coplanaire



Colinéaire



- Contact reactions are elastically driven (poorly affected by dislocation core).
- Additional degree of freedom are introduced along the lines at contact points.
- Junction zipping and unzipping is controlled by line tensions at the triple nodes.

Comparison with atomistic simulations

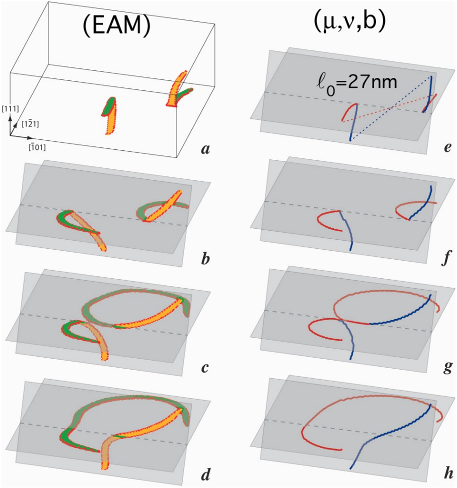
Collinear annihilation

Comparison between MD and DD (here Al).

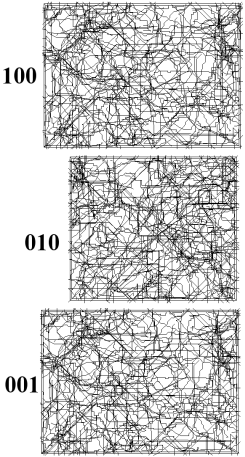
At critical curvature (b et f):

MD $\tau_c/\mu = 1.85\,10^{-2}$

DD $\tau_c/\mu = 1.67\,10^{-2}$



Periodic boundary conditions (PBC)

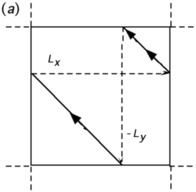


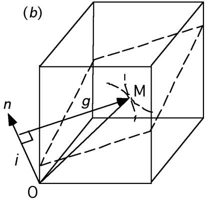
PBC

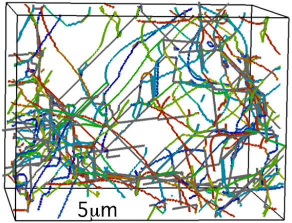
- Flux balance at boundaries
- Continuity of dislocation lines
- Infinite crystal mechanics

Dislocation mean free path

PBC artifact: dislocation self annihilation



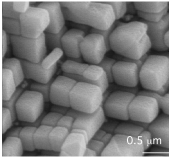


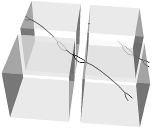


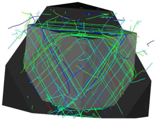
Complex boundary conditions

Surfaces and interfaces

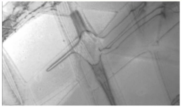
Exemple : superalliages



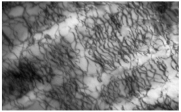




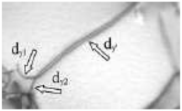
Confinement



Misfit

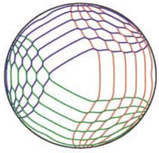


Multi-phases



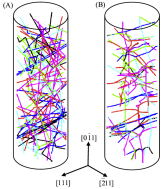
FEM and DD simulation coupling

Three solutions exist:

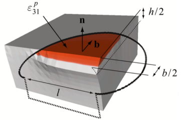


1. Superposition method (Vandergiessen:95):

$$\sigma_{dis} = \sigma_{dis\,\mathrm{inf}} + \sigma_{CL}$$



2. Discrete-continuous model (Lemarchant:01):
   Here a DD simulation is used instead of the FEM constitutive plastic law.



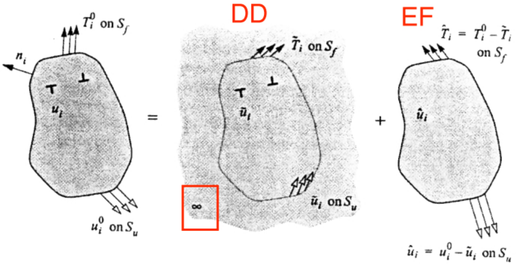
DD + FEM : Boundary value problem 1

Superposition principle

1995 -> van der Giessen, Needleman et al. (2D)

-> 3D Fivel, Weygand

$$\sigma_{dis} = \sigma_{dis\infty} + \sigma_{bc}$$



Dislocation singularities are moved to the surface

Stresses must be interpolated in the volume

DD + FEM : Boundary value problem 2

The Discrete - Continuous Model (DCM)