Coupled 3d dislocation dynamics at nano- and micro-scales

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Size effects in plasticity deformations

Compression of a micro-pillar

Sun et. al. Scripta Materialia 65 (2011)
Computational tools for dislocation dynamics

Multiscale problem

Discrete Dislocation Dynamics

- Simple representations
- Large domain sizes
- Comparable to experiments
- Long-range elastic field
- (-) Adhoc approach for nucleation
Computational tools for dislocation dynamics

Multiscale problem

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From 2D to 3D

CADD (2d) (Curtin’s group)
Shilkrot et.al.2004, Shiari et.al.2005

Hybrid dislocation

$\vec{t}_{\text{ext}}$
$\vec{u}_{\text{ext}}$

CADD3d project since 2013
PIs.: Curtin, Molinari and Anciaux

Hybrid dislocation should behave as one single dislocation
structure $\rightarrow$ Reciprocal boundary conditions
**CADD3d**

**Coupled Atomistic/Discrete Dislocations method in 3d**

From 2D to 3D

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**Diagram**

- **Indenter**
- **MD**
- **DD**
- **Infinite straight dislocation**

**Equations**

- \( \mathbf{t}_{\text{ext}} \)
- \( \mathbf{u}_{\text{ext}} \)

**Text**

- Hybrid dislocation should behave as one single dislocation structure → Reciprocal boundary conditions
Reciprocal boundary condition

Communications between MD and DD

- MD
- Pad atoms
- Slaved DD
- DD

Slaved DD

Detection zone

Pad atoms (slaved atoms)
Application of the BC during dynamics

Periodic synchronization of the BCs

Detection: DXA (Stukowski et al. 2012) & Centro-symmetry

Update pad atoms: Linear elasticity & core corrections

Exact mobility law compared to MD dislocations

\( M(\theta, T) \)
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Update pad atoms

Pad domain decomposition

Correction of core structure

linear elasticity +
core correction: Core structure $\bar{u}(\theta)$

$-\text{linear elasticity}$

pad

$\vec{r}_c$

$\theta$

Total 8 character angles $\theta$ were considered ($0^\circ \leq \theta \leq 90^\circ$).

The obtained MS core structures are validated by the analytic model (Peiers-Nabarro method).

The displacement meshes are stored in template forms.
Update pad atoms

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Mobility law

Mobility law as functions of characters angle and temperature

\[ v = \frac{F}{M}(\theta, T) \]

The various character angles \( \theta \) and temperatures (1, 100, 200 and 300K) are considered.

The mobility law (acceleration and gliding) is constructed.

It is implemented in the DDD engine (ParaDiS).
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Simulating engines

The third-party software components

- The three (open-source) codes communicate with each other through (open-source) LibMultiScale developed by Dr. G. Anciaux and co-workers.
- The (presented) MD↔DDD scheme is parallelized with MPI.
The various character angles $\theta$ are considered.

Several shear stresses $100\text{MPa} \leq \sigma \leq 1000\text{MPa}$ are applied in Burgers vector $\vec{b}$ direction on DD domain.

The corresponding strains $\epsilon$ are applied on MD atoms, and updated every coupling step.
Example: Mixed 30° dislocation, Shear stress 100MPa
Simulation result

Evolution of displacements and velocities

Example: Mixed 30° dislocation with 100MPa and 500MPa

All the cases with the various character angles and shear loading are successfully tested.
Test2: Hybrid dislocation loop

Perspective view and Top view

- DD
- MD
- $x[11\bar{2}]$
- $y[111]$
- $z[1\bar{1}0]$
- $\vec{b}$
- 140 Å

140 Å

140 Å
Simulation video

Example: shear stress 400MPa
Simulation results

Evolution of displacements and velocities along $x + z = 0$ axis
Test 3: Multiple dislocations

Perspective view and Top view

- Fixed DD loop
- Hybrid loop

$\vec{b}$
Simulation results

Evolution of displacements and velocities along $x + z = 0$ axis
Frank-Read source in Al-5%Mg alloy

- Nucleation source: a double Frank-Read source
- 5% magnesium substituents are randomly distributed in MD.
Simulation video (on-going)

Example: applied stress 1.0 GPa and $L_{DD}=0.5 \mu m$
Conclusions

Highlights of CADD3d

▶ Unique capability to handle dislocation dynamics coupled between MD and DD.
▶ Natural dislocation nucleation in DD.
▶ Enable infinite boundary condition in MD (no PBCs).

Outlook

▶ Possible application: single-arm Frank-Read source
▶ Future development: coupling with FEM → Indentation
Boundary conditions

Constant stress $\sigma_{ext}$

$$\vec{u}_{pad} = \vec{u}_{ext} + \vec{u}_{dislo}$$

$$\epsilon_{ext} = \sigma_{ext} / \mu$$

$$\sigma_{ext}$$

, where $\mu$ the shear modulus.
Connection between two slave DD nodes

Two strategies to close dislocation network
Simulation videos (test2 and test3)

Case0: partial detection
Case1: full detection
Case2: interaction
Validation (on-going)

Comparison between MD, DDD and CADD3d

Example: Aluminum, Single FR source, 700MPa, and L=50nm