Dislocation dynamics

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Christophe DEPRES, Chan Sun SHIN, Hyung-Jun CHANG

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Motivations: Metal forming: Viewed from Mechanics eyes

Continuum Mechanics

Finite Element simulations (Yield strain criterion: Von Mises)

Plasticity in crystalline materials

[Jaoul 1965]

Visible slip lines
**Numerical modelling:** (Finite Element Simulations):

\[
\text{div}\sigma + f_v = \rho \frac{\text{d}v}{\text{d}t}
\]

constitutive equations

**Example of constitutive equations (crystal plasticity):**

\[
\dot{\sigma} = f(\sigma, \varepsilon, \dot{\varepsilon})
\]

**Isotropic hardening:**

\[
\tau^s_c = r_0 + Q \sum_{r=1}^{N} h^{sr} [1 - \exp(-B v^r)], \quad \text{avec} \quad \dot{v}^s = |\dot{\gamma}^s|
\]

**Kinematic hardening:**

\[
x^s = c a^s, \quad \text{avec} \quad \dot{a}^s = \dot{\gamma}^s - d |\dot{\gamma}^s| a^s - \left(\frac{|a^s|}{M}\right)^m \text{signe} (a^s)
\]

**Very efficient BUT:**

*Phenomenological equations*

- **Lack of generality**

**Example:** Cailletaud, Forest et al.

**Need of information from the physics of plastic deformation**

**Crystal plasticity = dislocations motion**
**Multiscale Materials Modelling**

- Scanning Electron Microscope
- Transmission Electron Microscope
- Optical Microscope
- High Resolution Electron Microscope
- Eye

- Time [s]
- Size [m]

- Crystal plasticity (single crystals)
- Crystal plasticity (polycrystals)
- Homogenization technics
- Continuum mechanics
- Discrete dislocation dynamics
- Molecular dynamics

- Multiscale Materials Modelling
Dislocation dynamics simulations: 2D models

Seen in the slip plane:
- Interaction disloc/solutes
- precipitates, cavities,
- iirradiation defects
-...

Or…seen from line directions (edge):
- hardening
- films on substrates,
- composites
-...

Advantages: simple, fast

Drawback: 3D reality is missing
Line tension, junction, crossslip,…

2,5D ou 3D
3D modeling of dislocation dynamics

Françoise LOUCHET (Grenoble)

Thin foil (~200nm thick)

Slip plane
**Driving force** = elastic stress tensors (internal + applied)

\[ v = \frac{\tau b}{B} \]

**Dislocations** = edge and screw segments embedded in an elastic continuum

(Kubin, Canova and Bréchet 1992)

(similar to elastic inclusions)

**Example:**
Glissile dislocation loop

**Plastic deformation:** direct output
Modern 3D Discrete Dislocation Dynamics Codes (project NUMODIS (CNRS-CEA) L. Dupuy, M. Blétry)

Advantage: closer to reality

Frank-Read source + partials

Dislocation junctions

Stacking Fault Tetraedra

Nodal code

Drawback: Ten times slower

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Time [s]

Crystal plasticity (single crystals)
Discrete dislocation dynamics
Molecular dynamics

Crystal plasticity (polycrystals)
Homogenization technics
Continuum mechanics

Size [m]

Scanning Electron Microscope
Transmission Electron Microscope
Optical Microscope
High Resolution Electron Microscope
Multiscale Materials Modelling

Example of scale transition:
From dislocation dynamics to continuum mechanics
Identification of crystal plasticity constitutive equations
(Coll. L. Tabourot, C. Déprés, SYMME, Annecy)

\[
\dot{\gamma}^{(s)} = \dot{\gamma}_0^{(s)} \left( \frac{\tau^{(s)}}{\tau^{(s)}_{\mu}} \right)^{1/m} \\
\tau^{(s)}_{\mu} = \mu b \sqrt{\sum_{u=1}^{12} a_{su} \rho^{(u)}} \\
\rho^{(s)} = \frac{1}{b} \left\{ \frac{1}{K} \sqrt{\sum_{u=1}^{12} d_{su} \rho^{(u)}} \right\} \dot{\gamma}^{(s)}
\]

K = 32
\beta R = y_c \sim b

3D tensorial framework

\[
\dot{\tau}^{(s)} = \sum_{u=1}^{12} \left\{ \frac{\mu a_{su}}{2 \sqrt{\sum_{p=1}^{12} a_{sp} \rho^{(p)}}} \left( \frac{1}{K} \sqrt{\sum_{q=1}^{12} d_{uq} \rho^{(q)}} \right) - 2 \beta R \rho^{(u)} \right\} \dot{\gamma}^{(u)}
\]

soit
\[
\dot{\tau}^{(s)} = \sum_{u=1}^{12} h_{su} \dot{\gamma}^{(u)}
\]

Finite Element Implementation (ABAQUS : UMAT and VUMAT)

Example multicrystal Al

(Ph. D. Hyung-Jun CHANG (2009))
Crack initiation in fatigue
(111) Nanoindentation of Cu single crystal
(See also http://www.numodis.fr)
Creep of ice single crystals
Micro-compression of Mg pillars
Example of DD applications:
Ph.D. Chan Sun SHIN (2004)
Ph.D. Juliette CHEVY (2008)
Ph.D. Christophe DEPRES (2004)
Ph.D. Hyung Jun CHANG (2009)
Ph.D. Daniel GARCIA-RODRIGUEZ (2011)
Ph.D. Gyu Seok KIM (2011)
Ph.D. Thomas NOGARET (2007)
Ph.D. Gururaj KADIRI (2014)
Example of DD modelling
Clear channels in 316L steel
Plastic behavior of BCC Fe
(111) Nanoindentation of Cu single crystal
Ph.D. Hyung Jun CHANG (2009)
Main objective: Understand physical mechanisms at the origin of cracks

WHEN & WHY do cracks appear?

HOW do cracks propagate?
Discrete Dislocation Dynamics Modelling: Boundary conditions

Typical configuration
(motivated by thermal fatigue experiments)

Output:
- Dislocation microstructure
- Mechanical response
- Deformation of the free surface
- Internal stresses
- ...
Model validation: single slip ($\tau_p = 3\tau_d$)
Model validation: single slip ($\tau_p = 3\tau_d$)

Dislocation microstructure ✓
Model validation: single slip ($\tau_p = 3\tau_d$)

Single slip

Dislocation microstructure ✓
Mechanical response ✓
Model validation: single slip ($\tau_p = 3\tau_d$)

**Single slip**

**Double slip ($\tau_p = \tau_d$)**

Dislocation microstructure ✓
Mechanical response ✓
Strain localization mechanisms

- Strain spreading: Positive effect of x-slip
Strain localization mechanisms

Dipole formation:
Strain localisation
Negative effect of x-slip and dislocation interactions
Strain localization (double slip)

Effect of the grain size: $e \propto D^2$ ; $d \propto D$

Effect of the strain amplitude:

- $e_{cst} ; n \propto \Delta \varepsilon^P$ ; $d \propto 1/\Delta \varepsilon^P$
Mechanism for the formation of the persistent slip band

Dipolar wall (Vein structure)
Kinetics of the persistent slip band (snapshots at $\varepsilon=0$)

Mapping zone

Reversible slip lines

Irreversible slip

Strain localisation inside the Intense Slip Bands

Joint de grain

Free surface

Zero applied strain

PSB

Cycle no. 3

Cycle no. 8

Cycle no. 15

Cycle no. 23

PSB

Extrusion
Plastic slip occurs at the band interface (after stabilisation of disl. density ($N > 10$)).

**Kinetics of the persistent slip band (snapshots at $|\varepsilon| = \varepsilon_{\text{max}}$)**

- Lowest negative strain
- Highest positive strain

---

Mobile disl.  

Plastic slip occurs at the band interface (after stabilisation of disl. density ($N > 10$)).
Sweeping of the prismatic loops (multipoles) by mobile interface dislocations

Schematic description of the Persistent slip band

Mobile dislocations
Tangles
Multipoles (energy concentration)
Channels
Extrusions (stress concentration)

Primary system
Deviation system
Reversible versus irreversible slip

Quantification of the irreversibility:

\[ a_{\text{cum}} = \sum_{n_{\text{coin}}} \frac{L_i}{\cos \alpha} \]

\[ \gamma_{p}^{\text{surf}} = \frac{a_{\text{cum}} \cdot b \cdot \cos \alpha}{S} \]

\[ \gamma_{p}^{\text{surf}}(t) = \gamma_{p,\text{rev}}^{\text{surf}}(t) + \gamma_{p,\text{irr,cum}}^{\text{surf}}(t) \]

\[ \gamma_{p,\text{irr,cum}}(N) = K \sqrt{N} \]
Effect of different parameters

\[ \gamma_{p,irr,cum}(N) = K \frac{h_g}{D_g} \Delta \epsilon_{p}^{\text{VM}} f \left( \frac{\tau_{\text{dev}}}{\tau_{\text{prim}}} \right) \left( 1 + 2 \frac{|\epsilon_{p}^{\text{VM}}|}{\Delta \epsilon_{p}^{\text{VM}}} \right) \sqrt{N} \]
Distorsion energy in channels

Minimisation of mean energy

Increase of maximum energy

Densification of the multipole arrangements

$\langle e \rangle^2 (e + 2\sigma_e)^5$  $\langle e \rangle^2 (e + 2\sigma_e)^{19}$

Multipôles
Stress state in channels
Stress state in channels

Local shear stress

Local normal stress

Densification of the multipole arrangements

No increase of the opening component
Increase of the extrusion shape factor

Continuous increase of opening component at the surface due to stress concentrations

PSB Thickness = cst

PSB height = continuous increase
Crack initiation criterion

\[ h > \delta_{\text{threshold}} \]

\[ \int \int \int \sigma \varepsilon dV \]

\[ \sigma_{nn} > \sigma_{\text{SEPARATION}} \]

\[ N_{\text{init}} > \left( \frac{2k_2}{k_1} \delta_{\text{threshold}} \phi_{\text{grain}}^2 \frac{\tau_p}{\tau_d} \right) \left( \frac{1}{m} \right) \left( \frac{1}{2 + \frac{\Delta \varepsilon_p}{\Delta \varepsilon_p}} \right) \]
Multiscale Materials Modelling

Example of scale transition:
From atoms to continuum mechanics
Example of DD applications:
(See also http://www.numodis.fr)

Crack initiation in fatigue
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3D simulation of nanoindentation
Scale Transition #1: From MD to DD

DD coupled to FEM = ideal tool to investigate nanoindentation issues:
indentation size effect, pile-up vs sink in mechanism, microstructure formation,…

Problems:
I- Enforcing BC
   →Coupling DD to FEM
      - Superposition principle
      \[ [\sigma]^{\text{eff}} = [\sigma]^{\text{disl}} + [\sigma]^{\text{FE}} \]

II- Need of a nucleation criterion for dislocations:

1- What to put in?
2- When to put it in?

→ MD or experiments
**Problem I:** Enforcing boundary conditions: DD-FEM coupling method (superposition)


\[
\sigma_{\Omega} = \sigma_{\Omega}^{\text{ap}} + \sigma_{\Omega}^{\text{UD}}
\]

**Full problem**

\[
\left\{\begin{array}{l}
F_{\text{ap}} - F^D \\
d_2 \Omega
\end{array}\right.
\]

**DD sub-problem**

\[
\left\{\begin{array}{l}
\hat{\sigma}(M) \\
\hat{U}^D
\end{array}\right.
\]

**FE sub-problem**

\[
\left\{\begin{array}{l}
\hat{\sigma}(M) \\
\hat{U}^D
\end{array}\right.
\]

Dislocation theory

(\(\infty\) medium)

Coupling with Finite Elements

(CAST3M)
**Problem I:** Enforcing boundary conditions: DD-FEM coupling method (superposition)

*Application to nanoindentation*
Two possibilities:
- experimental observations (TEM) and measures (nanoindentation tests)
- atomic scale simulations (MD)

What to introduce?

**Prismatic loops?**

Interstitial loop
Two glide systems per prismatic loop

Problem II: Nucleation criterion: What to introduce?
(Molecular Dynamics modeling)

Simulation campaign:
- Material = Ni (EAM potential)
- Indenter = spherical repulsive potential
- Monitored in displacement
- 2 radii: R_{ind} = 60 Å and 120 Å
- 3 sizes: 174x198x163 Å³ (521.640 atoms)
  - 224x284x285 Å³ (1.675.080 atoms)
  - 301x301x200 Å³ (1.524.600 atoms)
Molecular Dynamic simulations of (111) indentation

The loading curves: study of the elastic part

Hertz prediction:

$$F = \frac{4}{3} \frac{E}{R_{ind}^2} \left(\frac{h}{R_{ind}}\right)^{3/2}$$

Atomistic results:

$$F = \alpha h^p$$

Where $1.65 < p < 1.75$ (p decreases as Zmax increases)

And $20.15 < \alpha < 30.65$ (when F in nN and h in Å)
Molecular Dynamic simulations

The dislocation structure: structure after the first pop in

More and more prismatic loops with larger size
Horizontal half loops propagate to accommodate the indentation print
Dislocation nucleation criterion: What to put in?

Atomistic simulations summarized:

Contact area

(111)

[110]

$b_3 = [110]$

$b_2 = [101]$

$b_1 = [011]$

Prismatic loops
**Problem II**: Nucleation criterion:

**What to put in?**

- Shape of Nucleation (MD,111)

**When to put it in?**

- Master curve (MD,111)

**What**: 3 Prismatic loops

**When**: Fit a master curve

- Good: Criterion without any experimental results
- Weak: MD response extrapolated for deeper indentation depth!

**Alternative nucleation criteria**: 
- Experimental master curve
- Geometrically necessary dislocations


Dislocation Dynamics simulations

Specimen

Copper single crystal (111 surface)

Tip geometries

Sphere (r=150nm)

Cone (angle = 71.2°)

Nucleation method

1. Global criterion: **Force** controlled Nucleation
   Master curve from MD (sphere) or Exp (cone)

2. GND criterion: **Depth** controlled Nucleation

Cross-slip probability

(Effect of Temperature)

\[ P = \beta \frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp\left(\frac{\tau^* - \tau_{III}}{kT/V}\right) \]

\[ \tau_{III} = \infty (no), \quad 640\text{MPa(Hard)}, \quad 32\text{MPa(Easy)} \]
Dislocation Dynamics simulations
(111) Spherical indentation
Dislocation evolution (MD global crit. + no cross-slip)

5nm depth
Contact area ↑ ➔ loop length ↑

10nm depth
σ > line tension ➔ F-R source

60nm depth
No space to nucleation

Nucleation only
(similar to MD)

Nucleation and
Frank-Read sources

Frank-Read sources only
(111) Spherical indentation
Cross-slip effect (MD global crit.)

Before unloading (60nm depth)

- No cross-slip
- Hard cross-slip
- Easy cross-slip

After unloading (60nm depth)

Cross-slip↑ ➔ more irreversible micro structure
(111) Conical indentation: Force-Displacement response (exp. Nucleation crit.)

**Total Force**
- MD global criterion
- GND criterion
- Exp. global criterion

**Hardness**
- MD global criterion
- Exp. global criterion
- GND criterion

**Softening mechanisms**
- Two phase behavior: Linear to parabolic
- Single behavior: Linear response

**Hardness**
- Decreases with depth

**Indentation Size Effect**
- Long range decreasing
3D simulation of nanoindentation
Scale Transition #2: From Dislocation Dynamics to Continuum Mechanics
Sample preparation

Crystal ILL : (110), (001), (111) surface orientation
Cut by spark erosion from bulk single crystal (high $\rho_{ini}$)

Crystal B. : (123), (111low) surface orientation
Grown from high purity Cu using Bridgman technique (low $\rho_{ini}$)

- 4 surface orientations
- 2 initial dislocation densities for (111) orientation
Strong effect of initial dislocation density & Weak effect of orientation

Experimental data (conical indentation)

Indentation loading curves
Experimental data (conical indentation)

Surface morphologies (AFM)

(001) Surface  (110) Surface  (123) Surface

(111) Surface (high\(\rho_{ini}\))  (111) Surface (low\(\rho_{ini}\))

Surface morphology strongly affected by Surface orientation

To check by FEM modelling
Crystal Plasticity Modeling

Nanoindentation procedure

**Experiment**
- Sapphire conical tip
- Tip angle = 71.2°
- Tip radius = 3.3 µm
- \( h_{\text{sphere}} = 200 \text{ nm} \)
- 4 Cu single crystals
- 5mm × 5mm

**FEM**
- Rigid body tip (identical)
- Indentation depth = 1400 nm

4 Specimens

**Nanoindentation procedure**

**Tip**

**Loading condition**
\[ \dot{\varepsilon} = 5 \times 10^{-2} / \text{sec} \]

**Strain rate control**

**Velocity control**
Crystal Plasticity Modeling

Dislocation density based model

\[ \dot{\gamma}^{(s)} = \dot{\gamma}_0 \left( \frac{\tau^{(s)}}{\tau^{(s)}_{\mu}} \right)^{1/m} \]

\[ \tau^{(s)}_{\mu} = \mu b \sqrt{\sum_{u=1}^{12} a_{su} \rho^{(u)}} \]

\[ \rho^{(s)} = \frac{1}{b} \left( \frac{\sqrt{\sum_{u=1}^{12} d_{su} \rho^{(u)}}}{K} - 2\beta R \rho^{(s)} \right) \dot{\gamma}^{(s)} \]

Crystal plasticity model

\[ \dot{\tau}^{(s)}_{\mu} = \sum_{u=1}^{12} \left\{ \frac{\mu a_{su}}{2 \sqrt{\sum_{p=1}^{12} a_{sp} \rho^{(p)}}} \left( \frac{\sqrt{\sum_{q=1}^{12} d_{uqp} \rho^{(q)}}}{K} - 2\beta R \rho^{(u)} \right) \right\} \dot{\gamma}^{(u)} \]

soit

\[ \dot{\tau}^{(s)}_{\mu} = \sum_{u=1}^{12} h_{su} \dot{\gamma}^{(u)} \]
Crystal Plasticity Modeling

Parameters used in the crystal plasticity model

Elastic properties for $T^* = C^E [E^*]$

<table>
<thead>
<tr>
<th></th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>168.4 GPa</td>
<td>121.4 GPa</td>
<td>75.4 GPa</td>
</tr>
</tbody>
</table>

From text book

Initial dislocation density and Surface orientation

From X-ray results

<table>
<thead>
<tr>
<th>Surface Orientation</th>
<th>FWHM (111) $\theta$ scan $^\circ$</th>
<th>Relative disl. density</th>
<th>Initial density (total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(011)</td>
<td>1.35</td>
<td>6 ~ 8</td>
<td></td>
</tr>
<tr>
<td>(111)</td>
<td>0.57</td>
<td>3 ~ 4</td>
<td></td>
</tr>
<tr>
<td>(001)</td>
<td>0.56</td>
<td>3 ~ 4</td>
<td></td>
</tr>
<tr>
<td>(123)</td>
<td>0.2</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(111low)</td>
<td>0.08</td>
<td>0.2 ~ 0.3</td>
<td></td>
</tr>
</tbody>
</table>

Hardening parameters

From DD theory

\[ \tau^s_{\mu} = \mu b \sqrt{\sum_{p=1}^{12} \alpha^p \rho^p} \]
\[ \dot{\rho}^s = \frac{1}{b} \left( \frac{\sum_{p=1}^{12} \alpha^p \rho^p}{K_g} - 2 y_c \rho^s \right) \] \dot{\gamma}

<table>
<thead>
<tr>
<th>$b$</th>
<th>$2.56 \times 10^{-10}$ m</th>
<th>$y_c$</th>
<th>$1.43 \times 10^{-9}$ m</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{1-6}$</td>
<td>Taylor</td>
<td>(0.09, 0.09, 0.09, 0.09, 0.09, 0.09)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Hetero</td>
<td>(0.122, 0.122, 0.07, 0.137, 0.122, 0.625)</td>
<td></td>
</tr>
<tr>
<td>$a_{1-6}$</td>
<td>Normal</td>
<td>(0.01, 0.4, 0.4, 0.75, 1.0, 0.4), K=36</td>
<td></td>
</tr>
<tr>
<td>$K$</td>
<td>Same</td>
<td>$a_{1-6}$ same as $\alpha_{1-6}$, K=36</td>
<td></td>
</tr>
<tr>
<td></td>
<td>High K</td>
<td>(0.01, 0.4, 0.4, 0.75, 1.0, 0.4), K=100</td>
<td></td>
</tr>
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</table>

Effect of orientation

Crystal Plasticity Modeling

Strong effect on surface displacement

Weak effect on loading curve

(Hetero / Same)
Effect of dislocation density for (111) orientation

Optimized initial dislocation density

\( \rho_{\text{ini}} = 6.0 \times 10^{12}/\text{m}^2 \) for (111\text{low})

\( \rho_{\text{ini}} = 1.2 \times 10^{14}/\text{m}^2 \) for (111\text{high})

Strong effect on surface shape

Strong effect on loading curve

What about the other orientations?
Crystal Plasticity Modeling / Comparison with experiments

Comparison of quantitative results

Optimized initial densities

<table>
<thead>
<tr>
<th>Orientation</th>
<th>( \rho_{ini} )</th>
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<tr>
<td>(110)</td>
<td>( 1.56 \times 10^{14} / \text{m}^2 )</td>
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<tr>
<td>(111)</td>
<td>( 1.20 \times 10^{14} / \text{m}^2 )</td>
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X-Rays
Effect of hardening parameters for (111) orientation

Crystal Plasticity Modeling / Comparison with experiments

Need to check for other orientation

Influence surface morphology

Hetero + Same

Taylor

$\alpha_{1-6}$

Hetero

Normal

Same

High K

Weak effect on loading curve

Obtained hardening parameter

$\alpha_{1-6}$
Comparison of Surface morphology (hetero / same)

Crystal Plasticity Modeling / Comparison with experiments

Confirmed hardening parameter

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<th>(y_c) (m)</th>
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<td>Same as (\alpha_{1-6}), (K=36)</td>
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Crystal Plasticity Modeling / Comparison with experiments

Comparison of pile up morphology
(hetero / same)

The hardening parameter (hetero/Same) is confirmed quantitatively
Conclusion: best set of parameters

**Elastic**

\[ T^* = C^E [E^*] \]

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**Hardening**

\[ \tau_{ij}^s = \mu b \sum_{p=1}^{12} a^{sp} \rho^p \]

\[ \dot{\rho}^i = \frac{1}{b} \left[ \frac{1}{\sum_{p=1}^{12} a^{sp} \rho^p} - 2 y_\epsilon \rho^i \right] \dot{\epsilon}^i \]

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Molecular Dynamics

Multi scale modelling of indentation

Dislocation dynamics

Finite Element Crystal plasticity

Experiments
Challenge & Perspectives

Too large computation time
- Limited cumulated strain

Large deformation, large rotations
- jogs, …

Polycrystal plasticity
- Static and dynamic interfaces

Taking into account climb

Dislocation core effect

Real materials
impurities, solutes, etc..

Parallel computing
- ParaDis, Paranoid, Tridis, Numodis,…

Updating Schmid factor
Updating dislocation positions, slip planes

Accounting for grain boundary

Coupling with diffusion theory
Dealing with heterogeneous time steps

Rules to be defined by MD or TEM

Rules needed from experiments