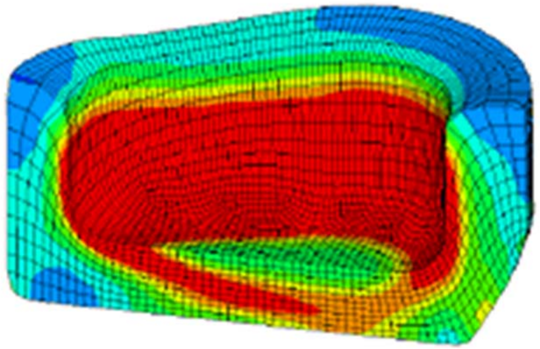
Dislocation dynamics

Marc FIVEL
SIMaP-GPM2, Grenoble INP / CNRS

Marc.Fivel@grenoble-inp.fr

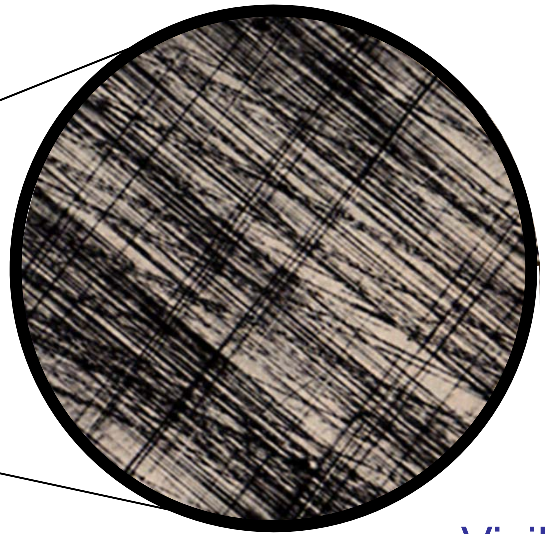
Marc VERDIER, Christian ROBERTSON, David RODNEY
Laurent DUPUY, Marc BLETRY
Edgar RAUCH, Yves BRECHET, François LOUCHET, Jean-Loup STRUDEL
Emmanuel CLOUET, Dan MORDEHAI
Christophe DEPRES,, Chan Sun SHIN, Hyung-Jun CHANG
…..

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) :

$$d\vec{i}v\,\underline{\underline{\sigma}} + \vec{f}_v = \rho\frac{d\vec{v}}{dt}$$

$$\dot{\underline{\underline{\sigma}}} = f\left(\underline{\underline{\sigma}}, \underline{\underline{\varepsilon}}, \dot{\underline{\underline{\varepsilon}}}\right)$$ Constitutive equations

Exple of constitutive equations (crystal plasticity):

R.J. Asaro, *Crystal plasticity,* J. Appl. Mech., **50**, pp. 921-934 (1983).

$$\dot{\gamma}^s = \left\langle \frac{|\tau^s - x^s| - \tau_c^s}{k} \right\rangle^n \text{signe}(\tau^s - x^s) \text{ avec } \langle\bullet\rangle = \begin{cases} \bullet & \text{si } \bullet > 0 \\ 0 & \text{si } \bullet \leqslant 0 \end{cases}$$

Isotropic hardening : $\tau_c^s = r_0 + Q\sum_{r=1}^{N} h^{sr}[1 - \exp(-B\upsilon^r)]$, avec $\dot{\upsilon}^s = |\dot{\gamma}^s|$

Kinematic hardening : $x^s = ca^s$, avec $\dot{a}^s = \dot{\gamma}^s - d\,|\dot{\gamma}^s|\,a^s - \left(\frac{|a^s|}{M}\right)^m \text{signe}(a^s)$

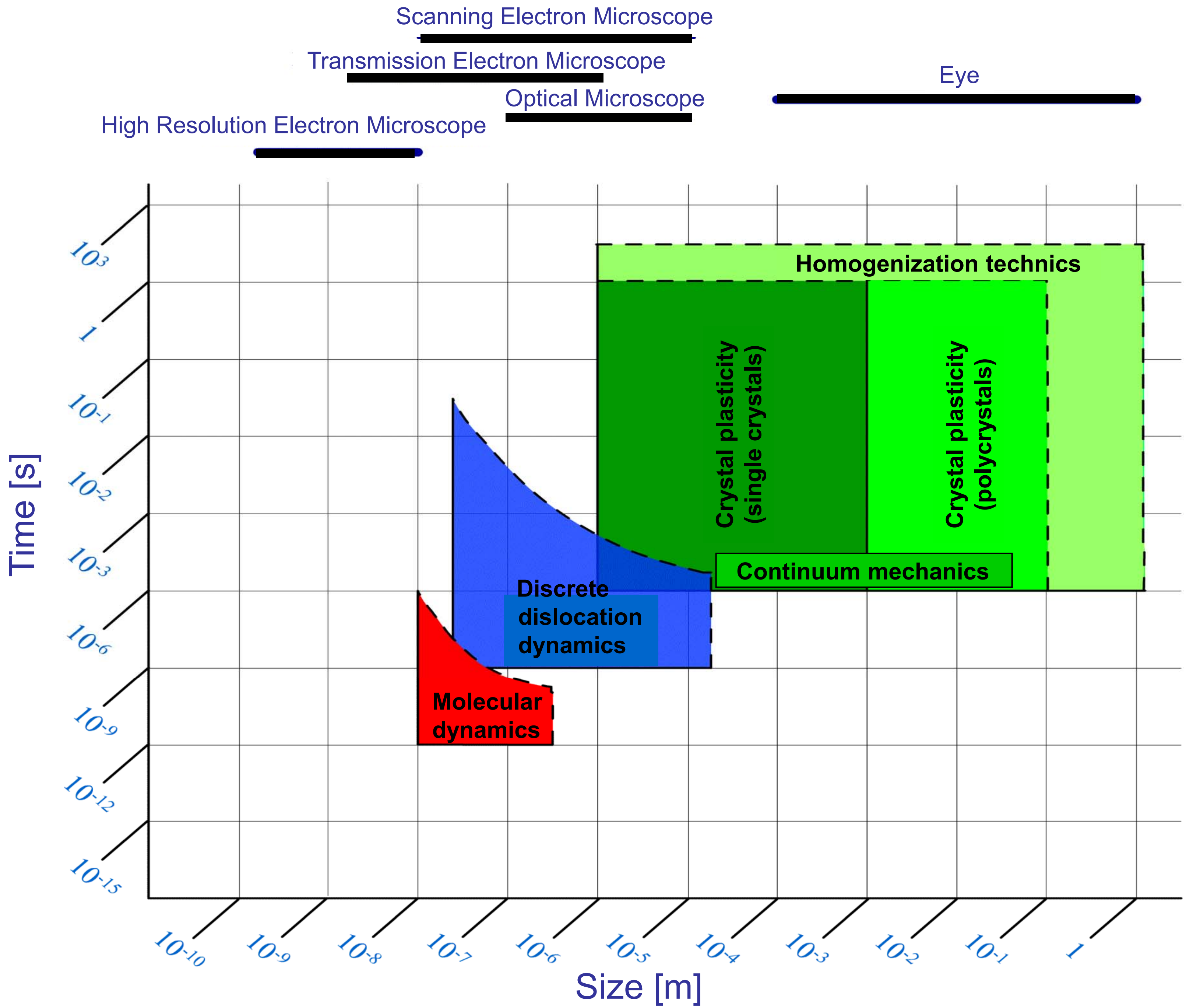
Very efficient **BUT** :
- Phenomenological equations
- Lack of generality

Exple : Cailletaud, Forest *et al.*

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

⇨ *Crystal plasticity = **dislocations motion***

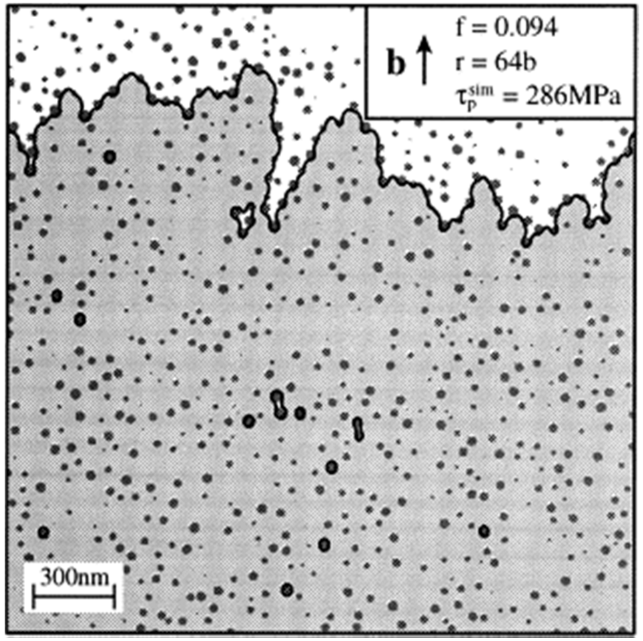
Multiscale Materials Modelling



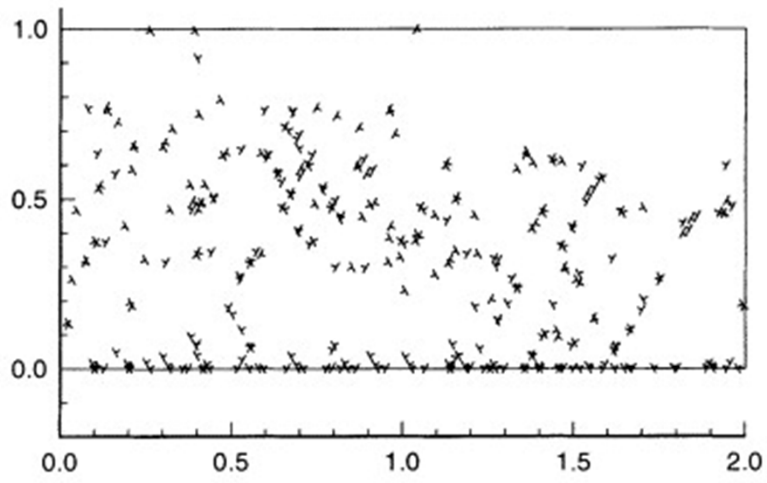
Dislocation dynamics simulations: 2D models

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

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



Foreman & Makin 1966

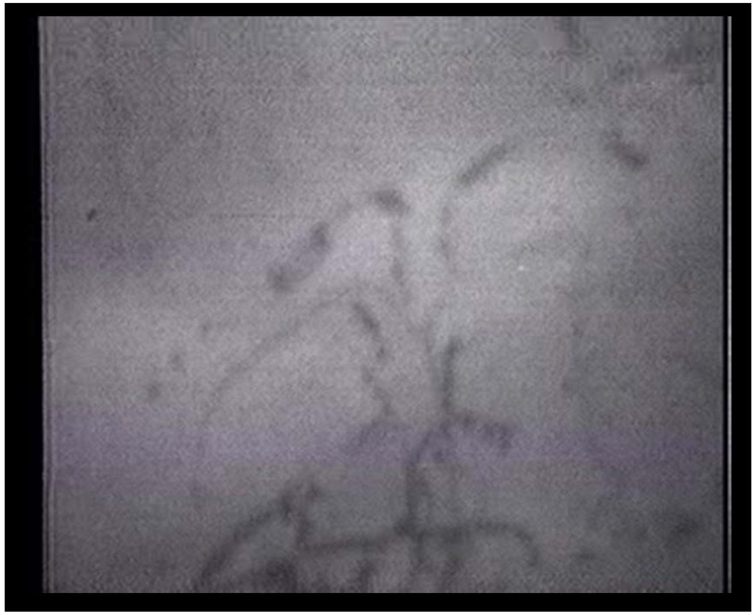


Van der Giessen & Needleman

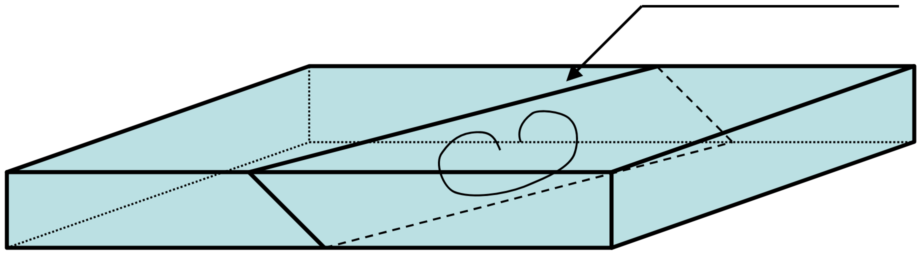
Advantages : simple, fast

Drawback: 3D reality is missing
Line tension, junction, crossslip,… ➡ **2,5D ou 3D**

3D modeling of dislocation dynamics

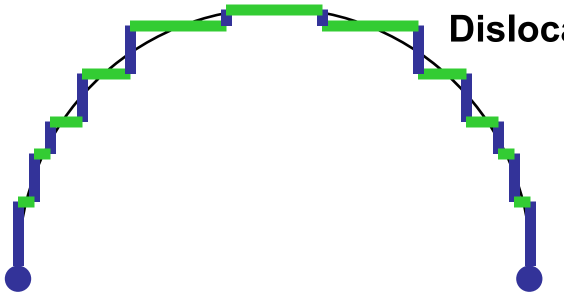


François LOUCHET (Grenoble)



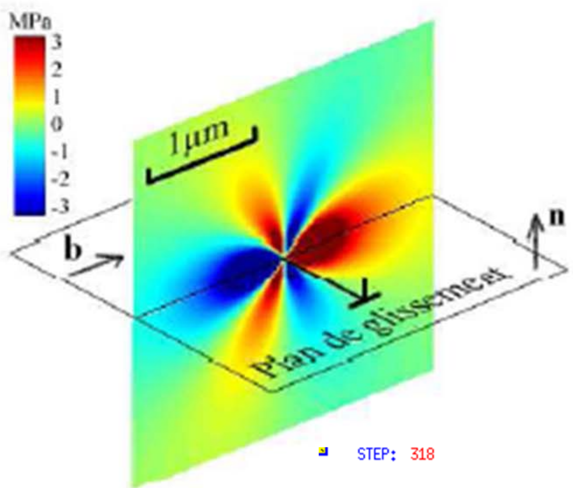
Thin foil (~200nm thick)

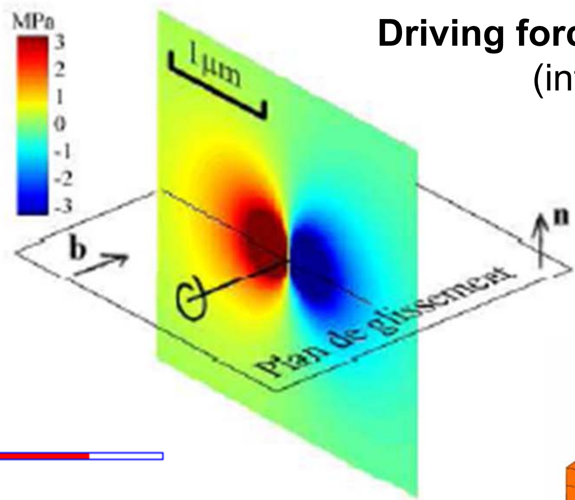
3D Discrete Dislocation Dynamics (code TRIDIS)



Dislocations = edge and screw segments embedded in an elastic continuum
(Kubin, Canova and Bréchet 1992)

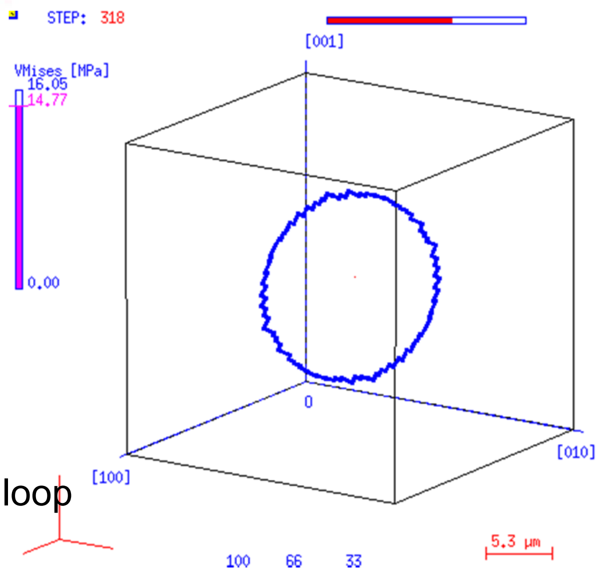
(similar to elastic inclusions)



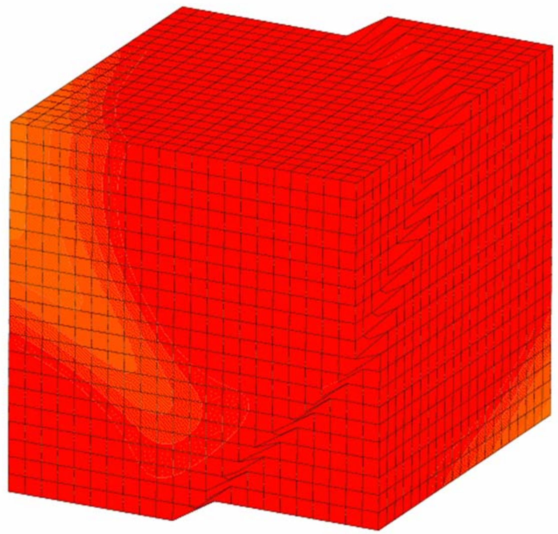


Driving force = elastic stress tensors
(internal + applied)

$$v = \frac{\tau b}{B}$$



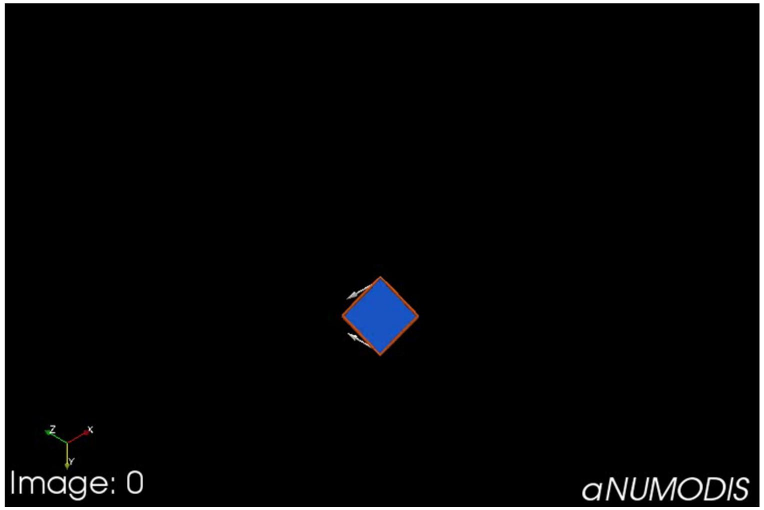
Example :
Glissile dislocation loop



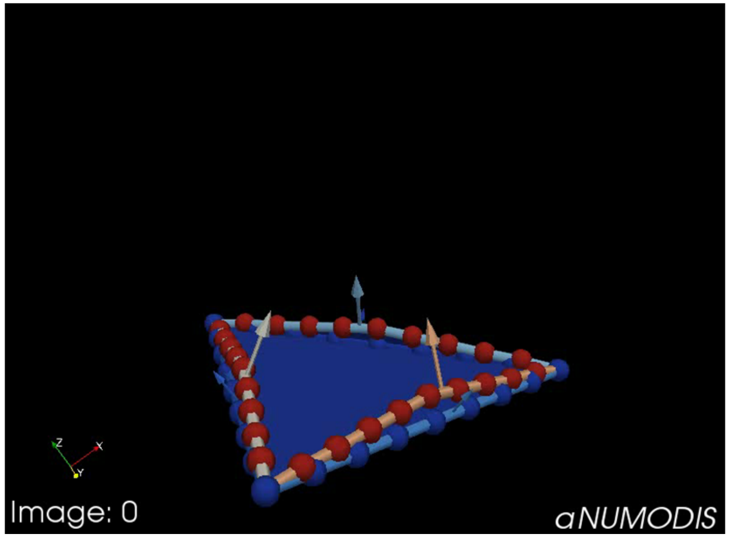
Plastic deformation: direct output

Modern 3D Discrete Dislocation Dynamics Codes
(project NUMODIS (CNRS-CEA) L. Dupuy, M. Blétry)

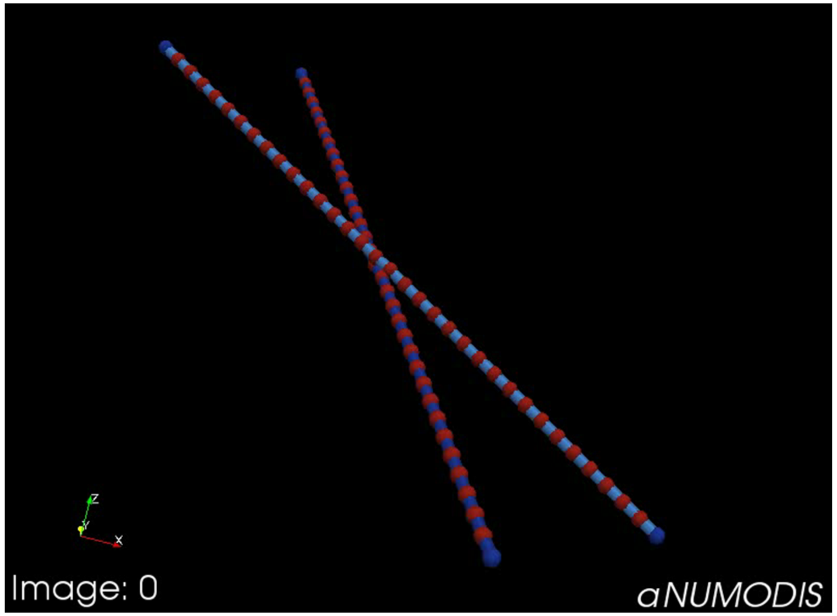
<u>Nodal code</u>



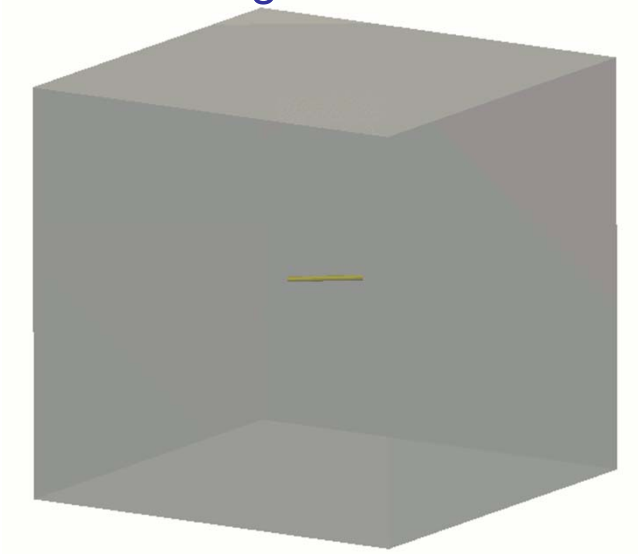
Frank-Read source + partials



Stacking Fault Tetraedra

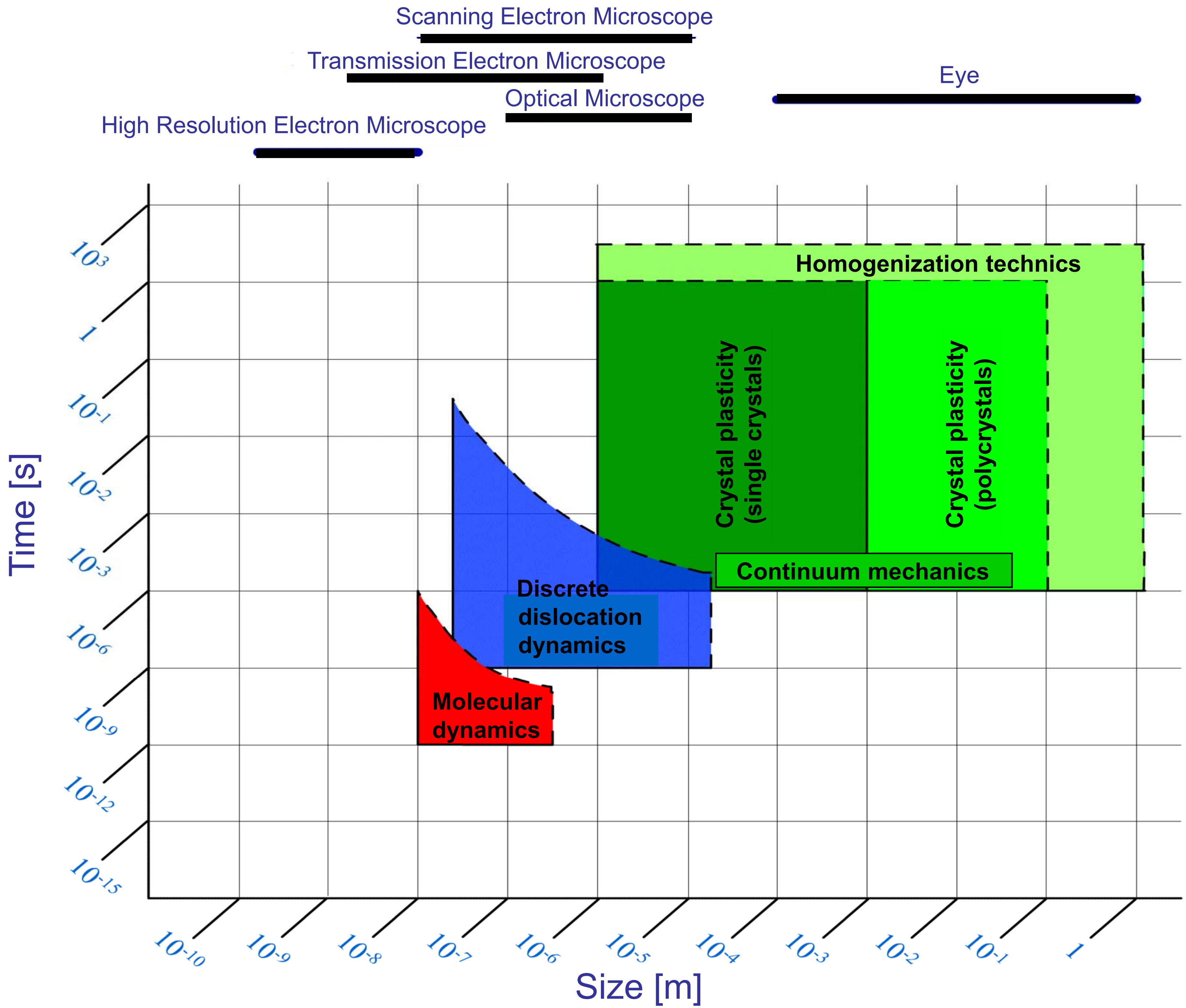


Dislocation junctions



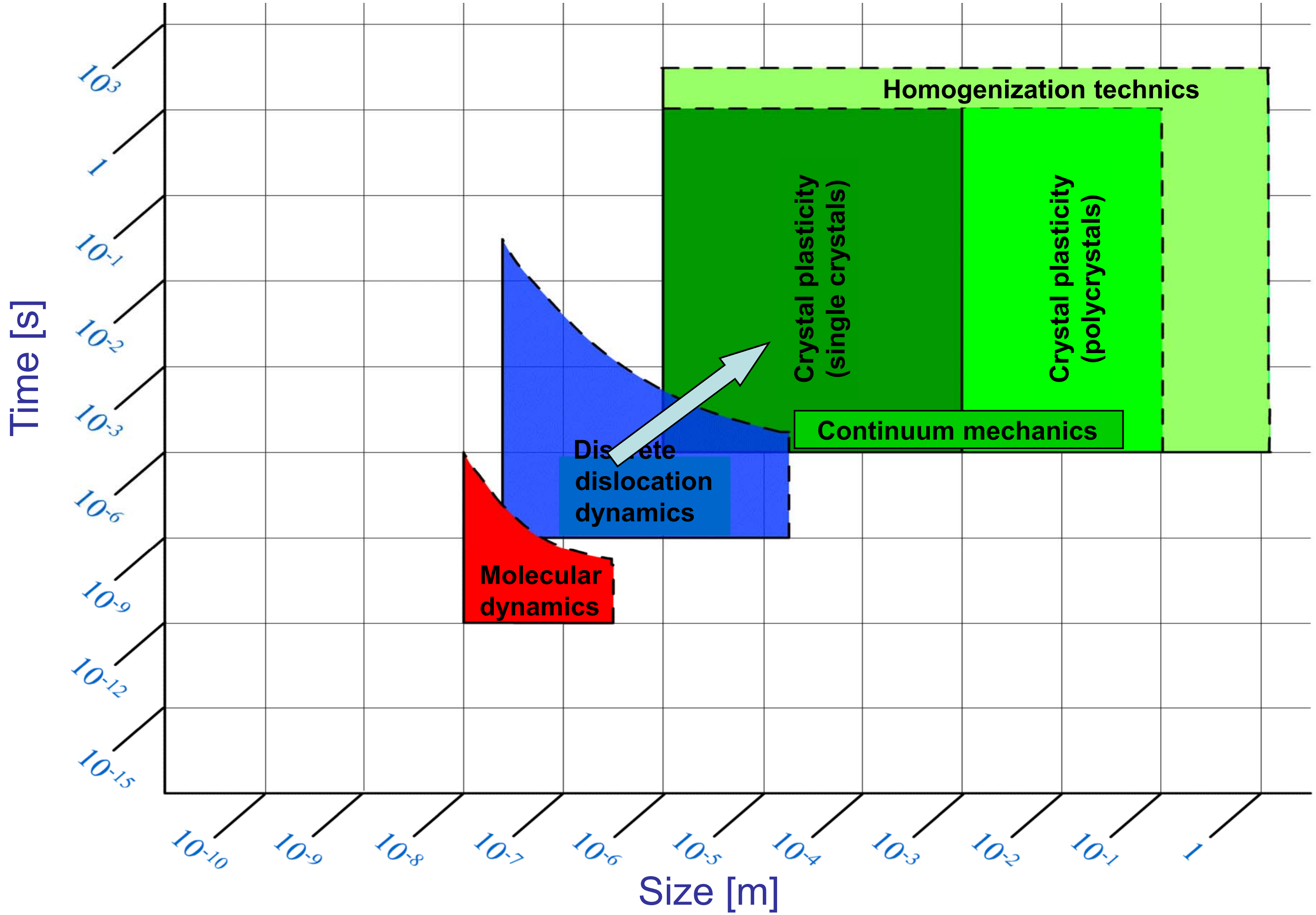
<u>Advantage :</u> closer to reality
<u>Drawback :</u> Ten times slower

Multiscale Materials Modelling



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)

$$\dot{\gamma}^{(s)} = \dot{\gamma}_0^{(s)} \left(\frac{\tau^{(s)}}{\tau_\mu^{(s)}} \right)^{1/m}$$

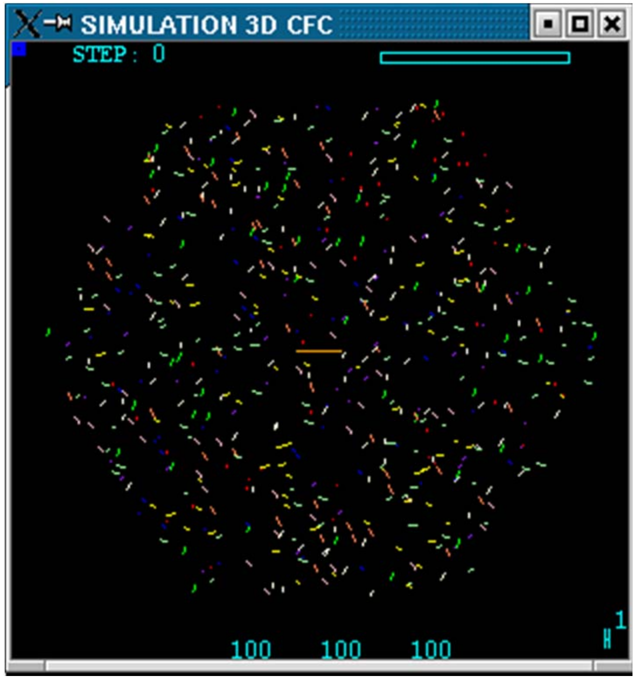
$$\tau_\mu^{(s)} = \mu b \sqrt{\sum_{u=1}^{12} a_{su} \rho^{(u)}}$$

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

$a_{su} \sim a = 0{,}09$

$K = 32$

$\beta R = y_c \sim b$



+ Recently revisited by : L. Kubin, B. Devincre and T. Hoc, Acta Mater., (2008)

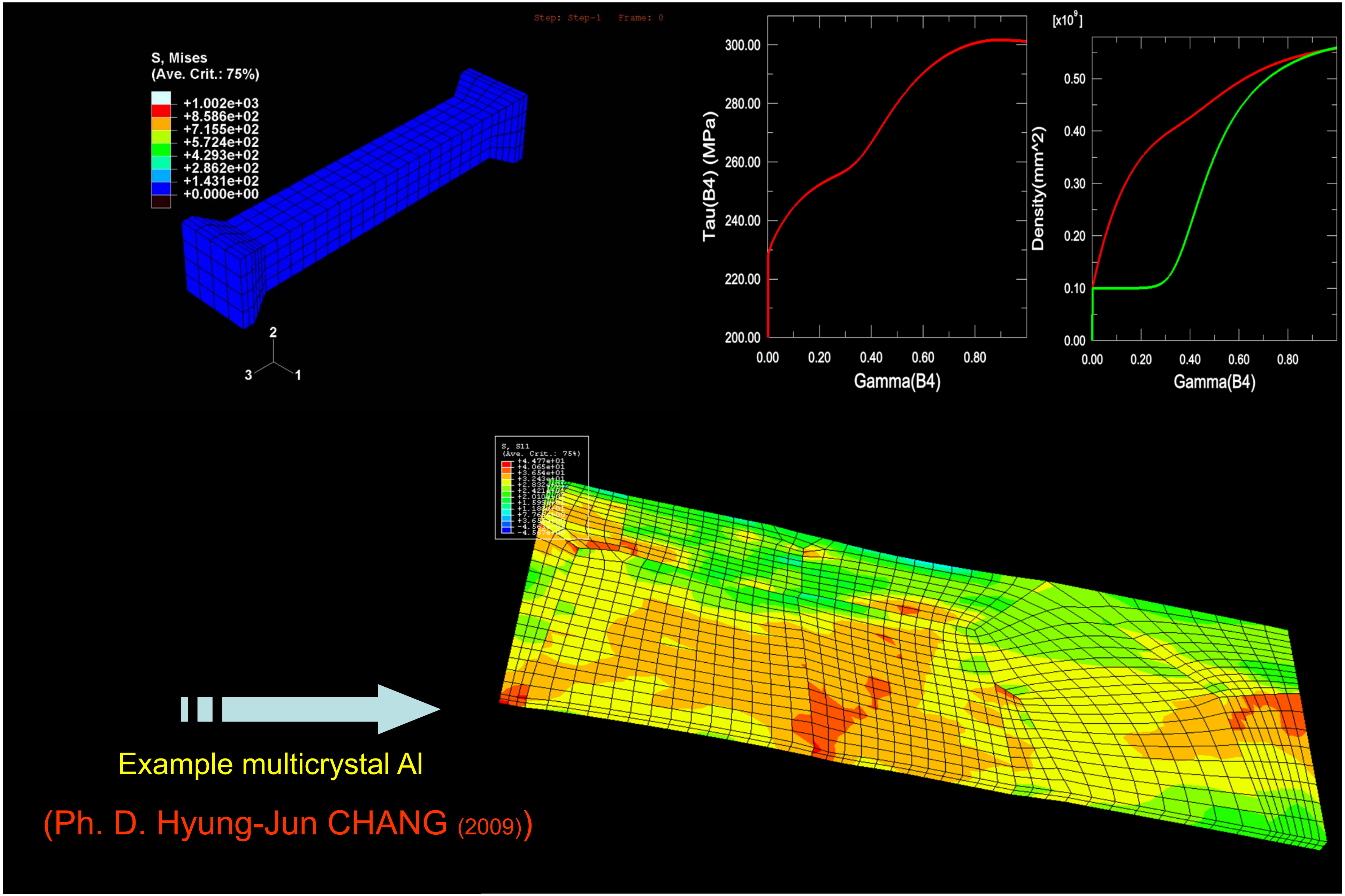
3D tensorial framework

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

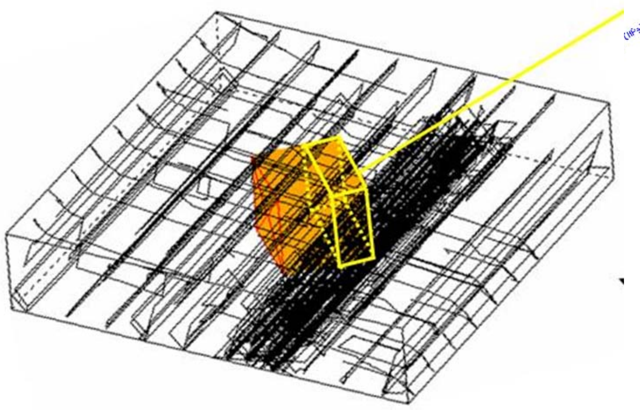
soit

$$\dot{\tau}_\mu^{(s)} = \sum_{u=1}^{12} h_{su} \dot{\gamma}^{(u)}$$

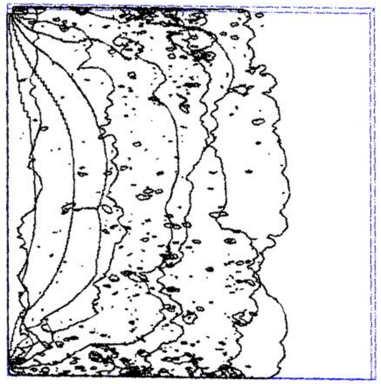
Finite Element Implementation (ABAQUS : UMAT and VUMAT)



Example of DD applications:
(See also http://www.numodis.fr)

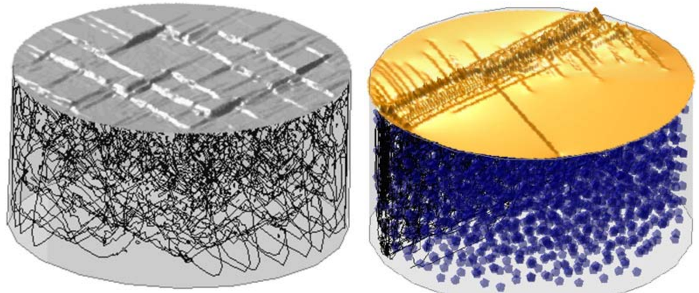


Plastic behavior of BCC Fe
Ph.D. Julien CHAUSSIDON (2007)
Ph.D. Daniel GARCIA-RODRIGUEZ (2011)

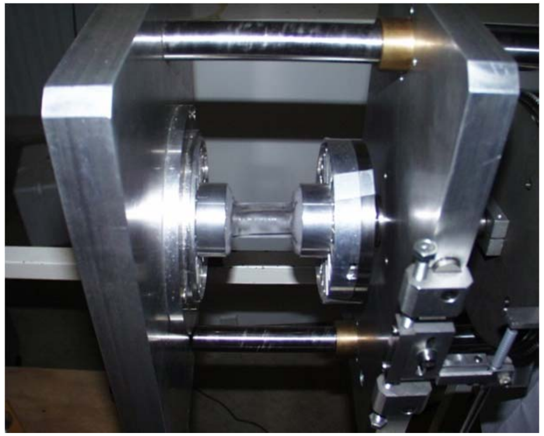


Clear channels in 316L steel
Ph.D. Thomas NOGARET (2007)
Ph.D. Gururaj KADIRI (2014)

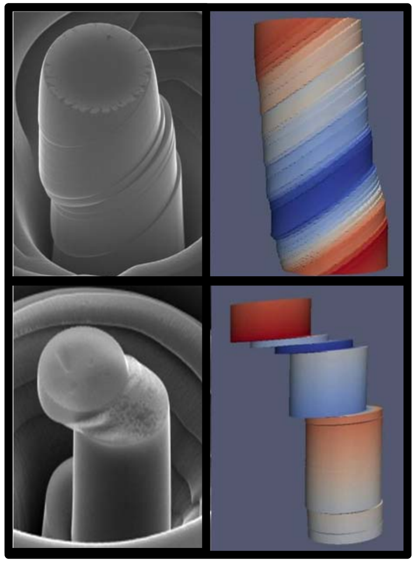
Example of DD modelling



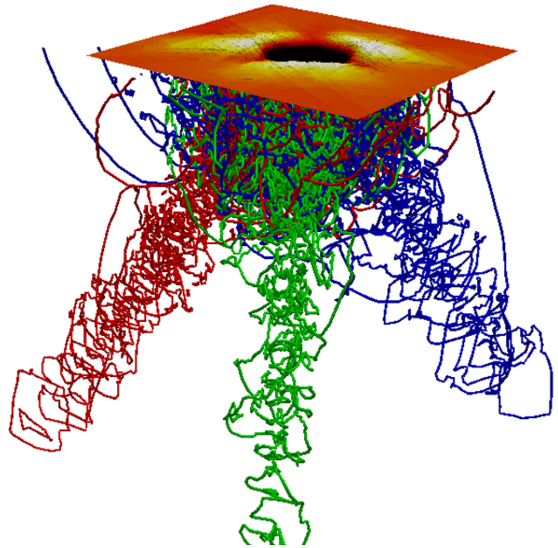
Crack initiation in fatigue
Ph.D. Christophe DEPRES (2004)
Ph D. Chan Sun SHIN (2004)



Creep of ice single crystals
Ph.D. Juliette CHEVY (2008)

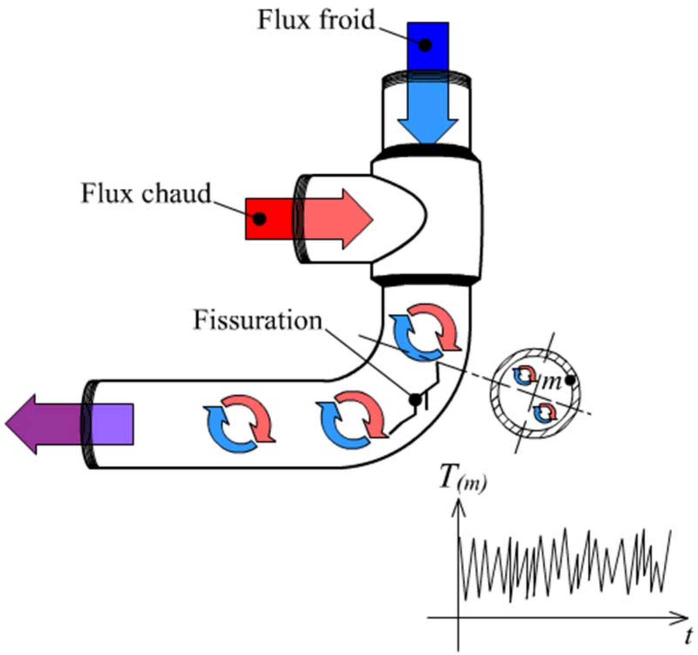


Micro-compression of Mg pillars
Ph.D. Gyu Seok KIM (2011)

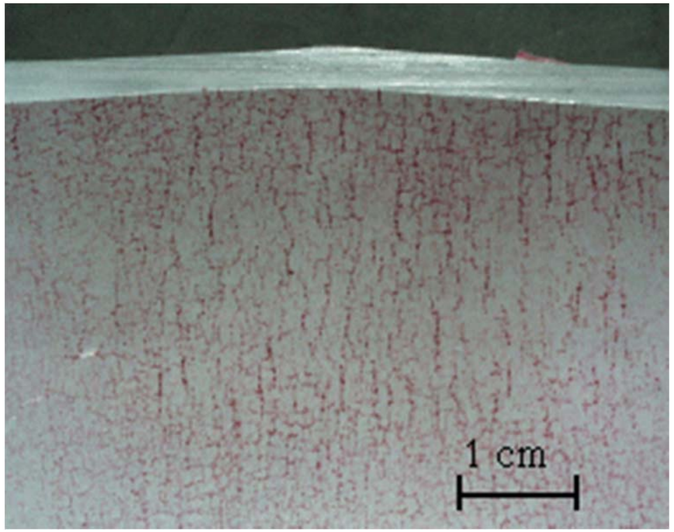


(111) Nanoindentation of Cu single crystal
Ph.D. Hyung Jun CHANG (2009)

'Engineering' application: How do cracks initiate in fatigue ?
(AISI 316L surface grains)



Incident Civaux1
May 1998 :
leak 30m³/h



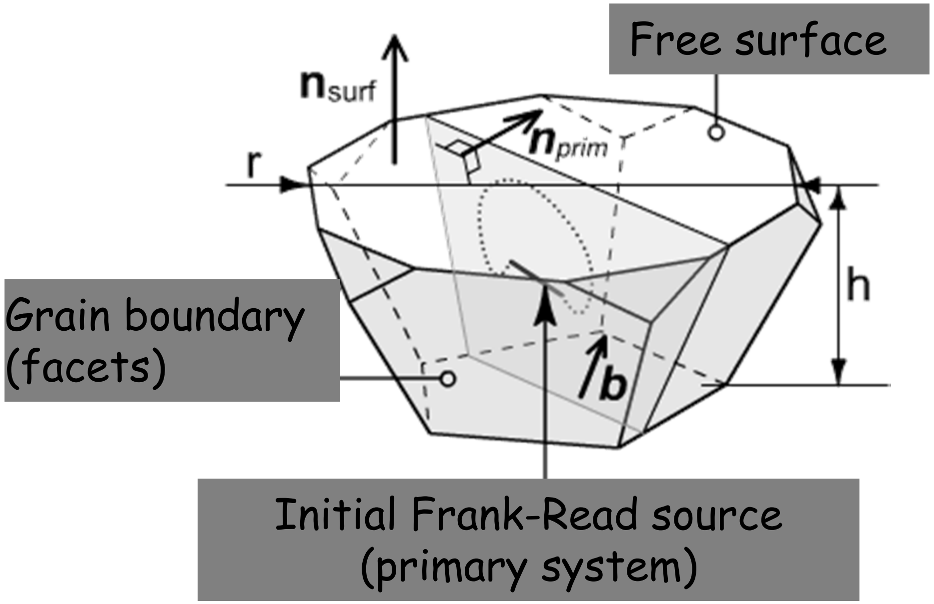
Transgranular crack network

<u>Main objective :</u> Understand physical mechanisms at the origin of cracks

WHEN & WHY do cracks appear ?

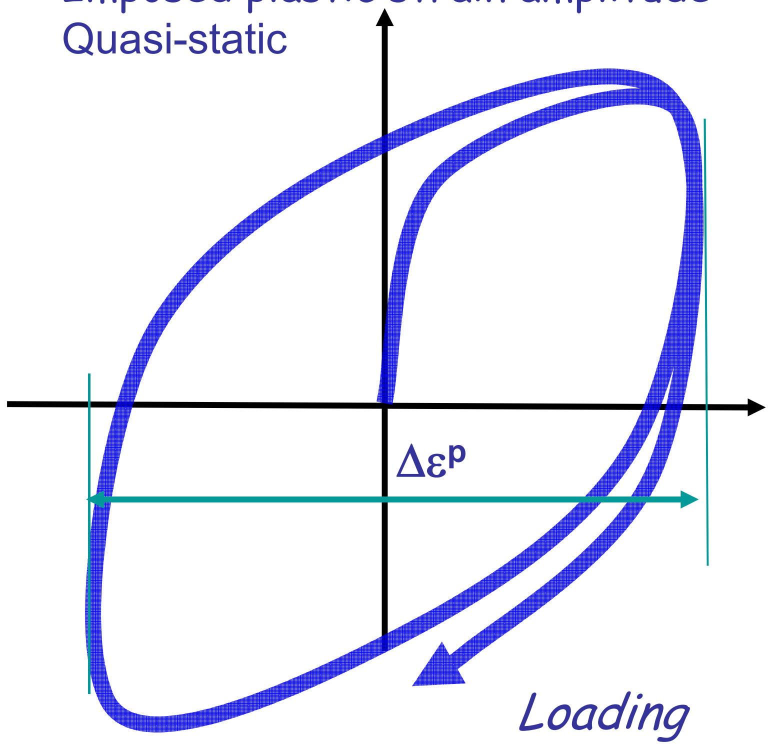
HOW do craks propagate ?

Discrete Dislocation Dynamics Modelling: Boundary conditions



Typical configuration
(motivated by thermal fatigue experiments)

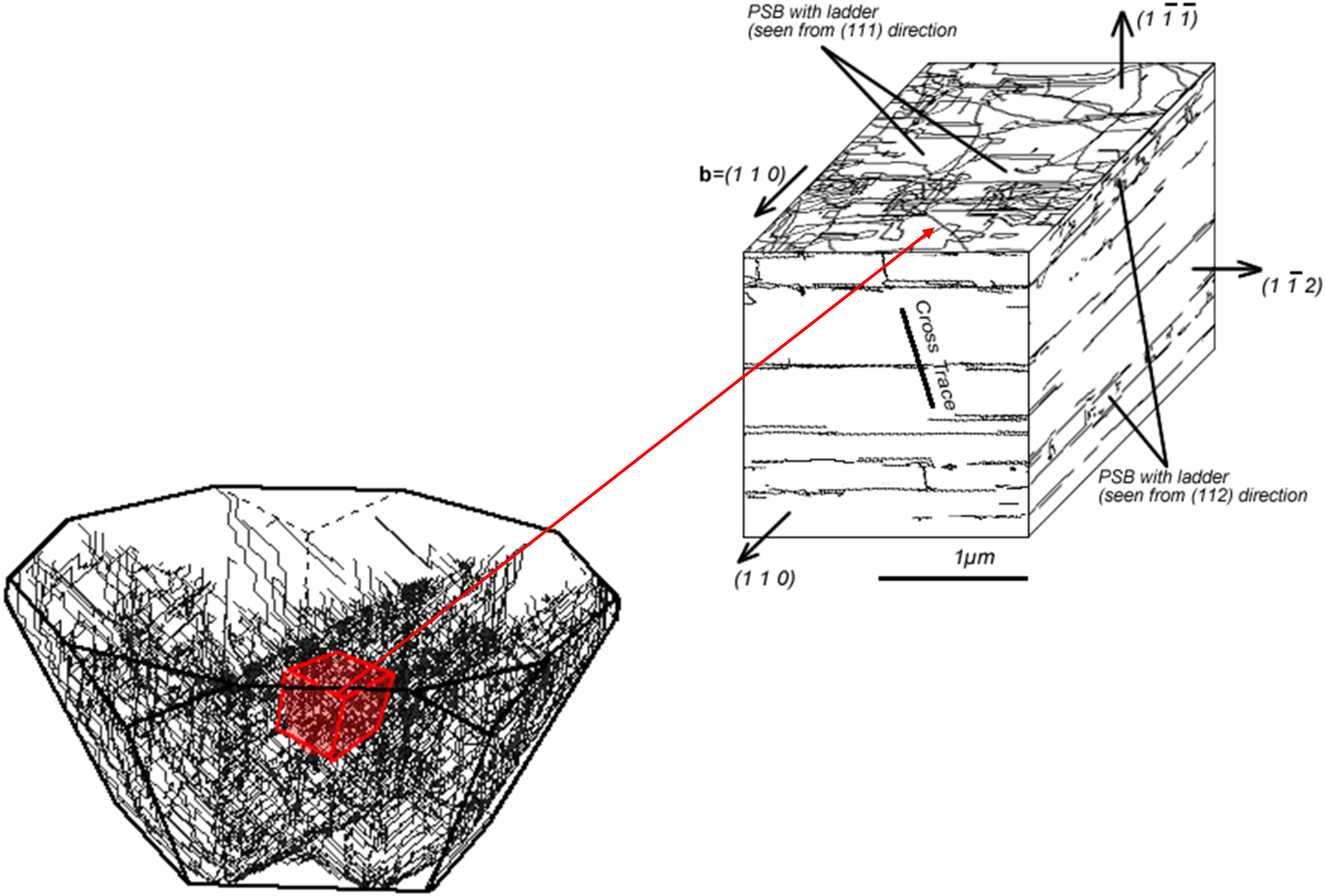
Imposed plastic strain amplitude
Quasi-static



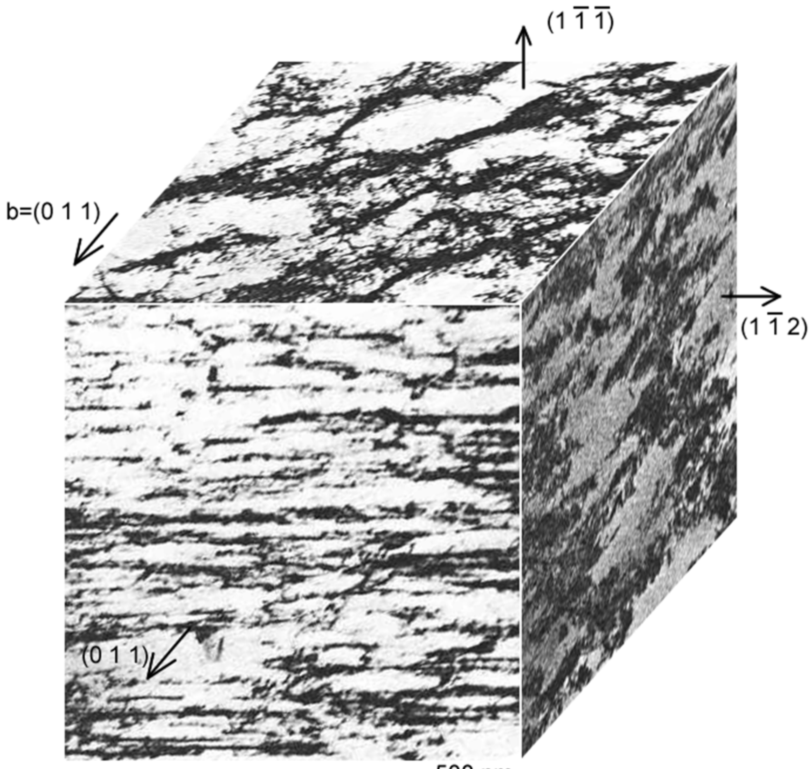
Output :

Dislocation microstructure
Mechanical response
Deformation of the free surface
Internal stresses
...

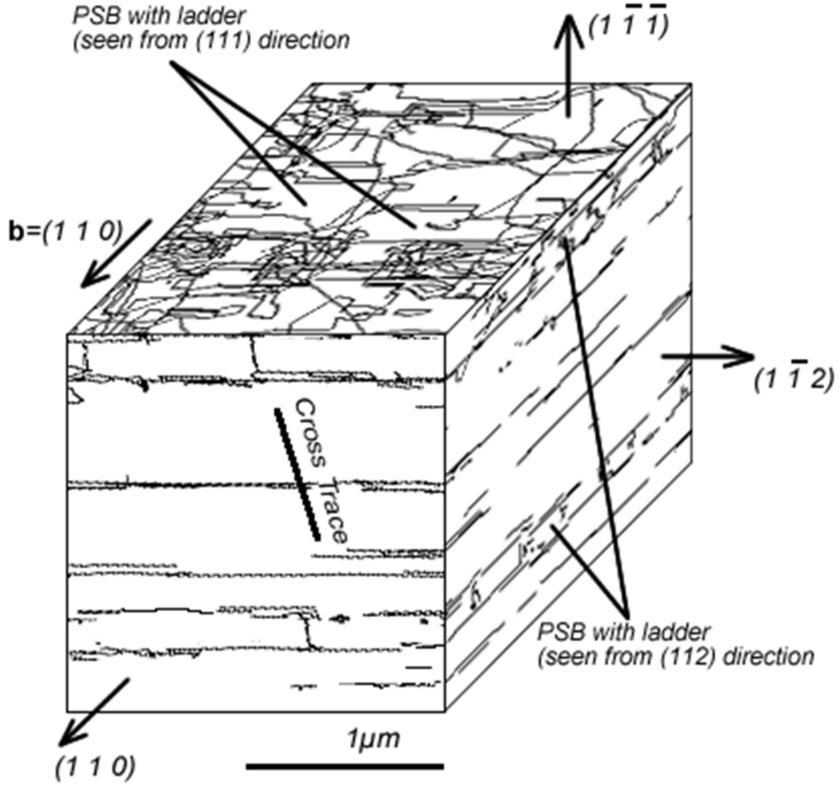
Model validation : single slip ($\tau_p = 3\tau_d$)



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



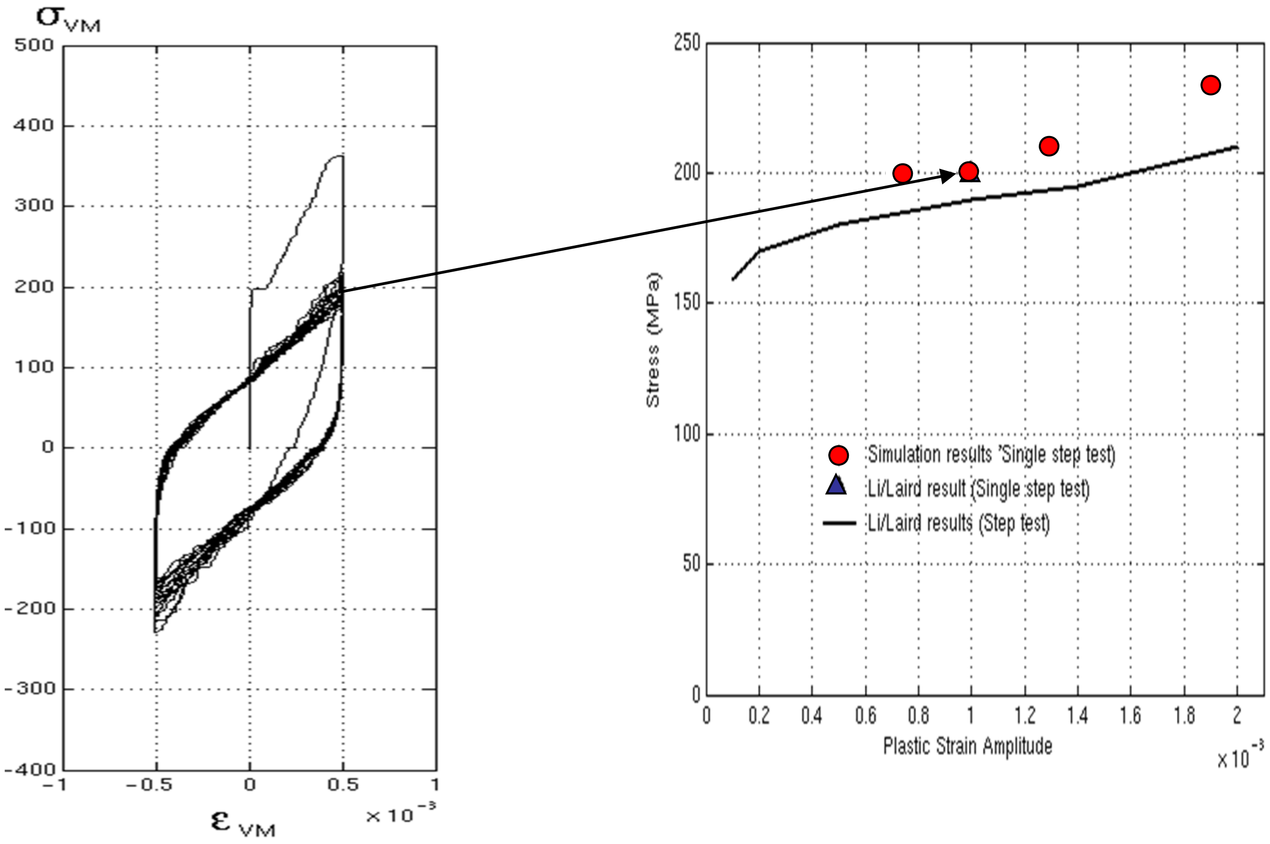
Obrtlik & al. (1994)



Dislocation microstructure ☑

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

Single slip

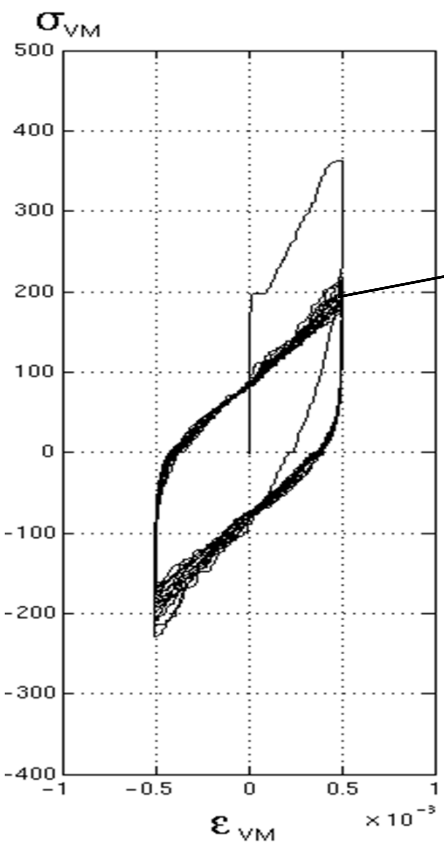


Dislocation microstructure ☑

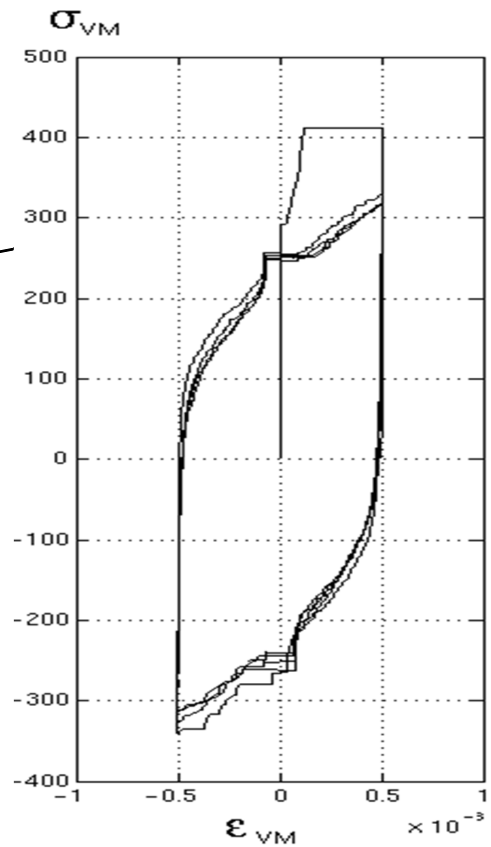
Mechanical response ☑

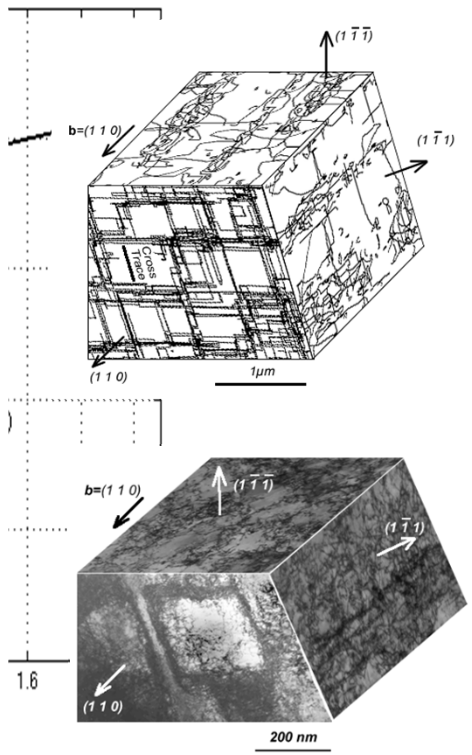
Model validation : single slip ($\tau_p = 3\tau_d$)

Single slip



Double slip ($\tau_p=\tau_d$)

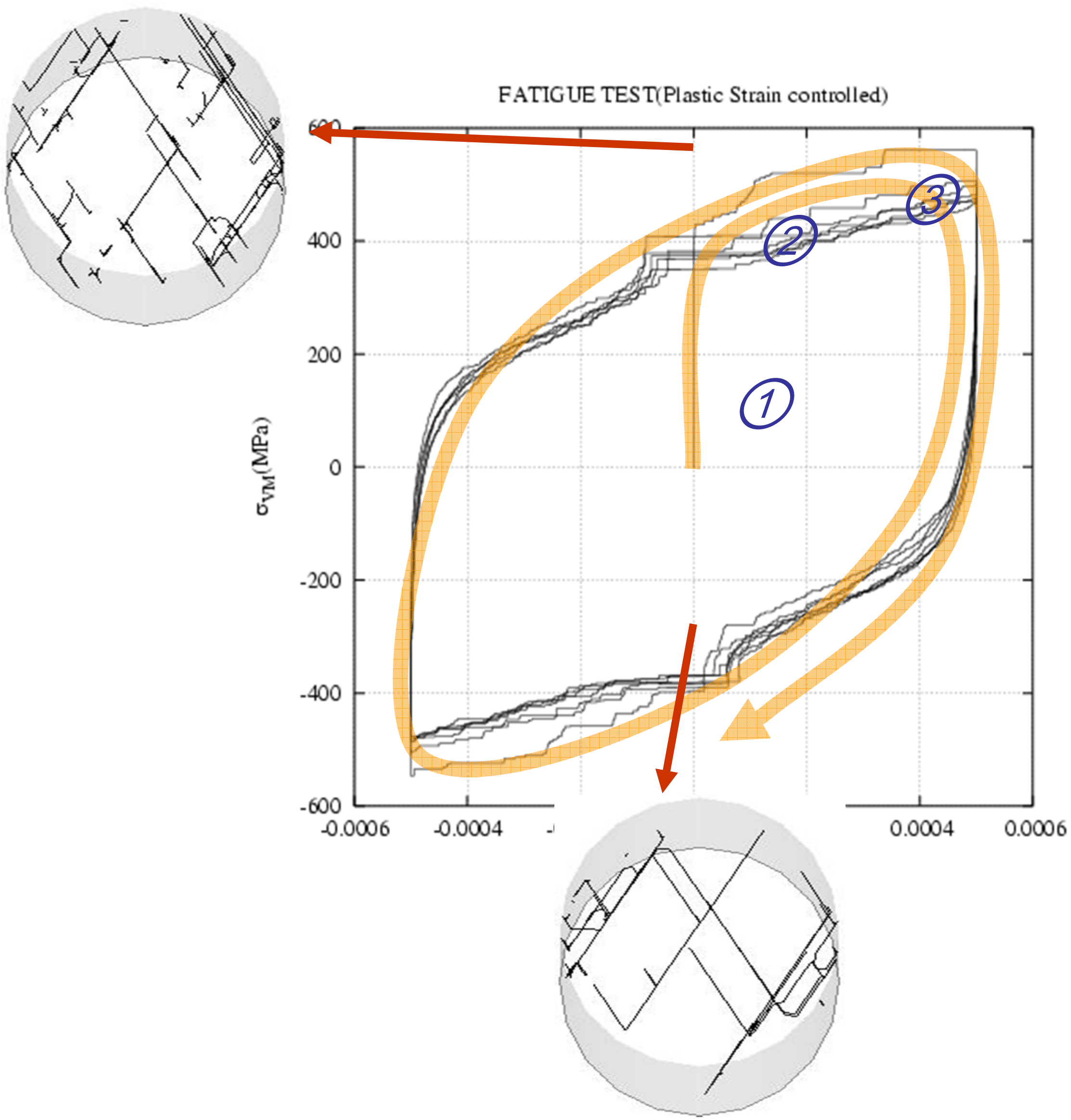


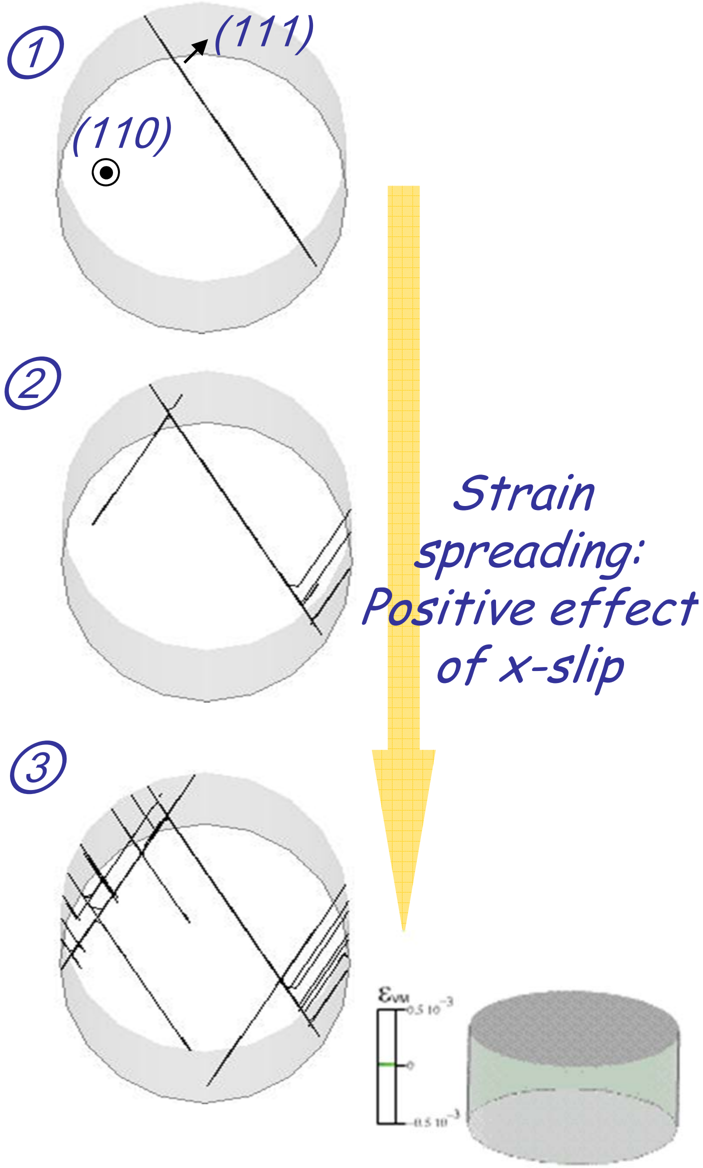


Dislocation microstructure ☑

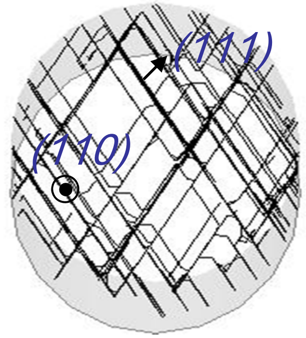
Mechanical response ☑

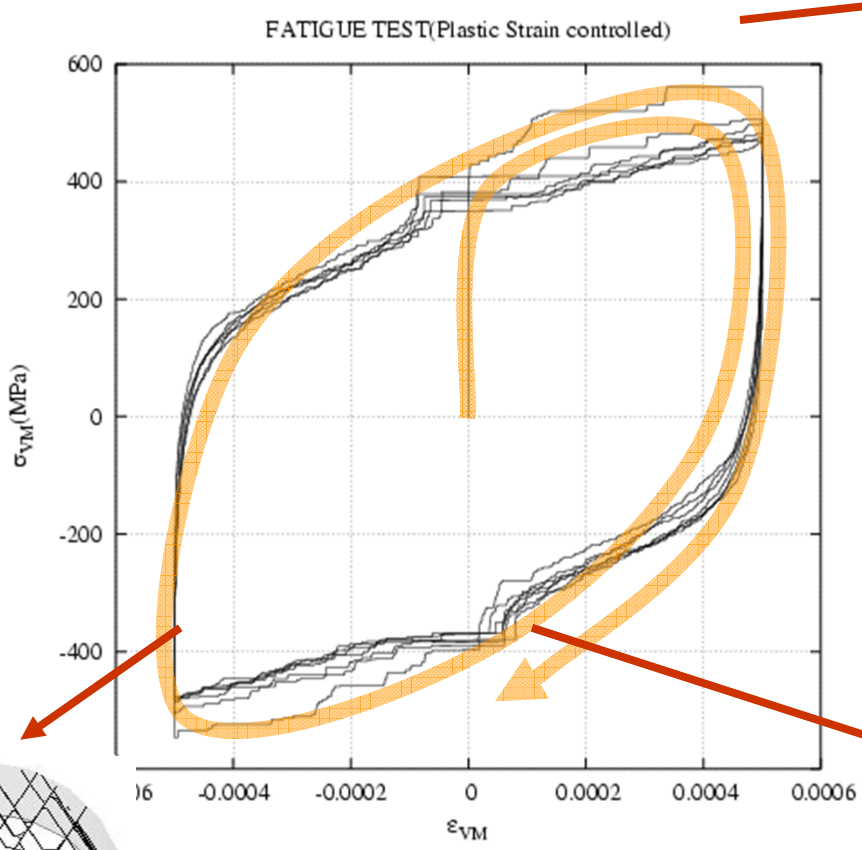
Strain localization mechanisms



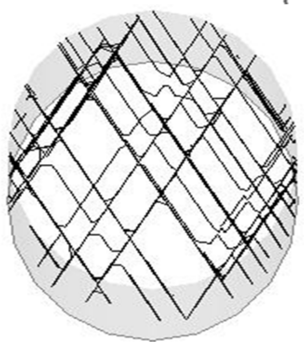


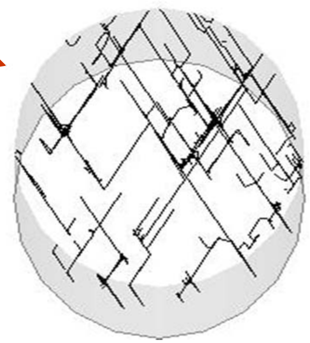
Strain localization mechanisms



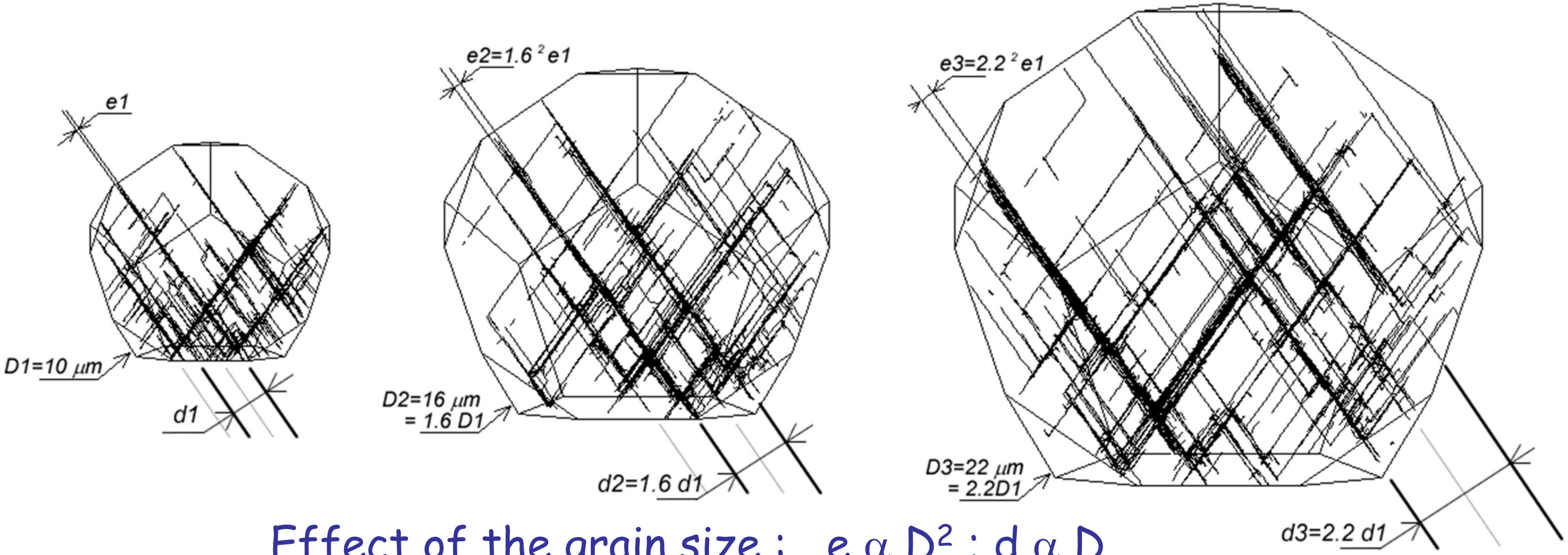


Dipole formation:
Strain localisation
Negative effect of x-slip
and dislocation interactions

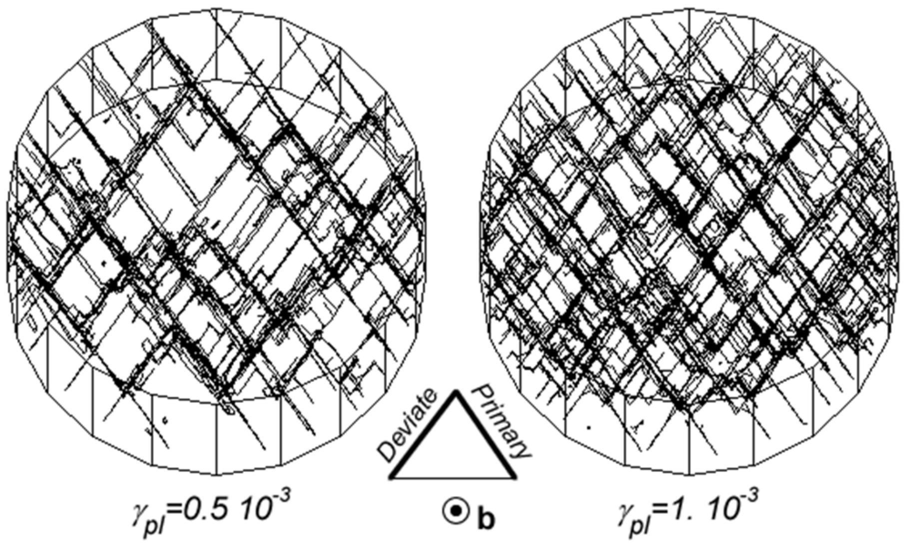




Strain localization (double slip)

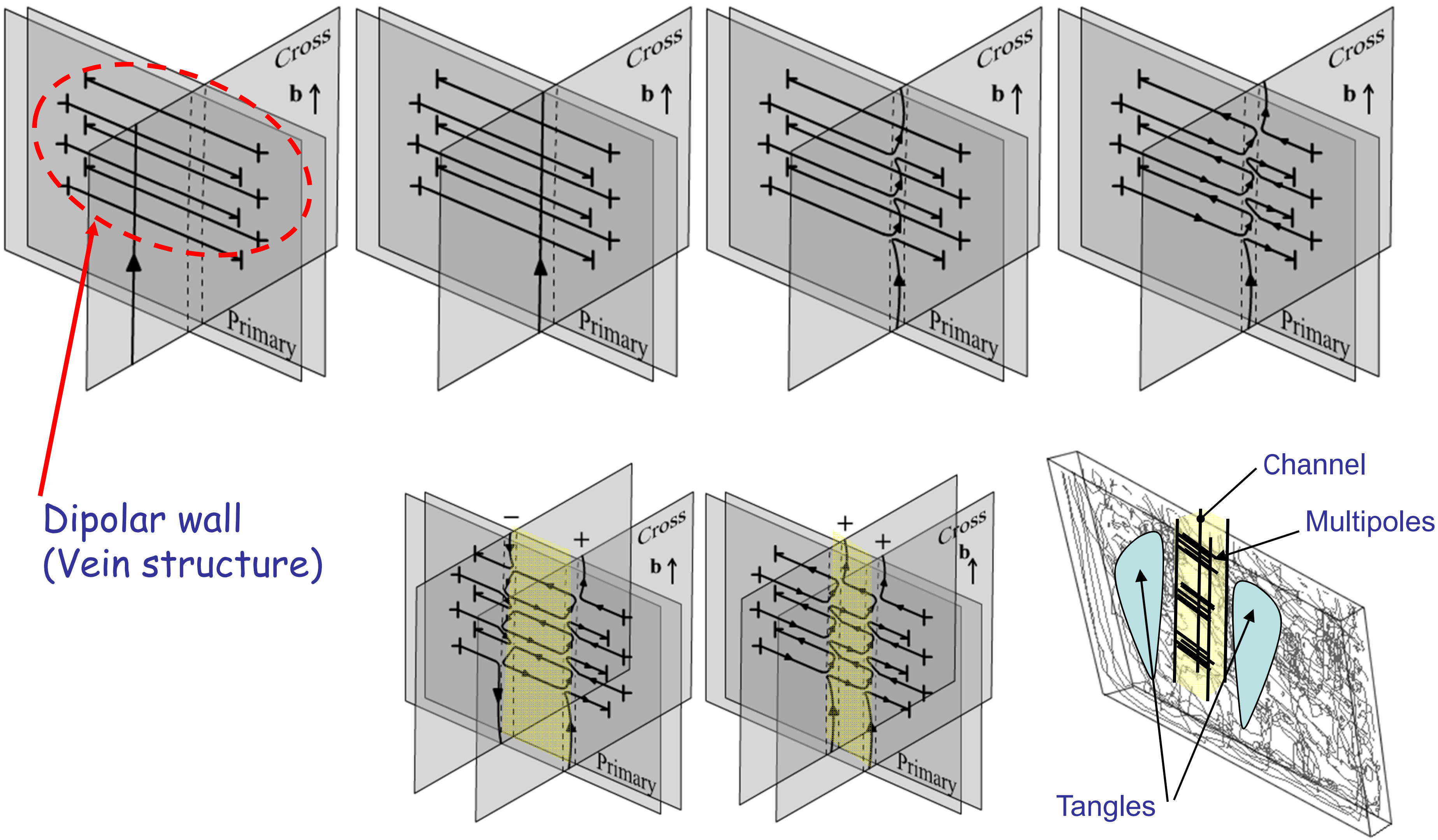


Effect of the grain size : $e \propto D^2$; $d \propto D$

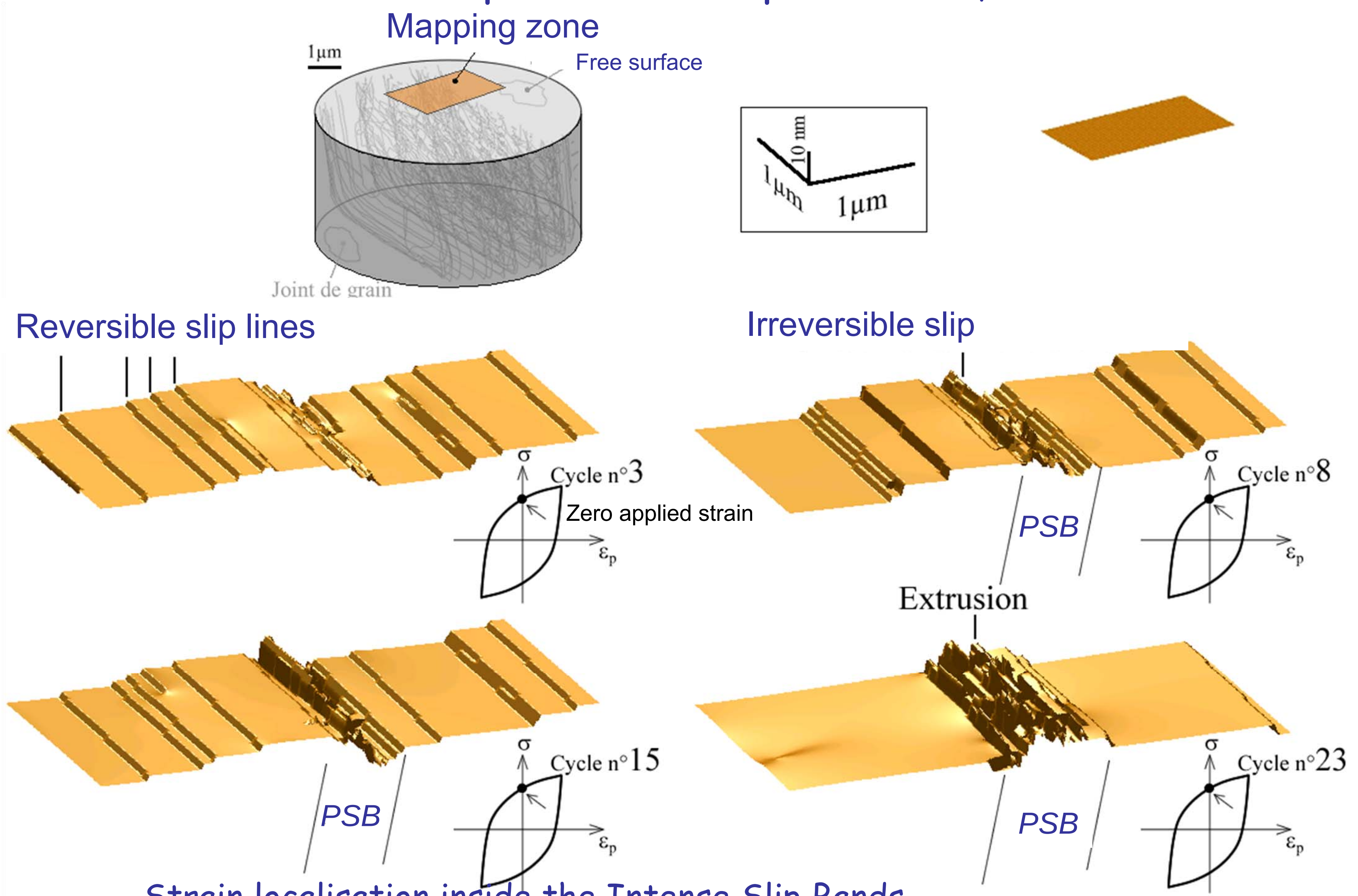


Effect of the strain amplitude :
e cstt ; $n \propto \Delta\varepsilon^p$; $d \propto 1/\Delta\varepsilon^p$

Mechanism for the **formation** of the persistent slip band

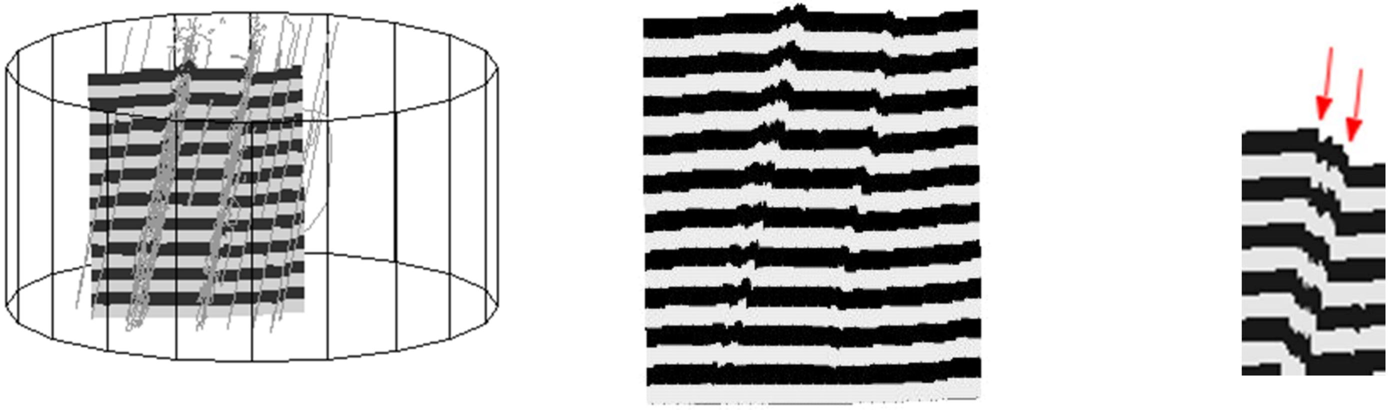


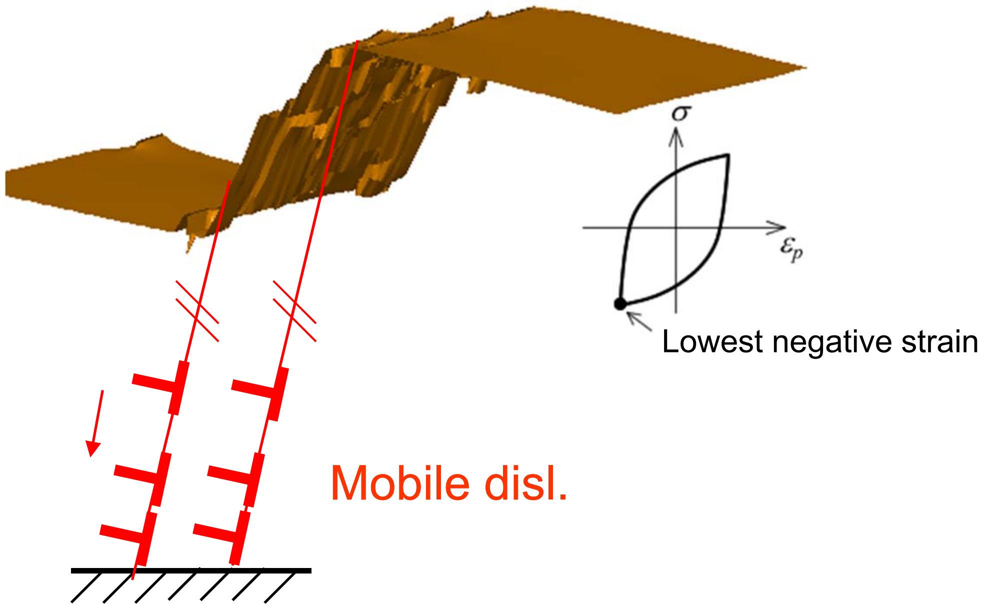
Kinetics of the persistent slip band (snapshots at ε=0)

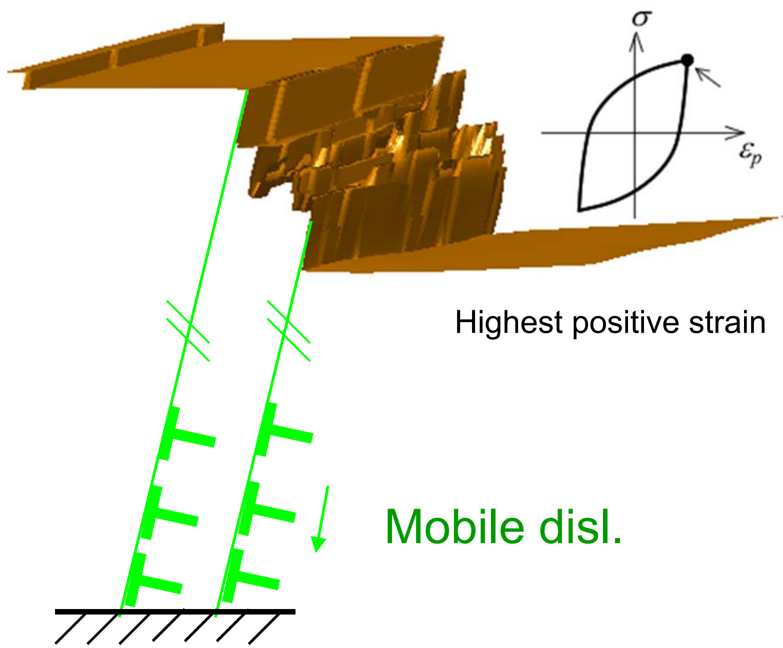


Strain localisation inside the Intense Slip Bands

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

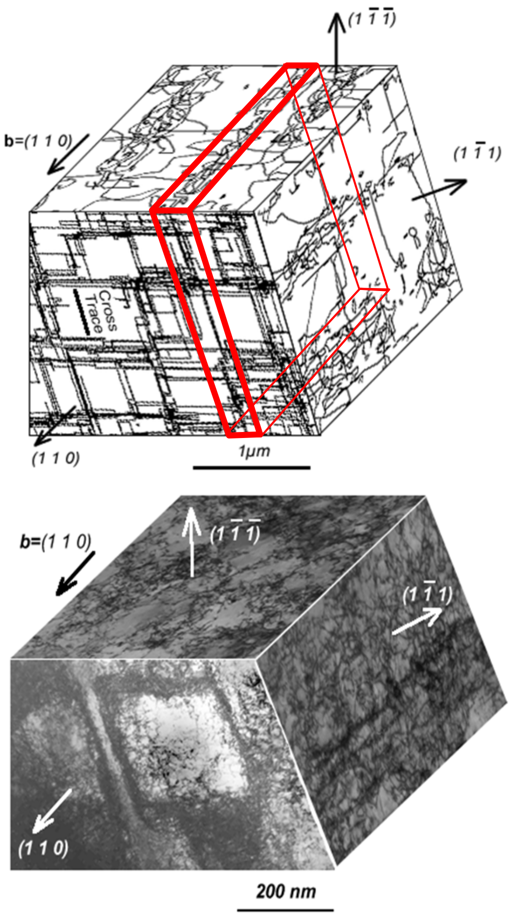


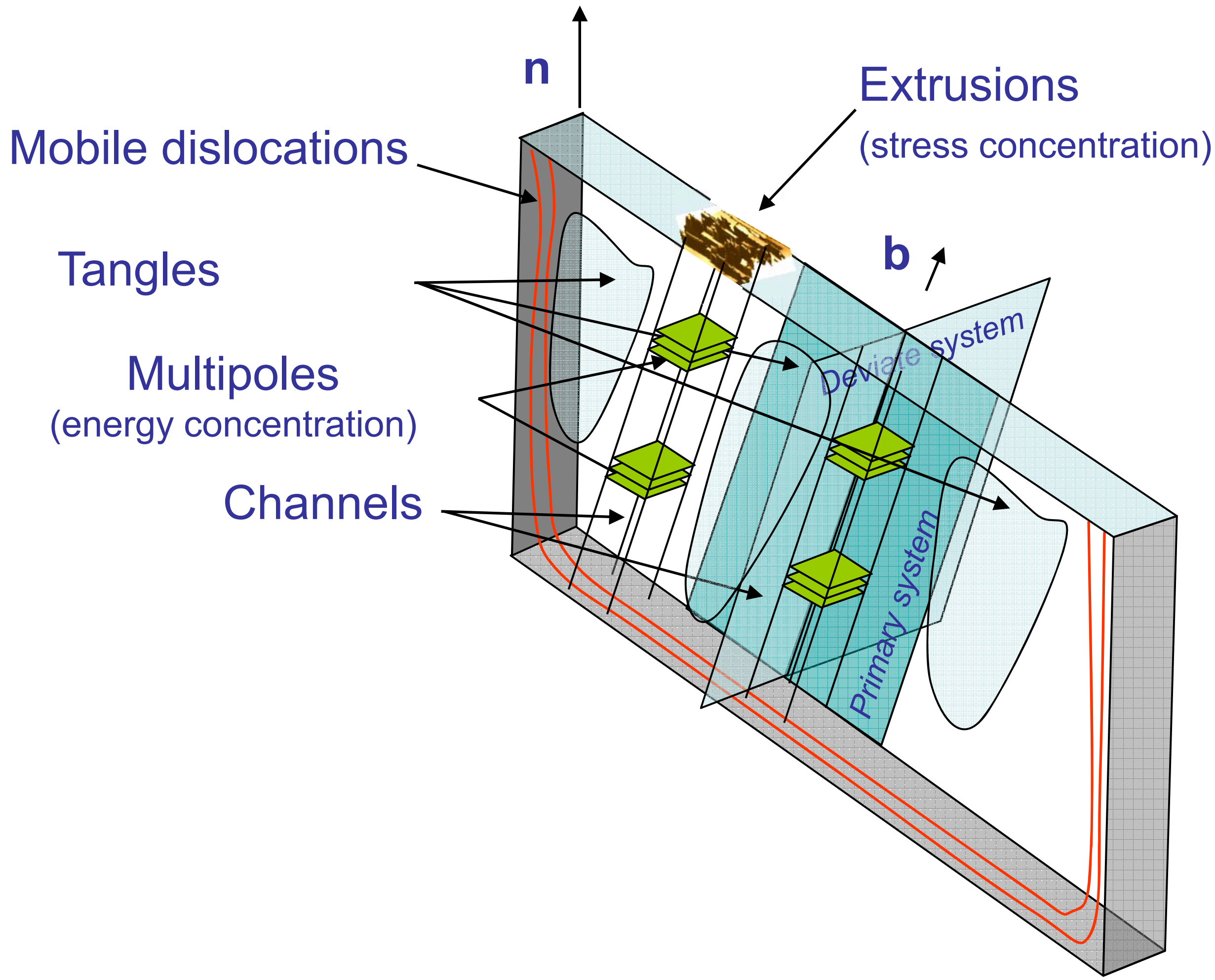




➡ Plastic slip occurs at the band interface
(after stabilisation of disl. density (N> 10))

Schematic description of the Persistent slip band

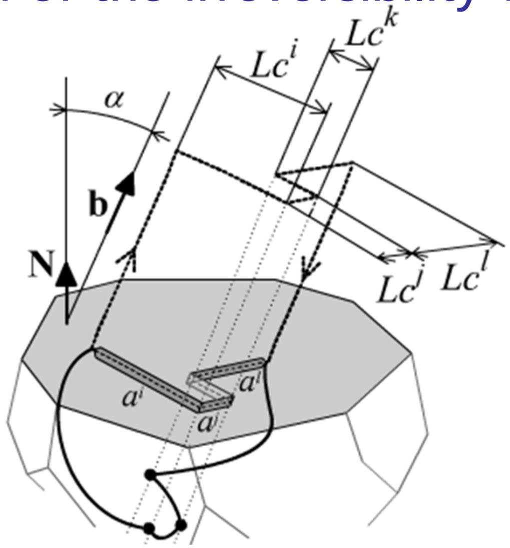




Sweeping of the prismatic loops (multipoles) by mobile interface dislocations

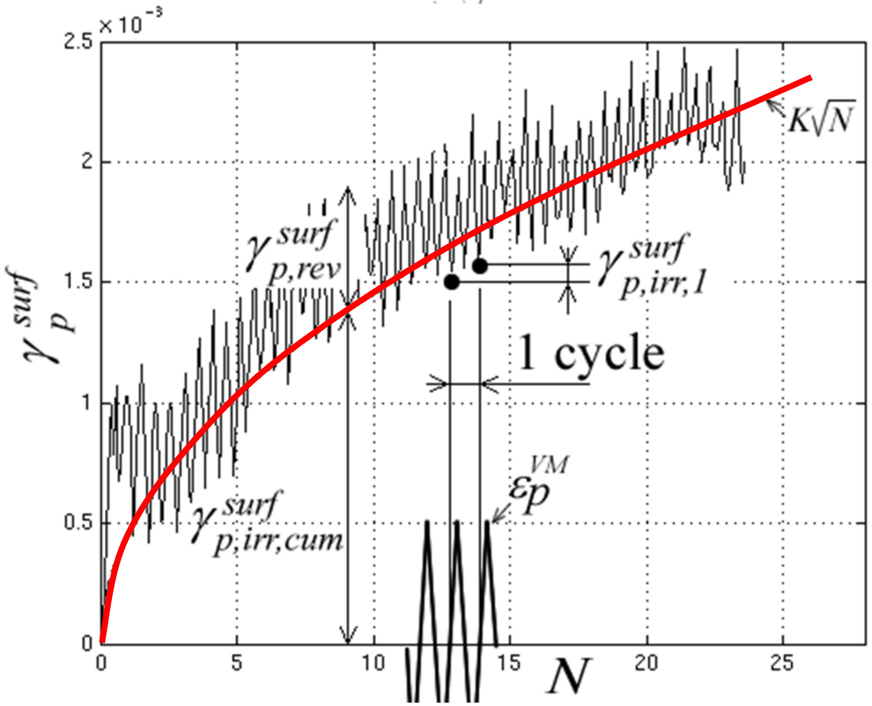
Reversible versus irreversible slip

Quantification of the irreversibility :



$$a_{cum} = \sum_{n_{coin}} \frac{L_c^i}{\cos\alpha}$$ = cumulated height

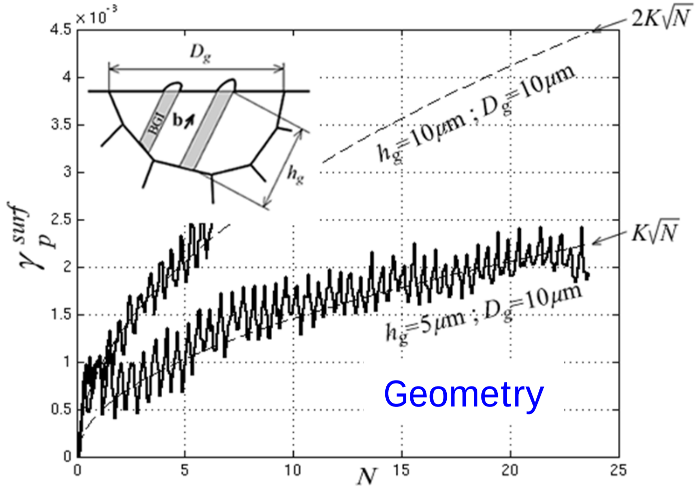
$$\gamma_p^{surf} = \frac{a_{cum}.b.\cos\alpha}{S}$$

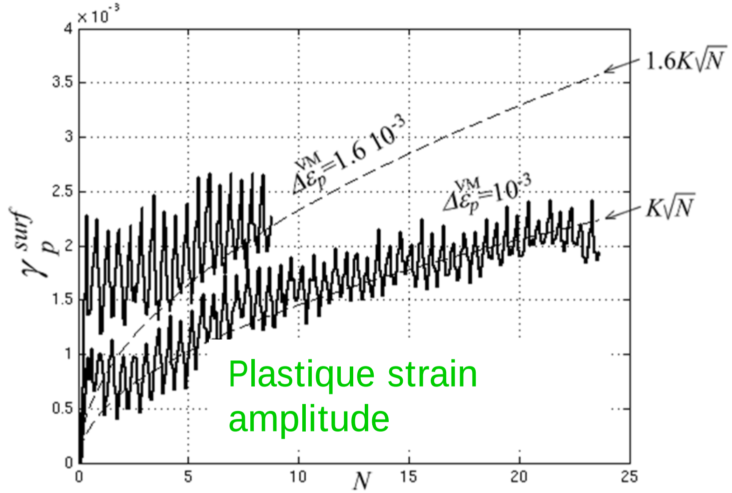


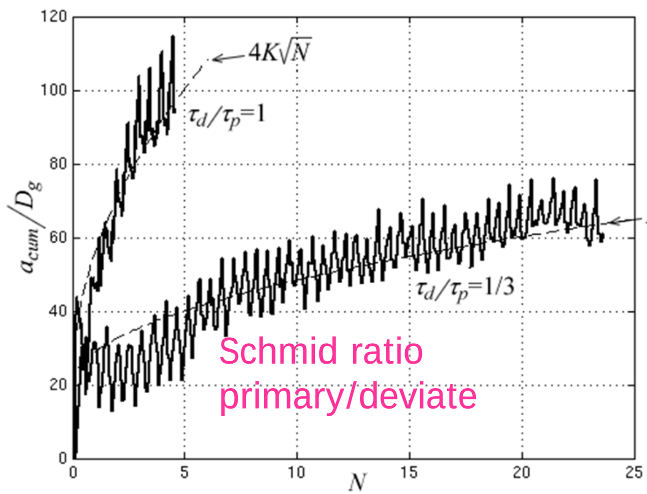
$$\gamma_p^{surf}(t) = \gamma_{p,rev}^{surf}(t) + \gamma_{p,irr,cum}^{surf}(t)$$

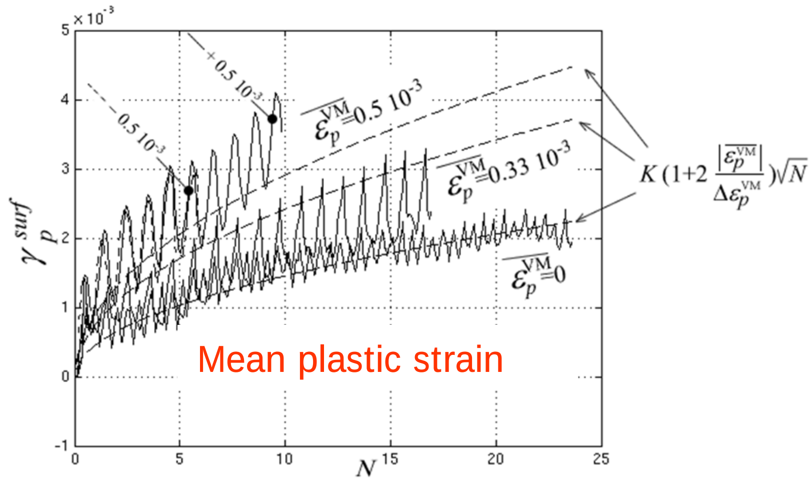
$$\gamma_{p,irr,cum}^{surf}(N) = K\sqrt{N}$$

Effect of different parameters



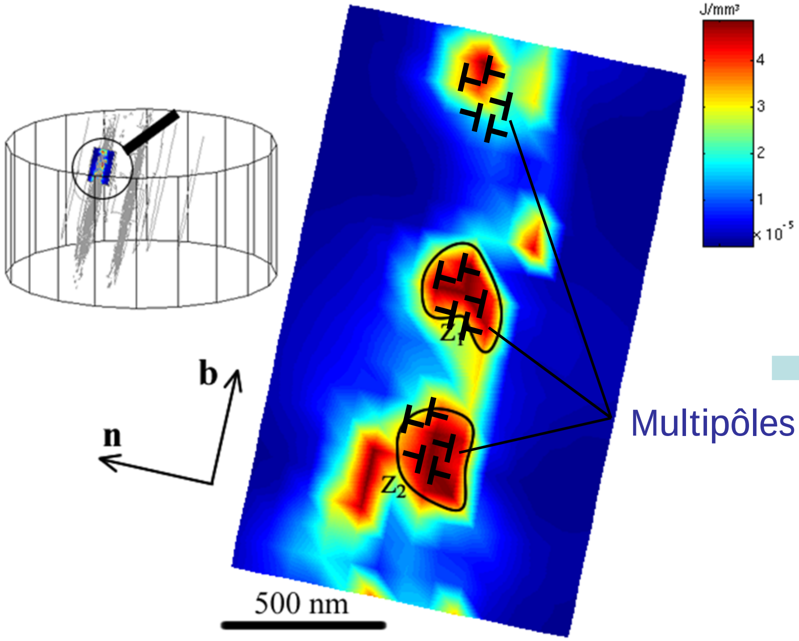


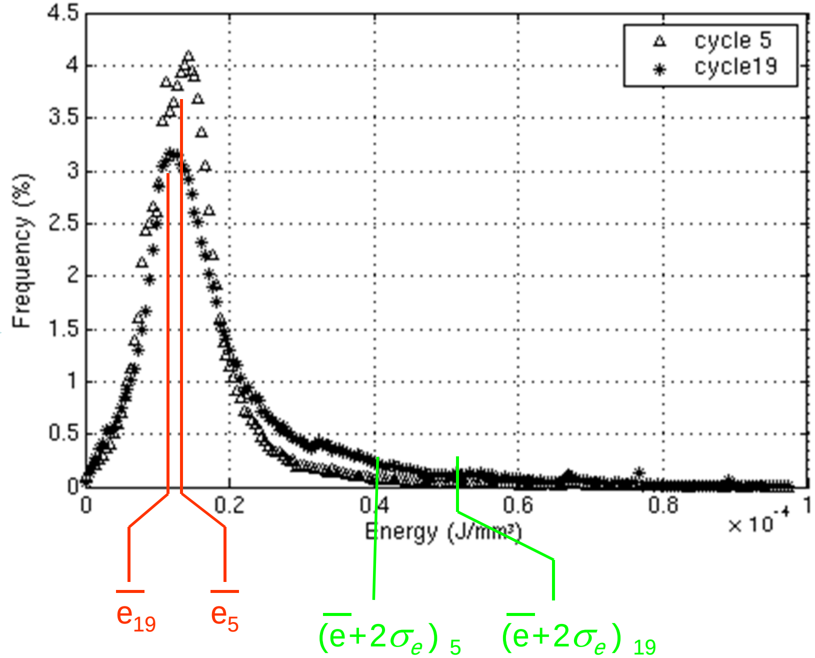


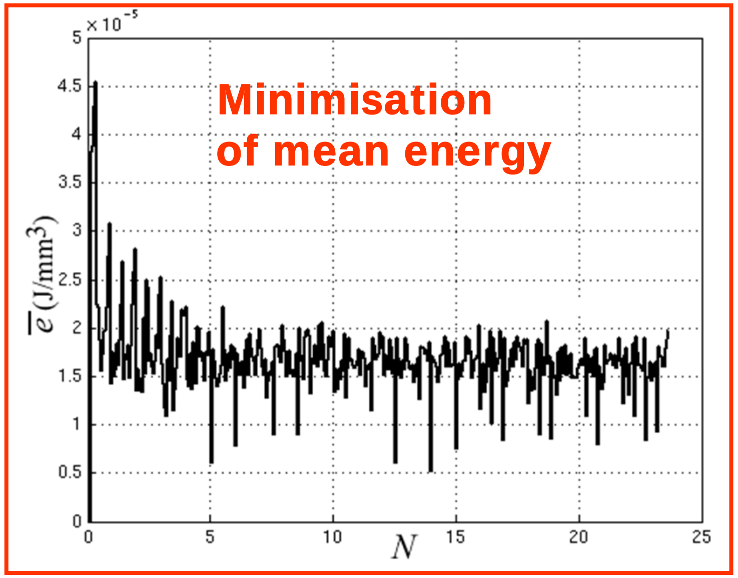


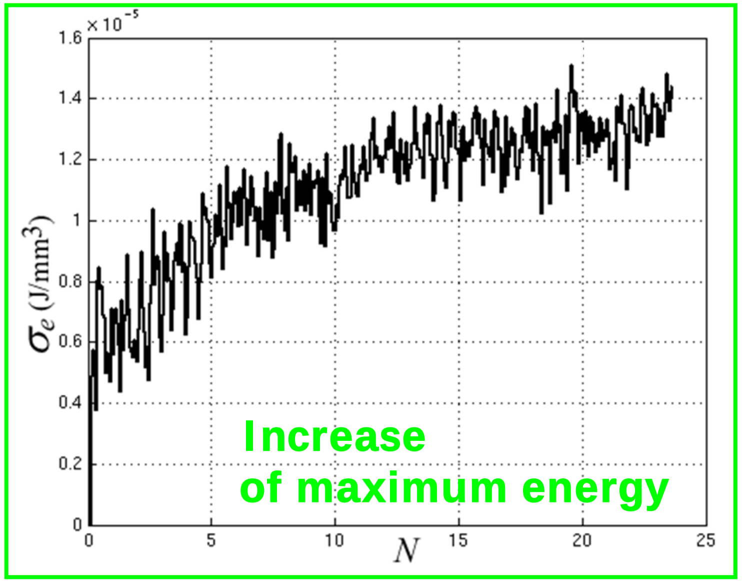
$$\gamma_{p,irr,cum}^{surf}(N) = K\frac{h_g}{D_g}\Delta\epsilon_p^{VM} f\left(\frac{\tau_{dev}}{\tau_{prim}}\right)\left(1+2\frac{|\overline{\epsilon_p^{VM}}|}{\Delta\epsilon_p^{VM}}\right)\sqrt{N}$$

Distorsion energy in channels

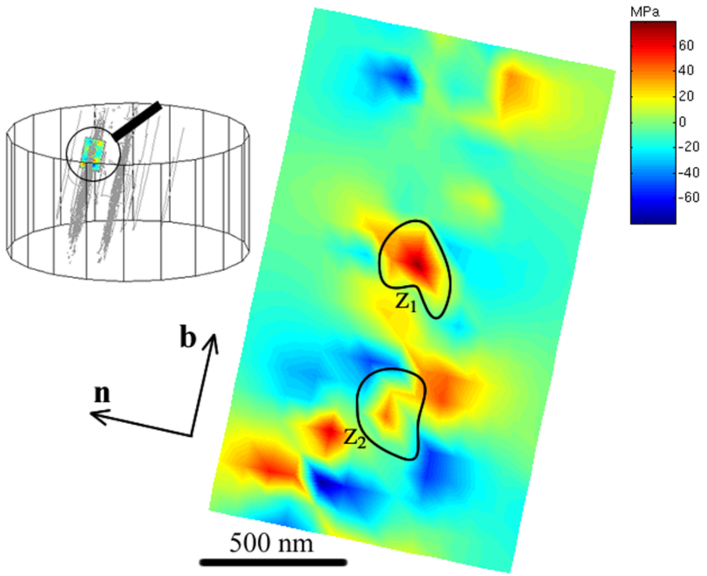


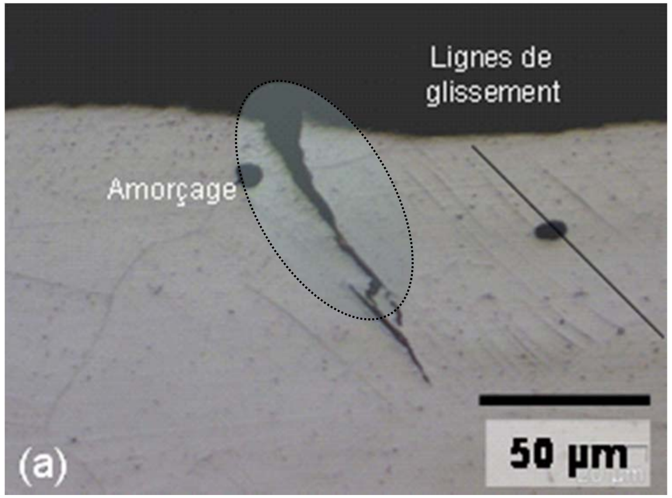


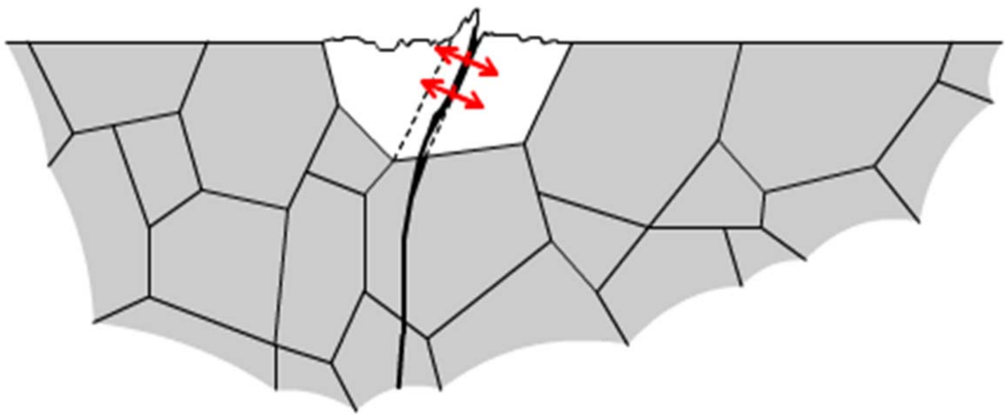




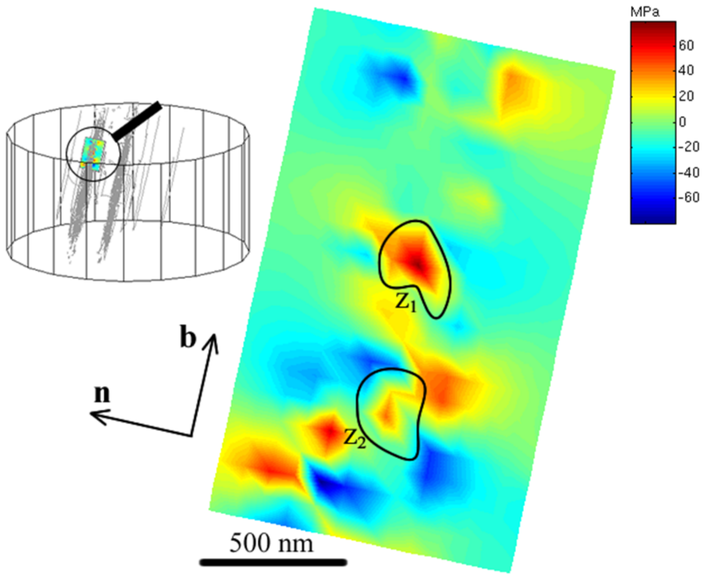
Stress state in channels

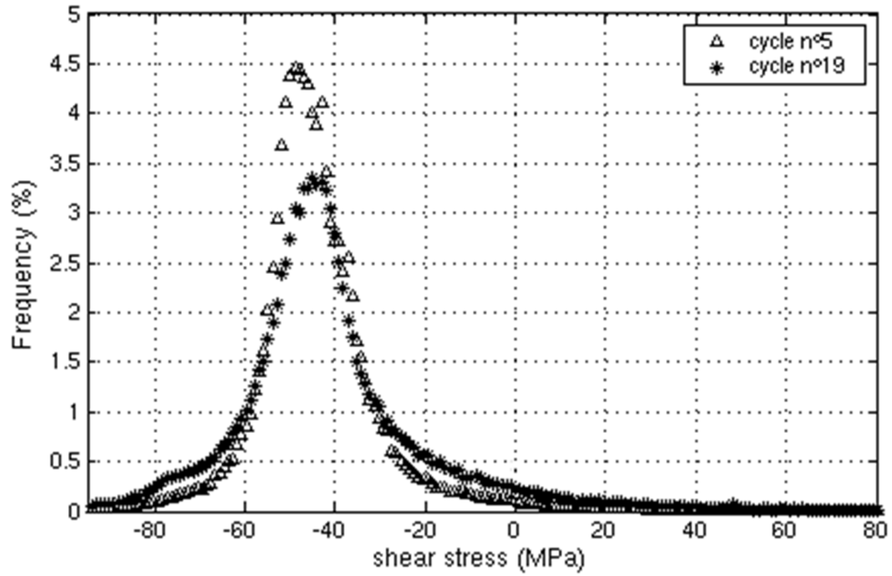


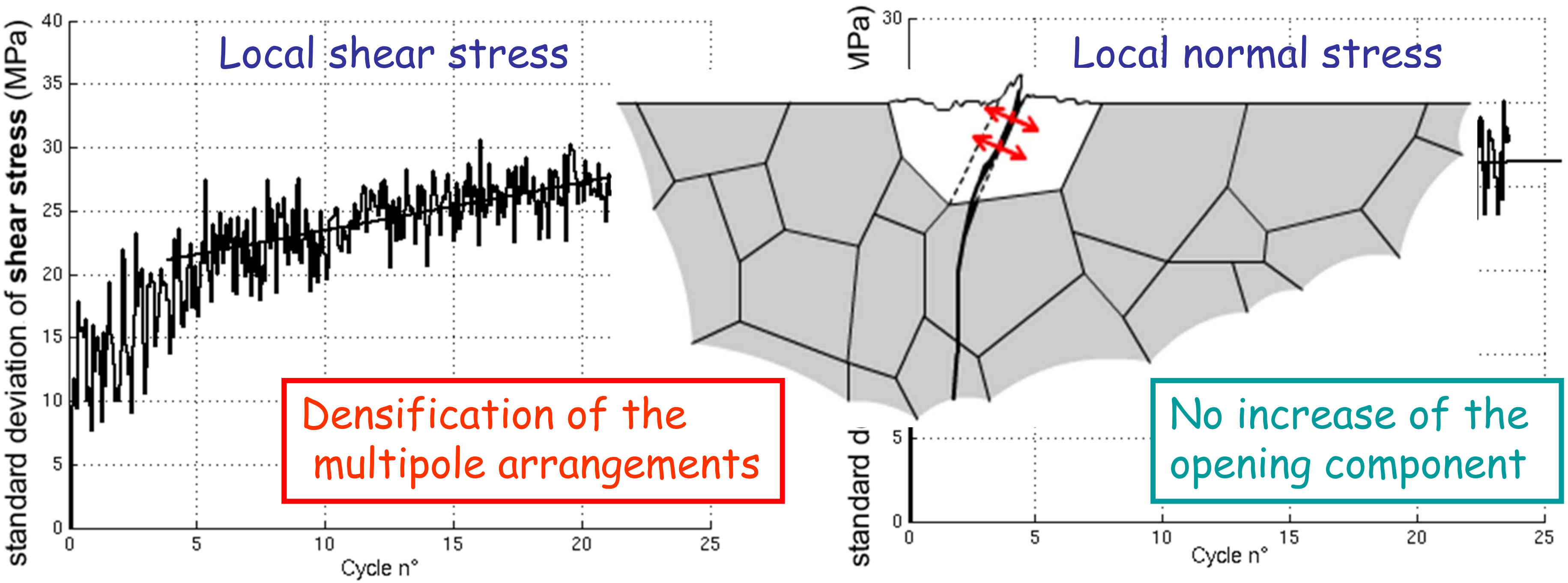




Stress state in channels

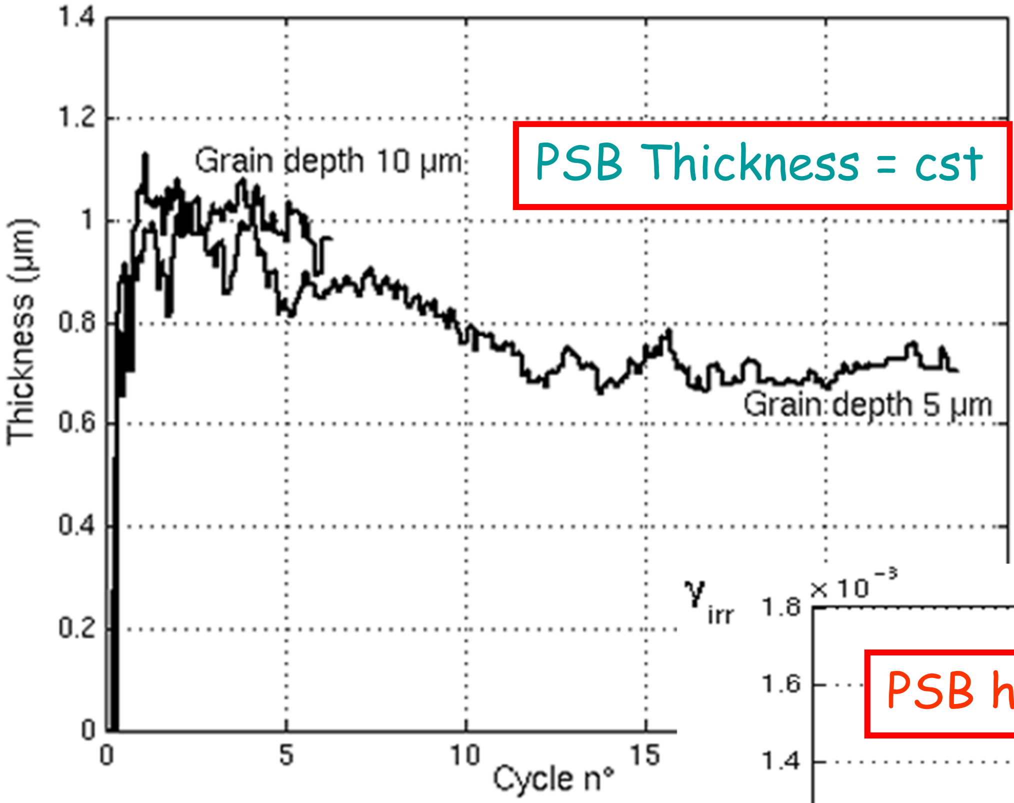


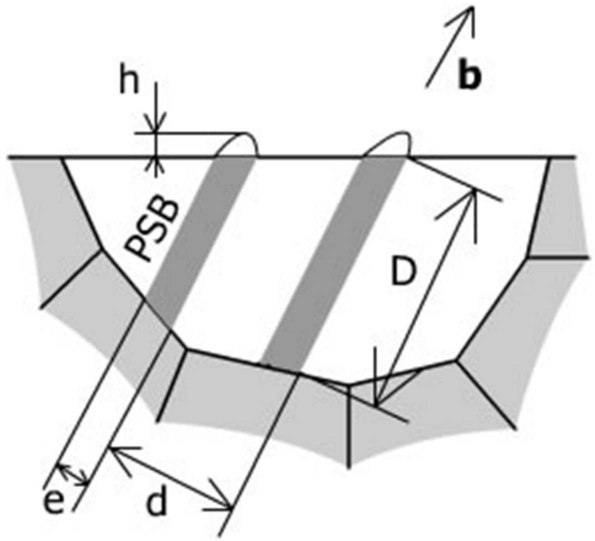


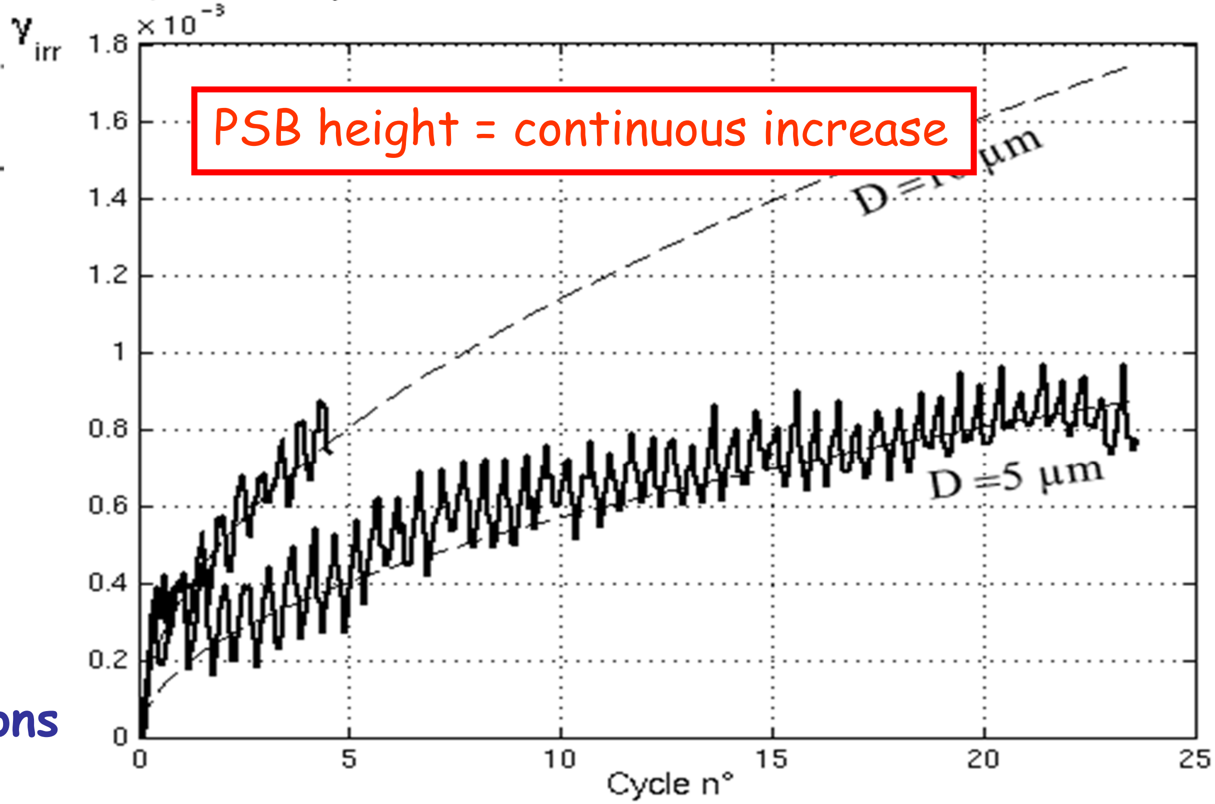


Densification of the multipole arrangements

No increase of the opening component



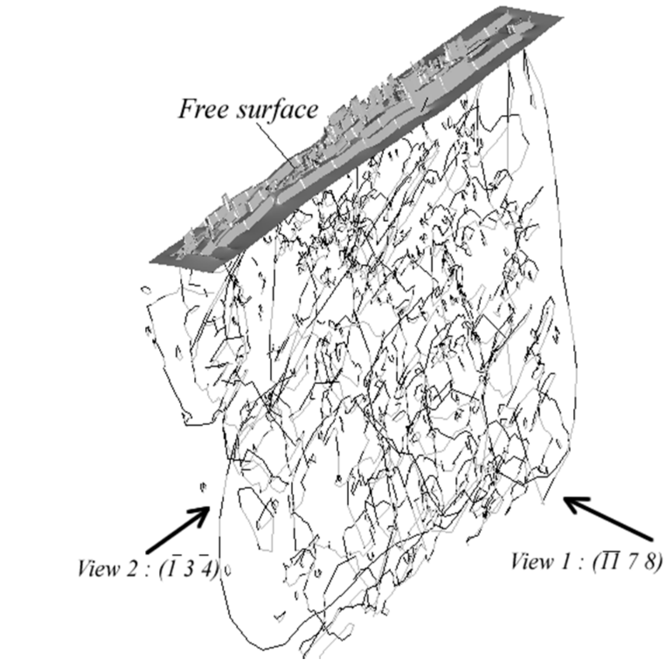


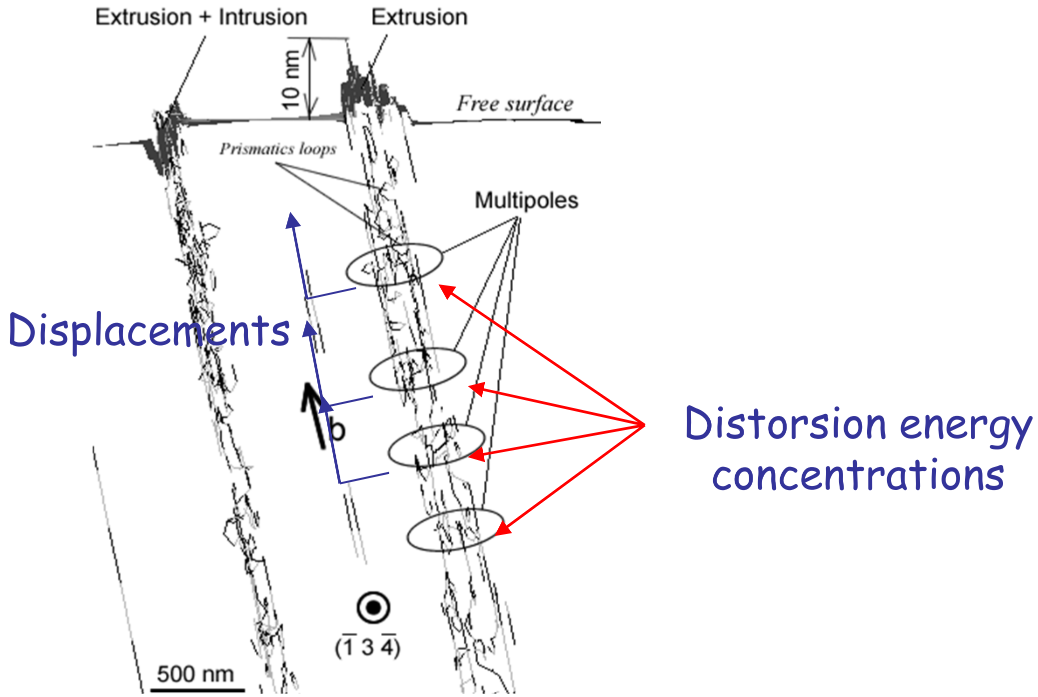


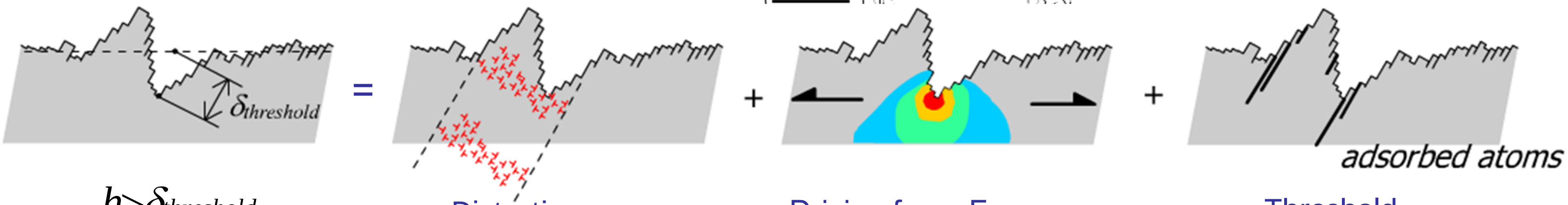
Increase of the extrusion shape factor

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

Crack initiation criterion







$h > \delta_{threshold}$

Distortion energy concentrations

$$\iiint_V \underline{\underline{\sigma}} : \underline{\underline{\varepsilon}}\, dV$$

Driving force Fm
Evolution of h/e

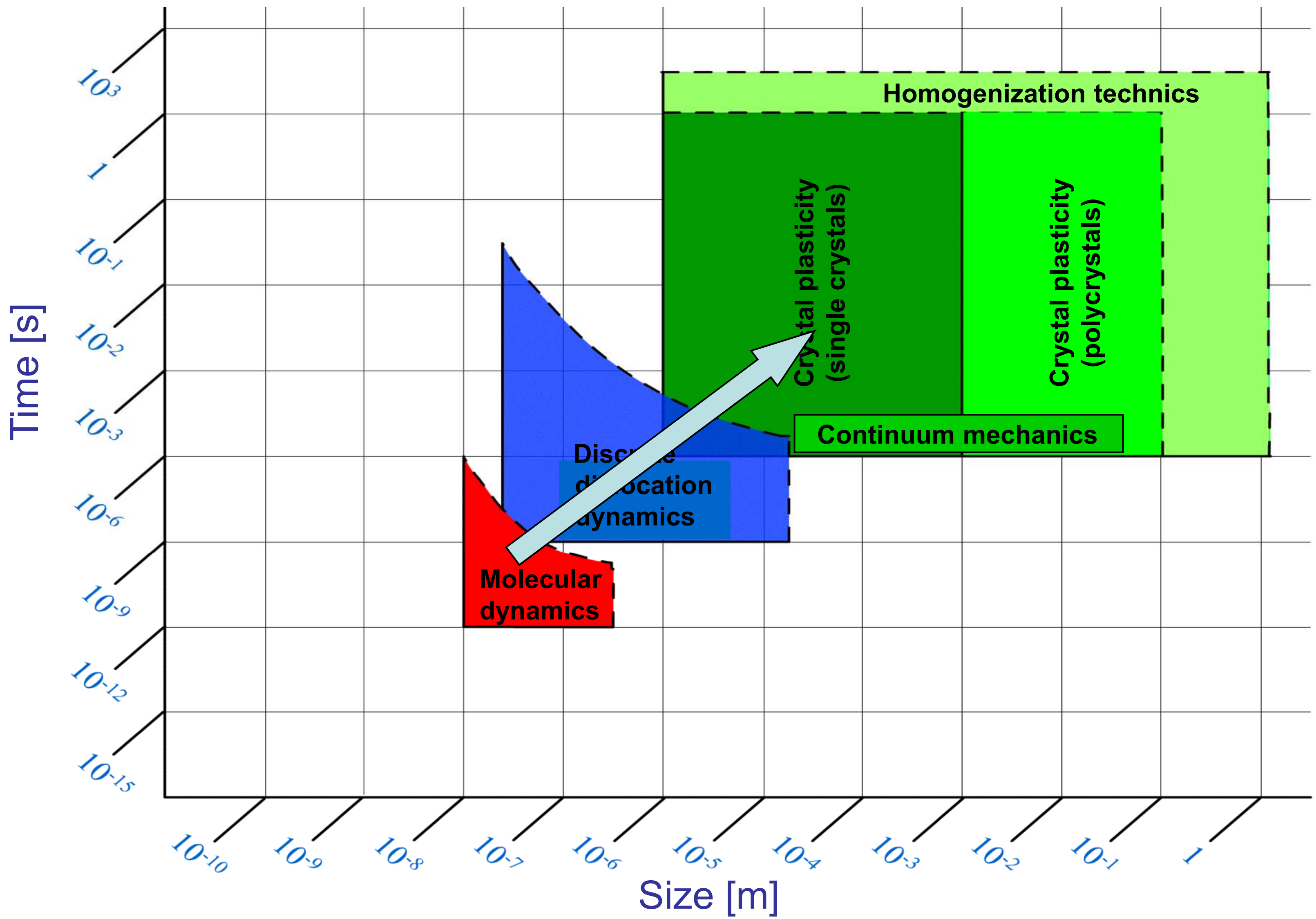
$$\sigma_{nn} > \sigma_{SEPARATION}$$

Threshold diminution

$$N_{init} > \left(2\frac{k_2}{k_1} \frac{\delta_{threshold}\,\phi_{grain}^2}{V_{grain}} \cdot \left(\frac{\tau_p}{\tau_d}\right)^{\frac{1}{m}} \right)^{\frac{1}{\frac{1}{2}+\frac{\varepsilon_{moy}}{\Delta\varepsilon_p}}}$$

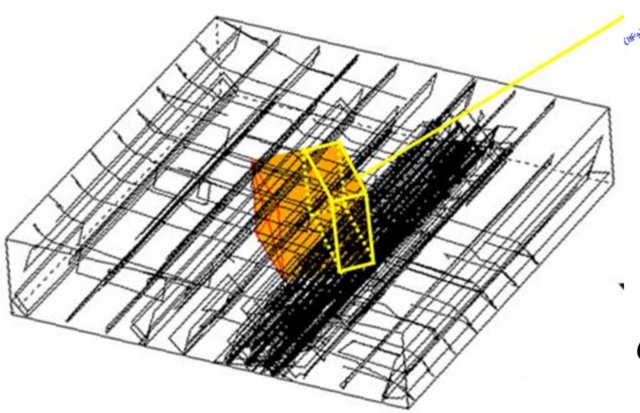
Multiscale Materials Modelling

Example of scale transition :
From atoms to continuum mechanics



Example of DD applications:

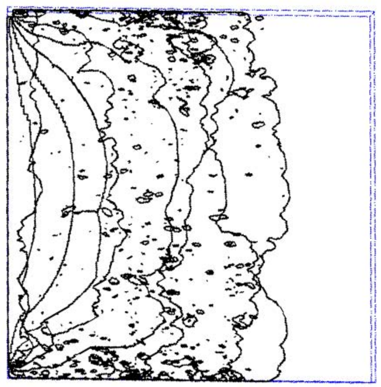
(See also http://www.numodis.fr)



Plastic behavior of BCC Fe

Ph.D. Julien CHAUSSIDON (2007)

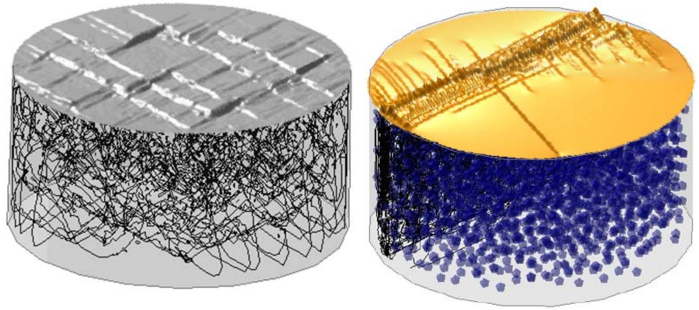
Ph.D. Daniel GARCIA-RODRIGUEZ (2011)



Clear channels in AISI 316L steel

Ph.D. Thomas NOGARET (2007)

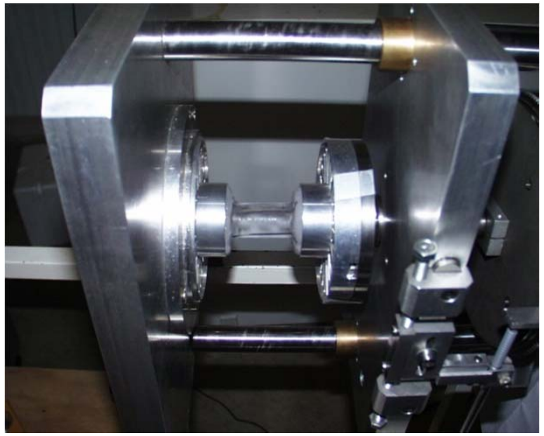
Ph.D. Gururaj KADIRI (2014)



Crack initiation in fatigue

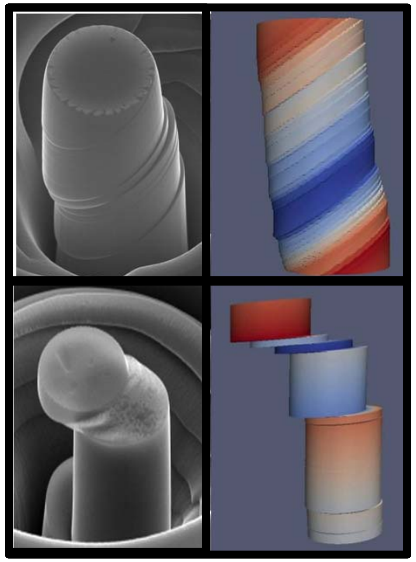
Ph.D. Christophe DEPRES (2004)

Ph D. Chan Sun SHIN (2004)



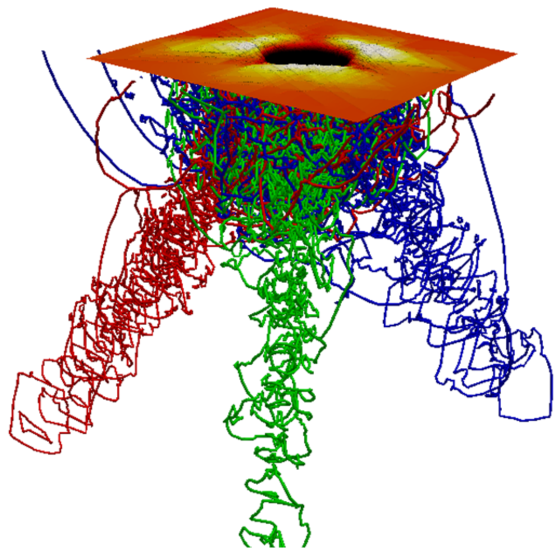
Creep of ice single crystals

Ph.D. Juliette CHEVY (2008)



Micro-compression of Mg pillars

Ph.D. Gyu Seok KIM (2011)

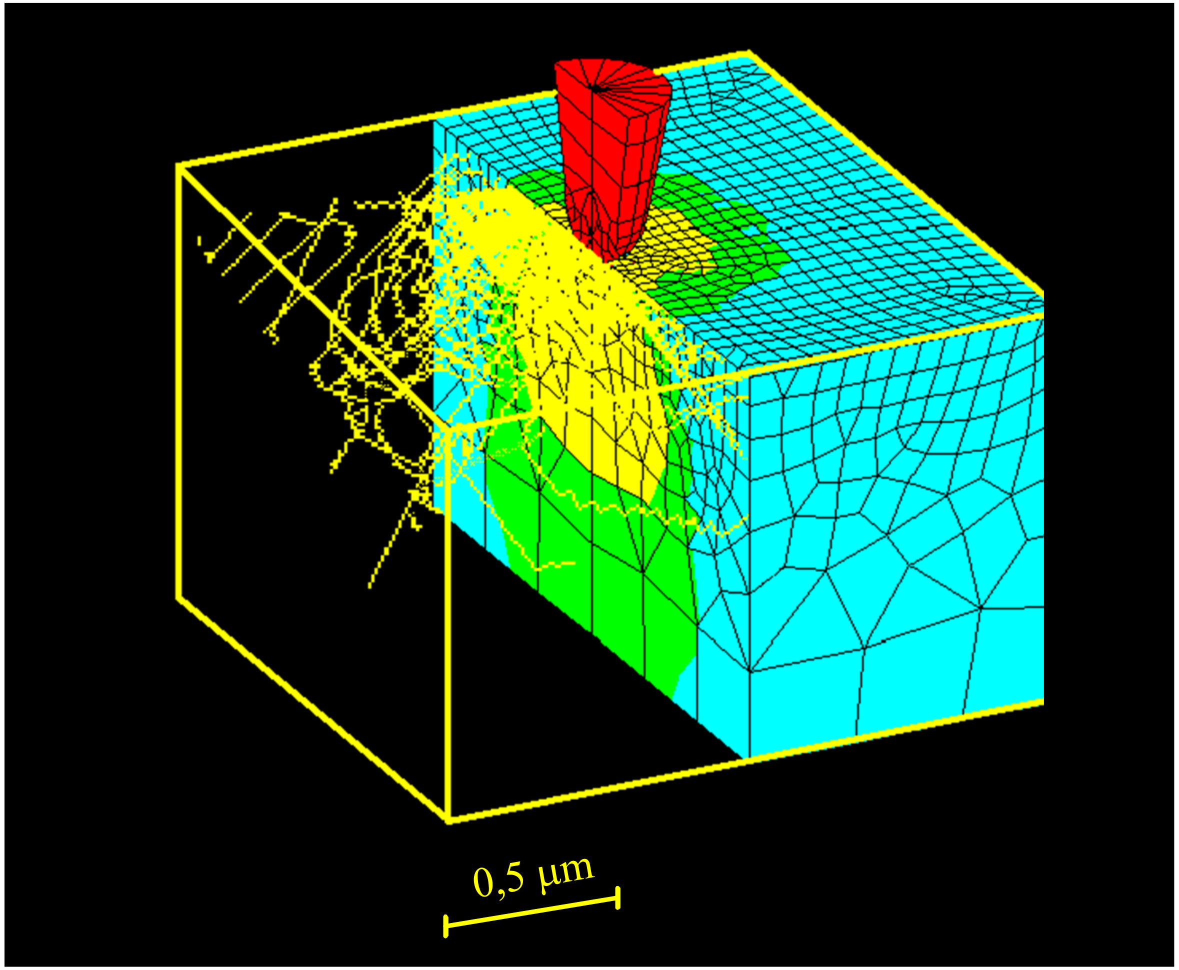


(111) Nanoindentation in Cu single crystal

Ph.D. Hyung Jun CHANG (2009)

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

$$[\sigma]^{\mathrm{eff}} = [\sigma]^{\mathrm{disl}} + [\sigma]^{\mathrm{FE}}$$

II- Need of a nucleation criterion for dislocations:

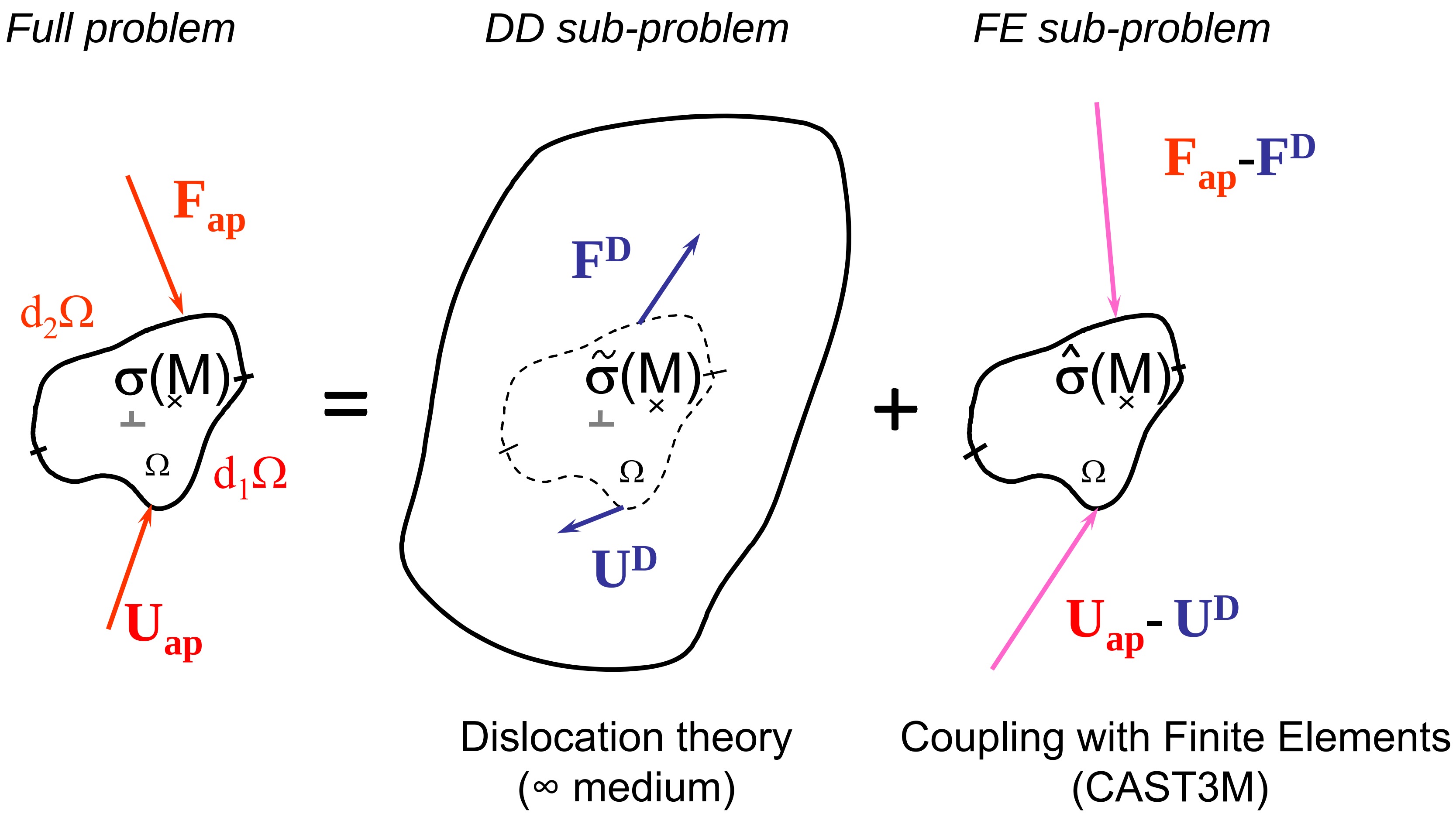
1- What to put in ?

2- When to put it in ?

⇨ MD or experiments

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

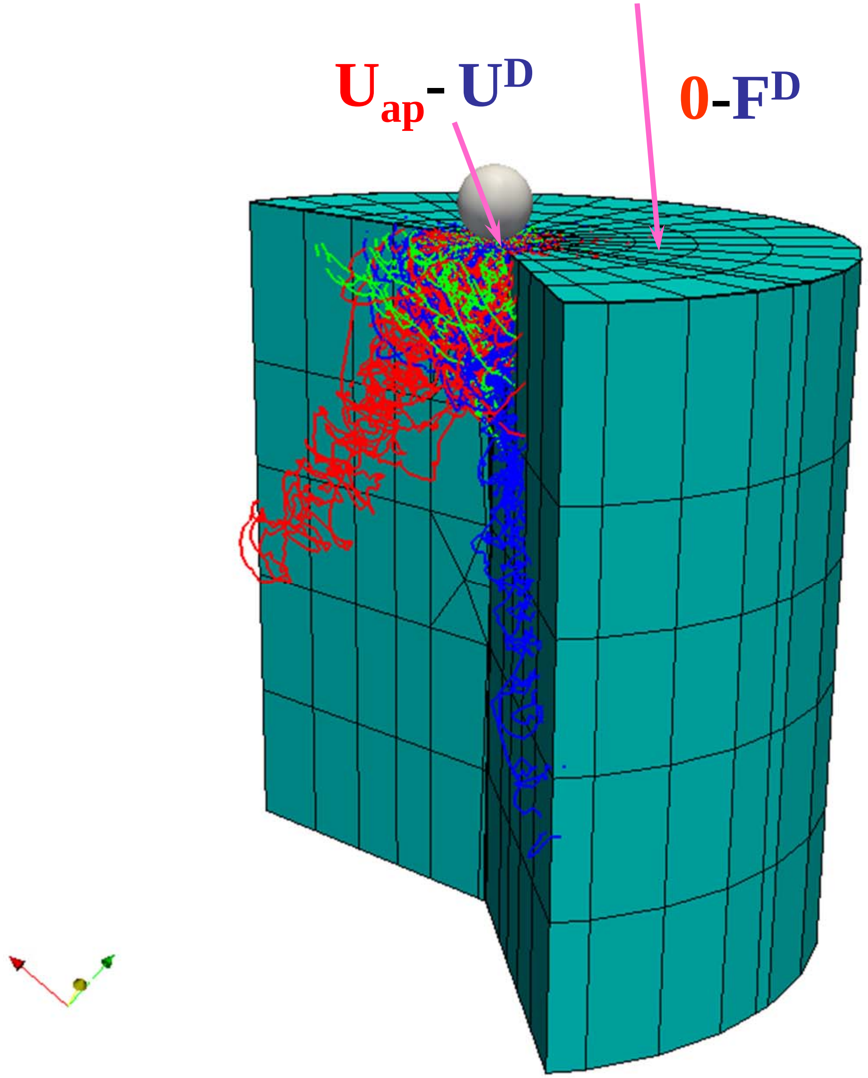
E. van-der-Giessen, A. Needleman, Mater. Sci. Eng. , (1995)



$$\underline{\underline{\sigma}} = \underline{\underline{\hat{\sigma}}} + \underline{\underline{\tilde{\sigma}}}$$

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

Application to nanoindentation



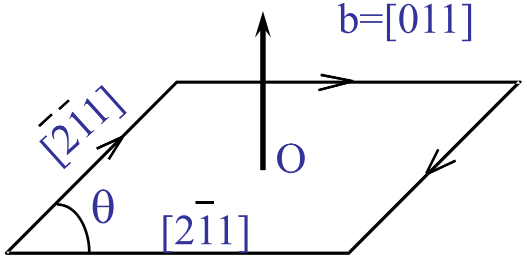
Problem II: Nucleation criterion : What to introduce ?
(Experimental evidences)

Two possibilities :

- experimental observations (TEM) and measures (nanoindentation tests)
- atomic scale simulations (MD)

What to introduce ?

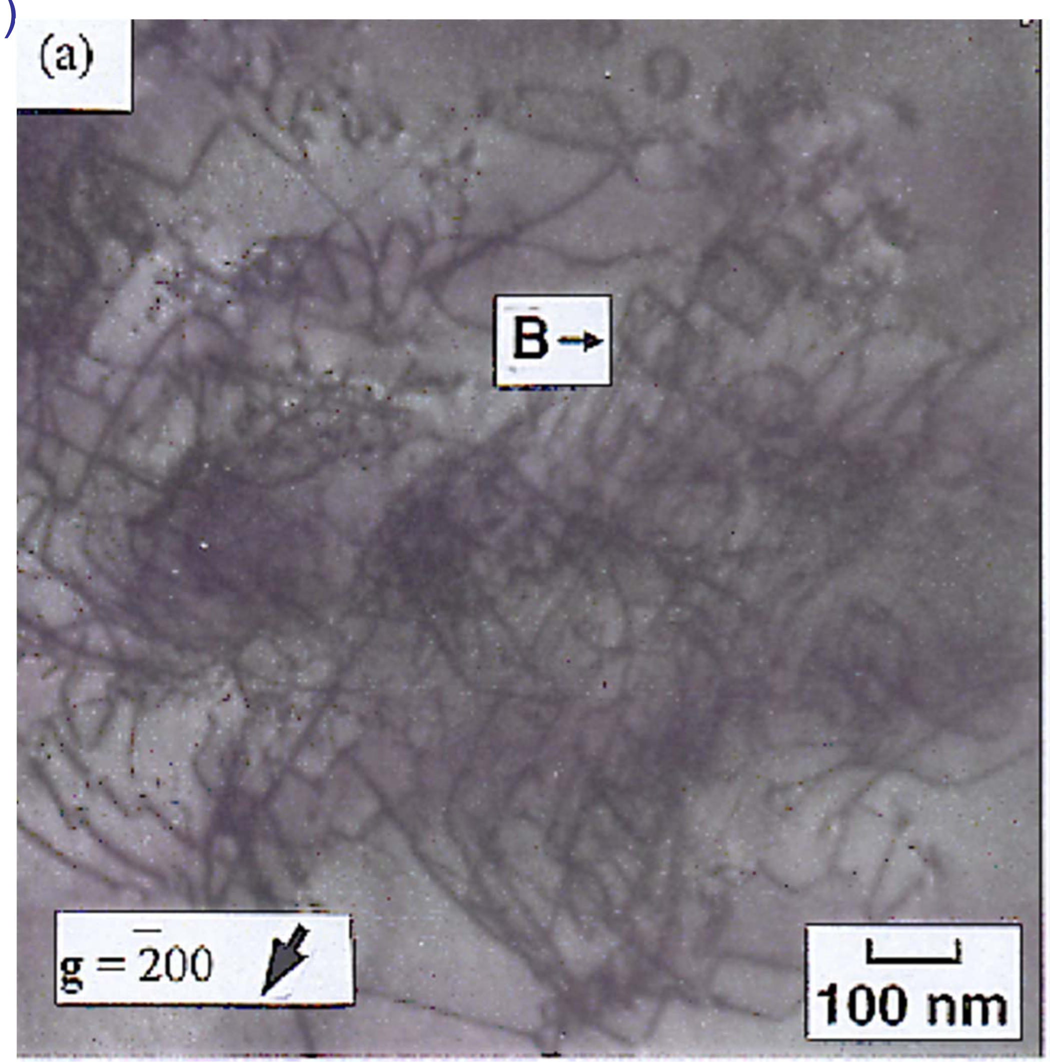
Prismatic loops ?



Interstitial loop

Two glide systems per prismatic loop

(Acta Mater **46**(17), pp.6183-6194, 1998)



Low penetration on 316L (C. Robertson)

Problem II: Nucleation criterion : What to introduce ?

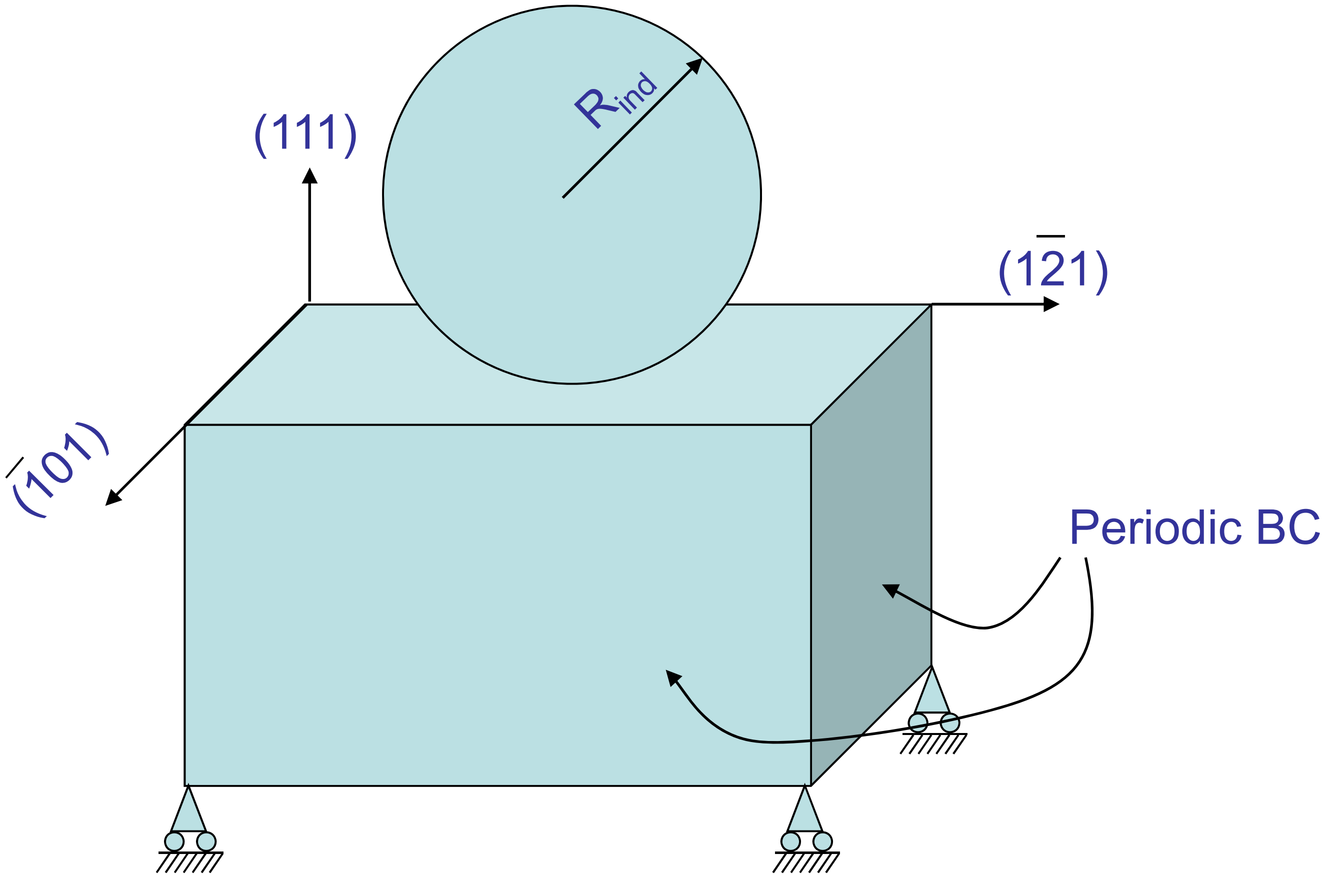
(Molecular Dynamics modeling)

Simulation campaign :

- Material = Ni (EAM potential)
- Indenter = spherical repulsive potential
  Monitored in displacement

2 radii : Rind = 60Å and 120 Å

3 sizes : 174x198x163 Å^3 (521.640 atoms)
224x284x285 Å^3 (1.675.080 atoms)
301x301x200 Å^3 (1.524.600 atoms)



Molecular Dynamic simulations of (111) indentation

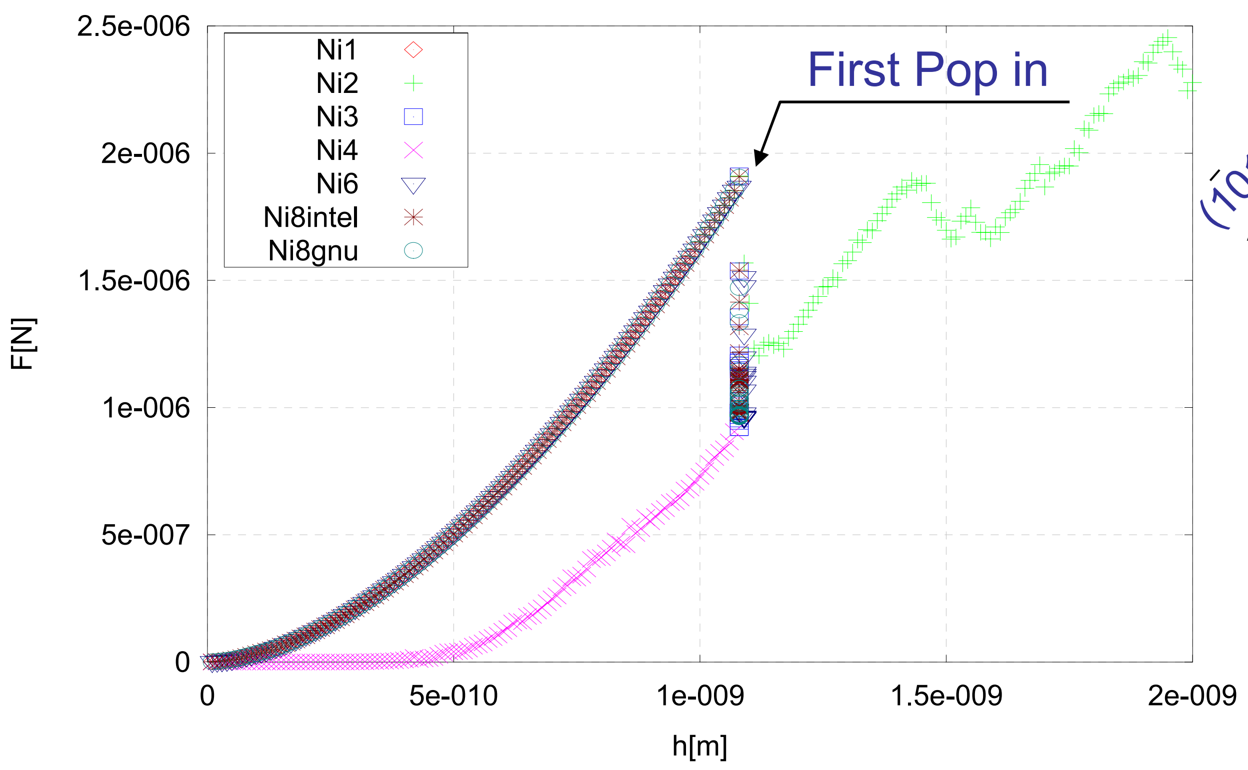
The loading curves : study of the elastic part

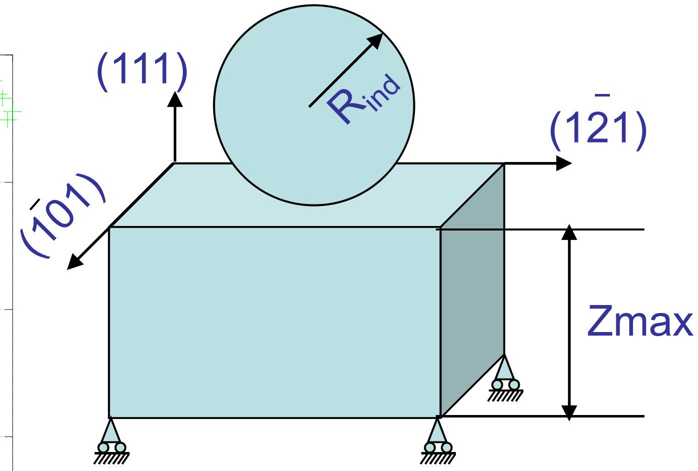
Hertz prediction : $$F = \frac{4}{3}\frac{E}{1-\nu}R_{ind}^2\left(\frac{h}{R_{ind}}\right)^{3/2}$$

Atomistic results : $$F = \alpha h^p$$

Where 1,65 < p < 1,75 (p decreases as Zmax increases)

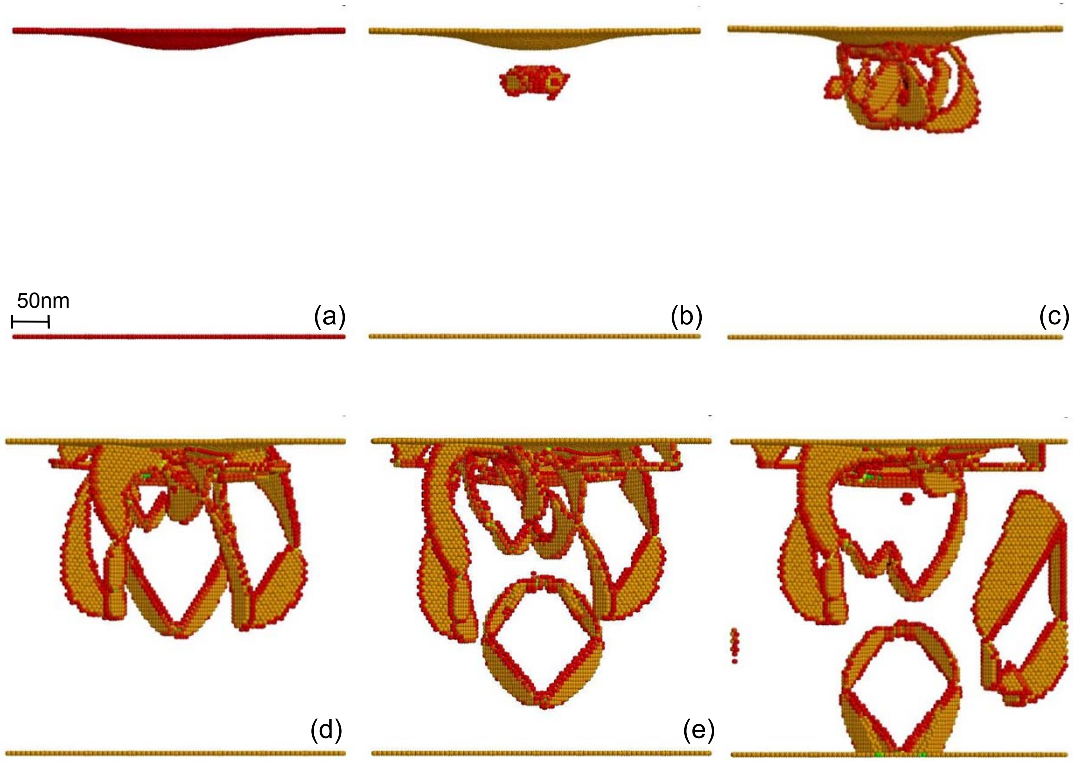
And 20,15< α < 30,65 (when F in nN and h in Å)

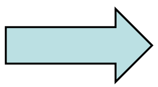




Molecular Dynamic simulations

The dislocation structure : structure after the first pop in

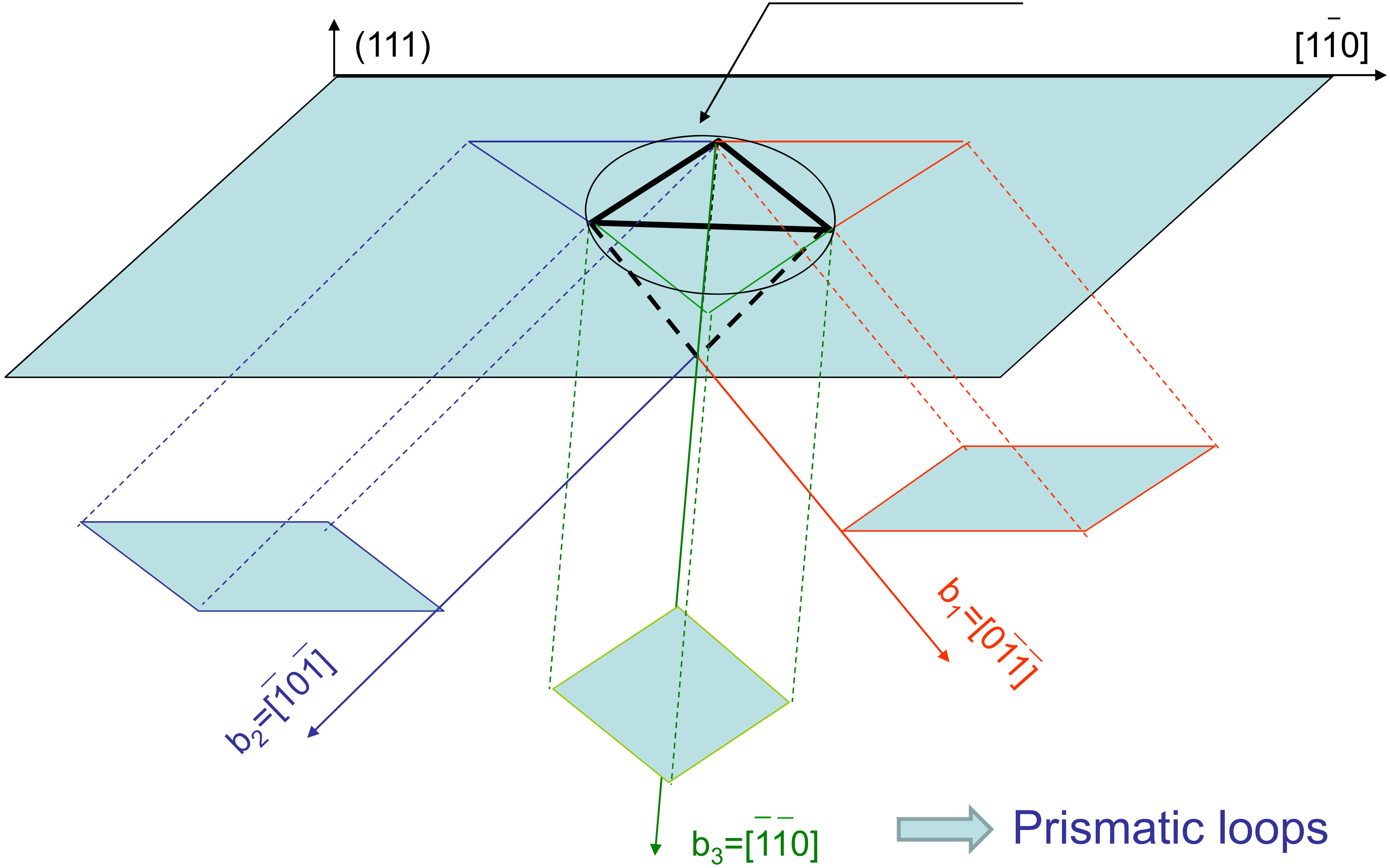




More and more prismatic loops with larger size
Horizontal half loops propagate to accommodate the indentation print

Dislocation nucleation criterion : What to put in ? ☑

Atomistic simulations summarized :

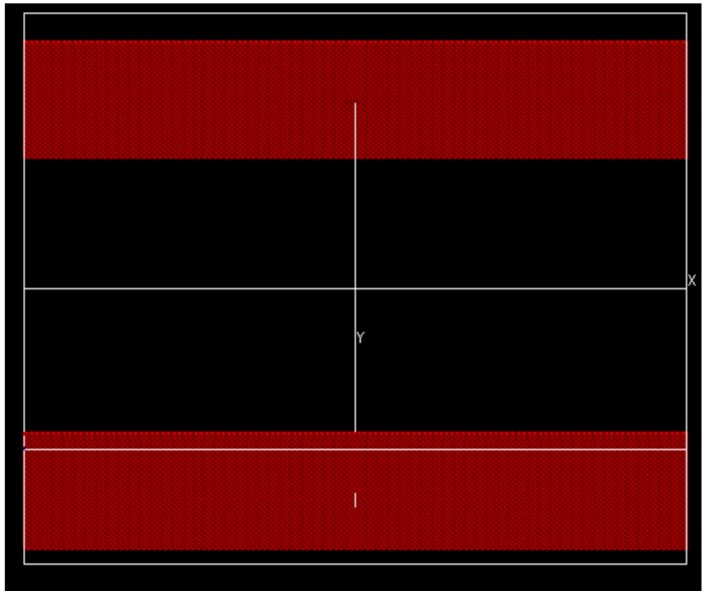


⇨ Prismatic loops

Problem II: Nucleation criterion :

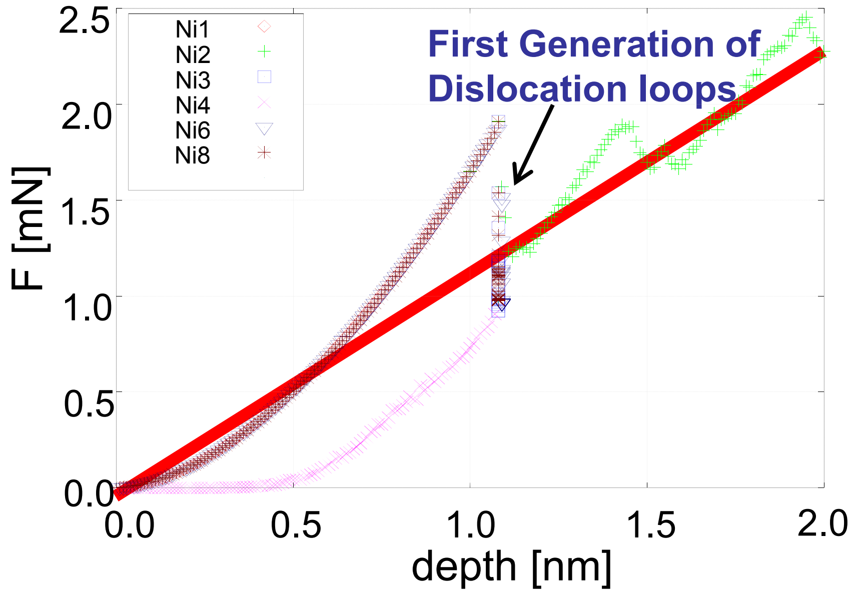
What to put in ? When to put it in ?

Shape of Nucleation (MD,111)



What : 3 Prismatic loops

Master curve (MD,111)



When : Fit a master curve

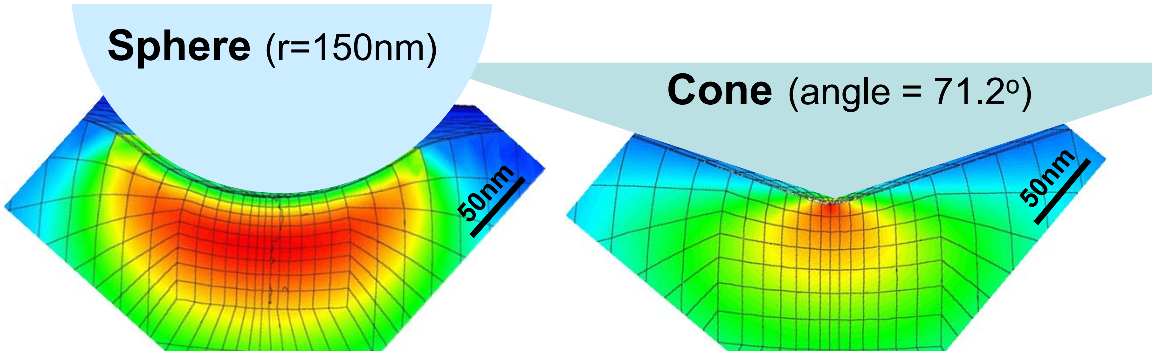
Good : Criterion without any experimental results
Weak : MD response extrapolated for deeper indentation depth !

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

Dislocation Dynamics simulations

Specimen — **Copper single crystal (111 surface)**

Tip geometries



Nucleation method

1. Global criterion : **Force** controlled Nucleation

   Master curve from MD (sphere) or Exp (cone)

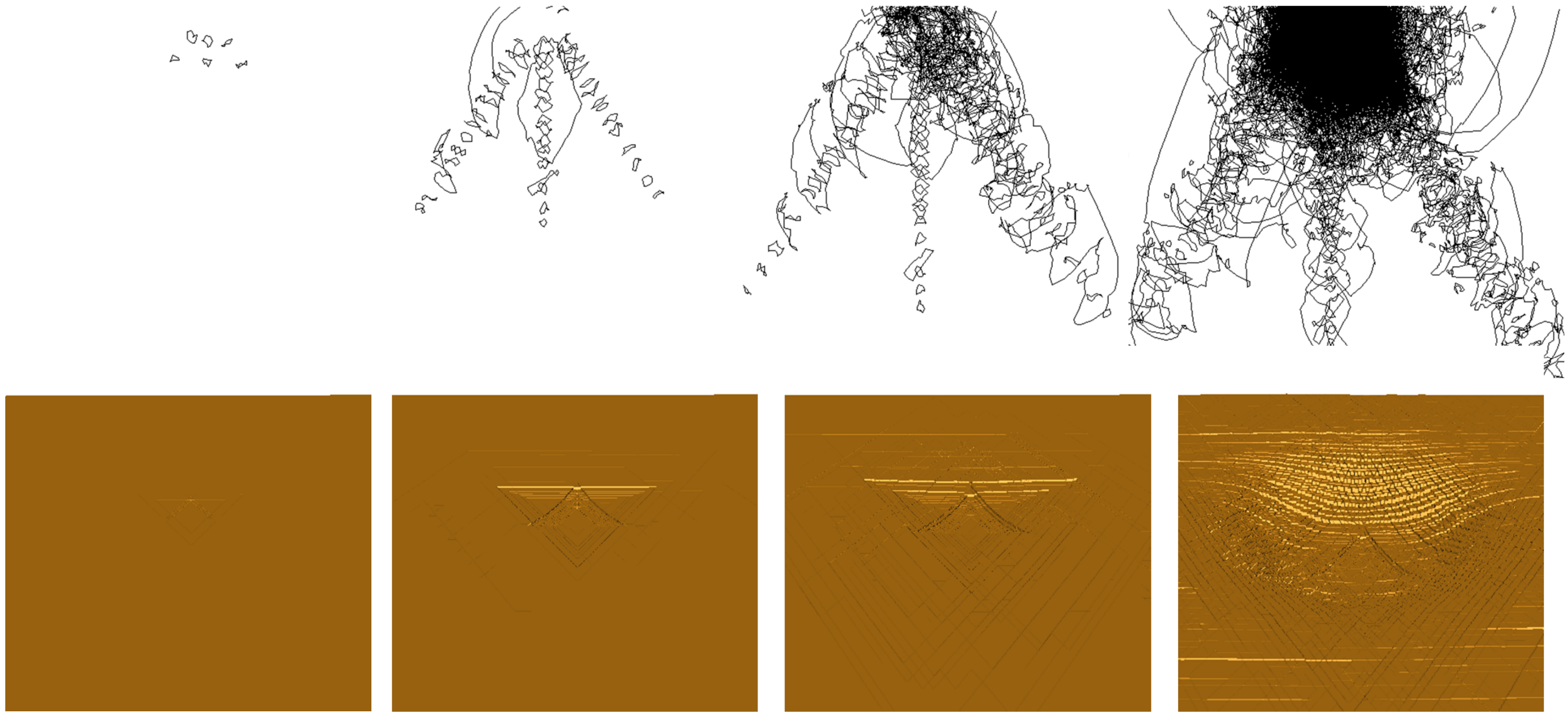
2. GND criterion : **Depth** controlled Nucleation

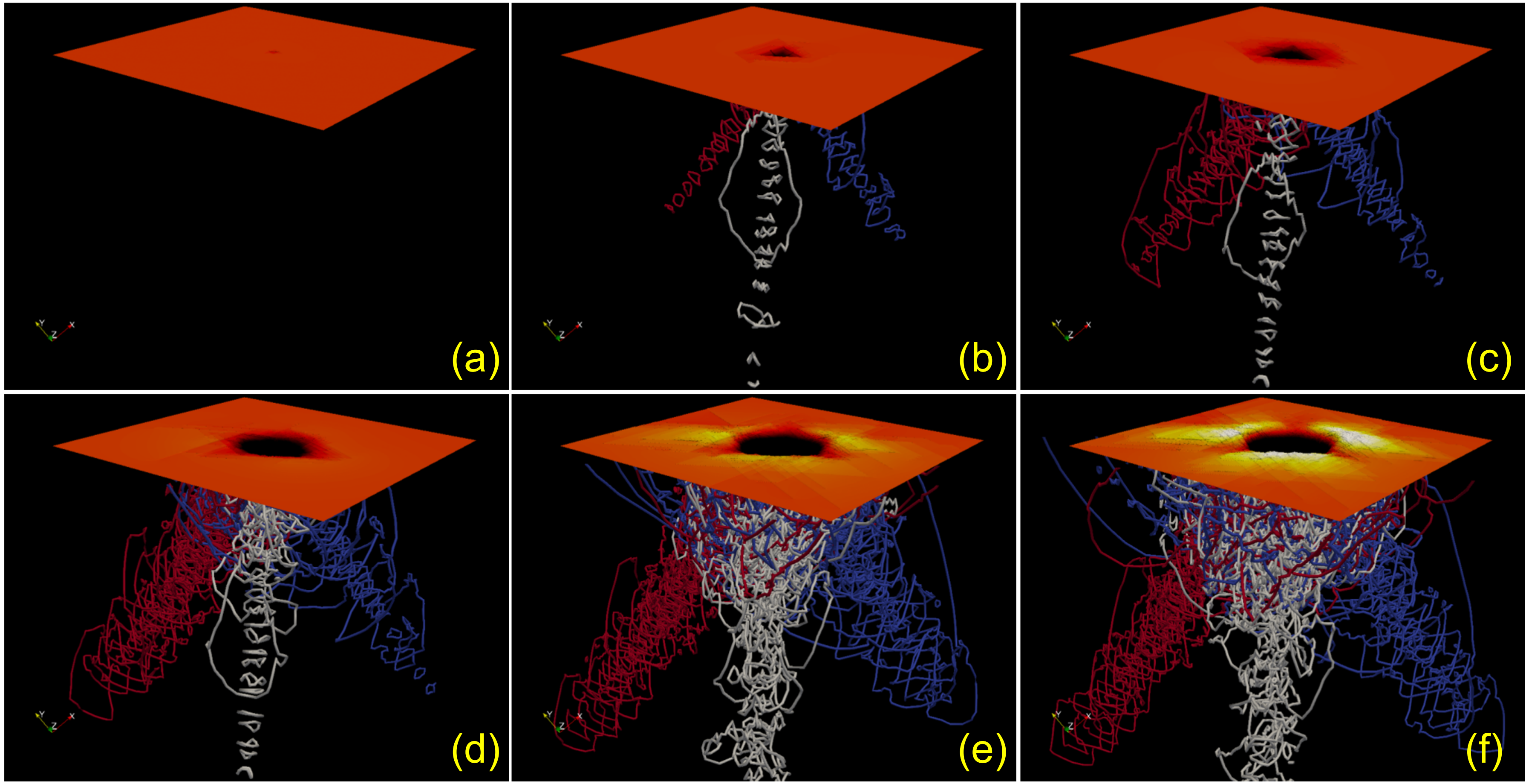
Cross-slip probability
(effect of Temperature)

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

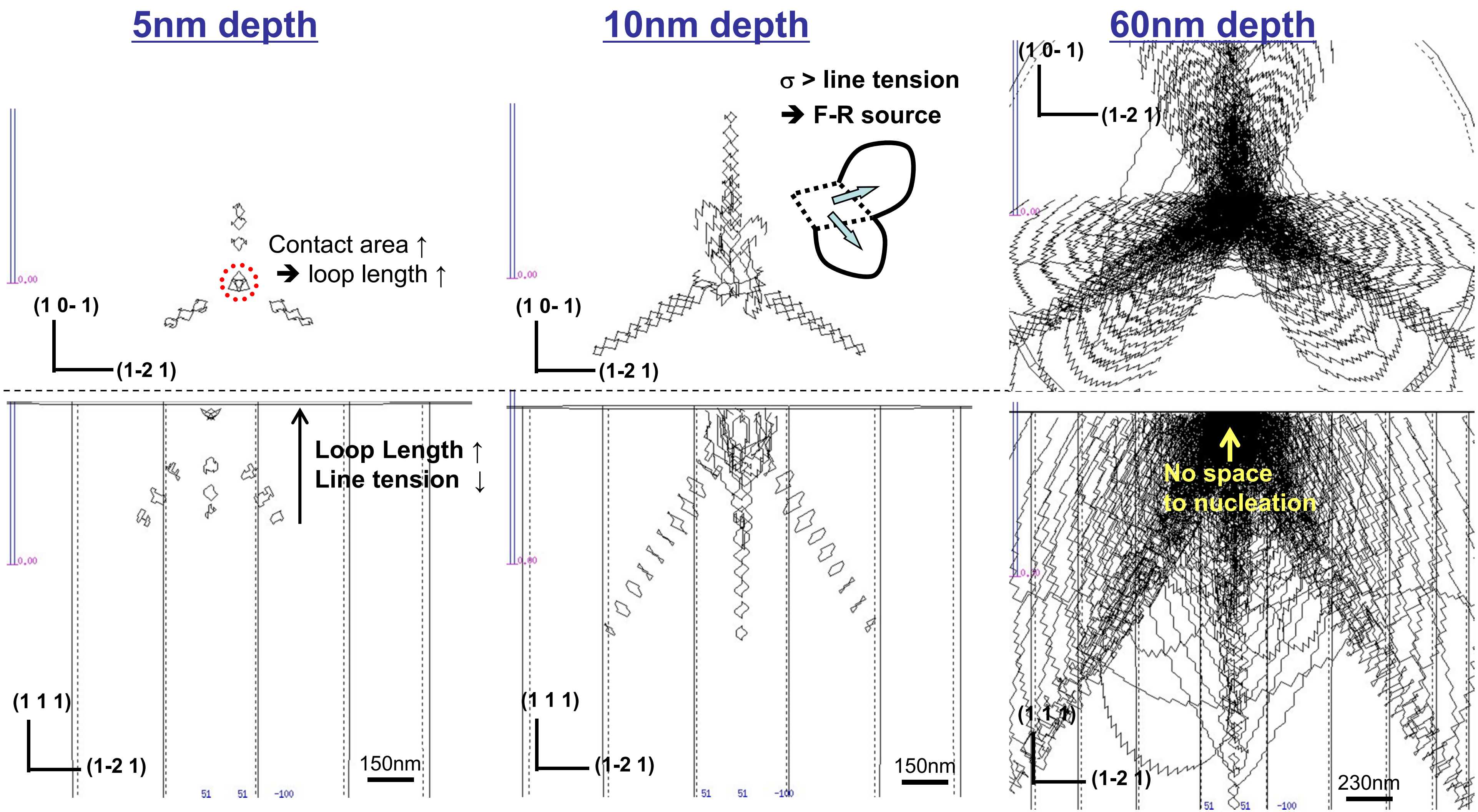
$$\tau_{III} = \infty(no), \quad 640MPa(Hard), \quad 32MPa(Easy)$$

Dislocation Dynamics simulations




(a)
(b)
(c)
(d)
(e)
(f)

(111) Spherical indentation
Dislocation evolution (MD global crit. + no cross-slip)



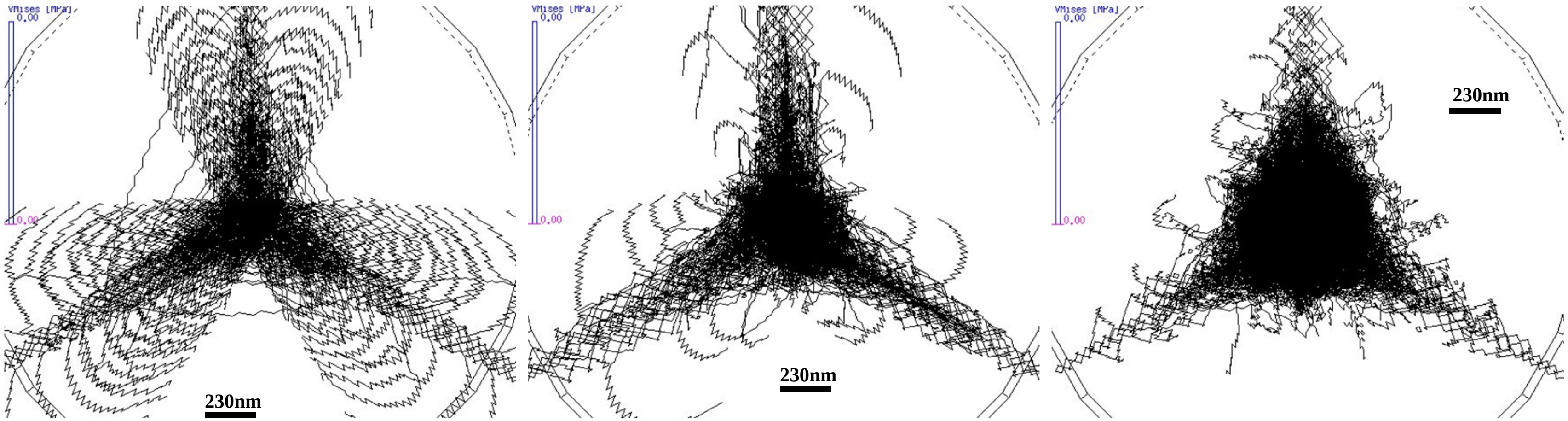
Nucleation only
(similar to MD)

Nucleation and
Frank-Read sources

Frank-Read sources only

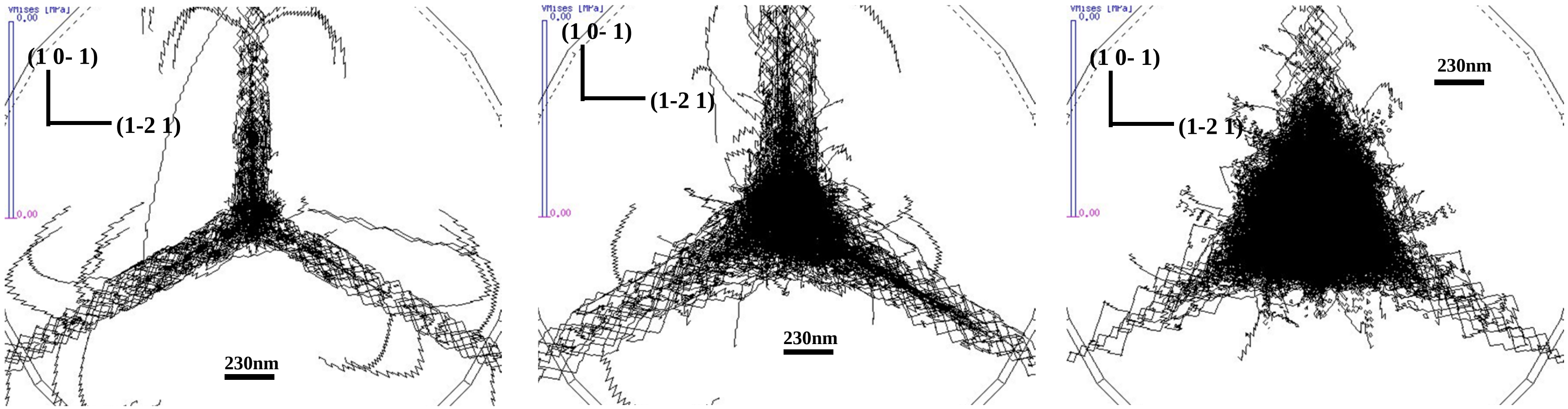
(111) Spherical indentation
Cross-slip effect (MD global crit.)

Before unloading (60nm depth)



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

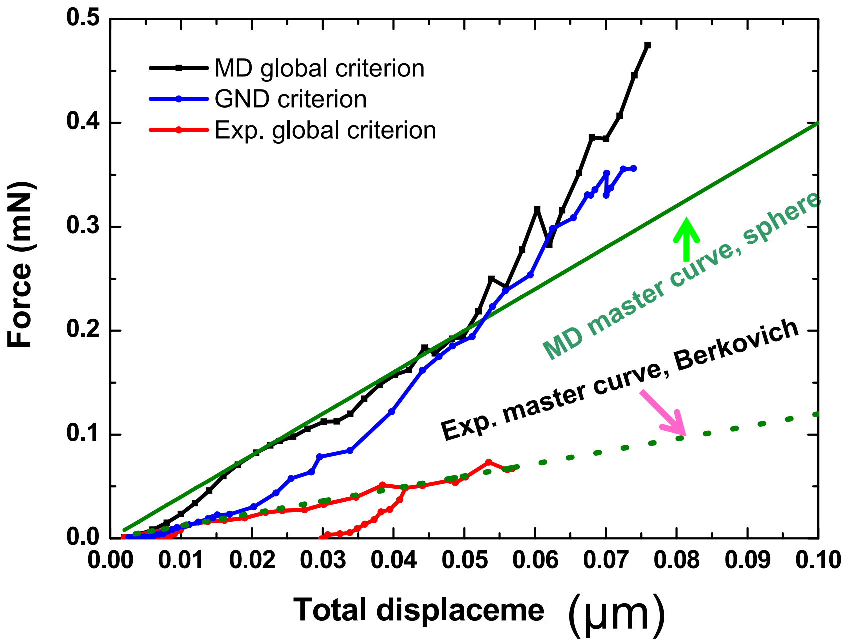
After unloading (60nm depth)



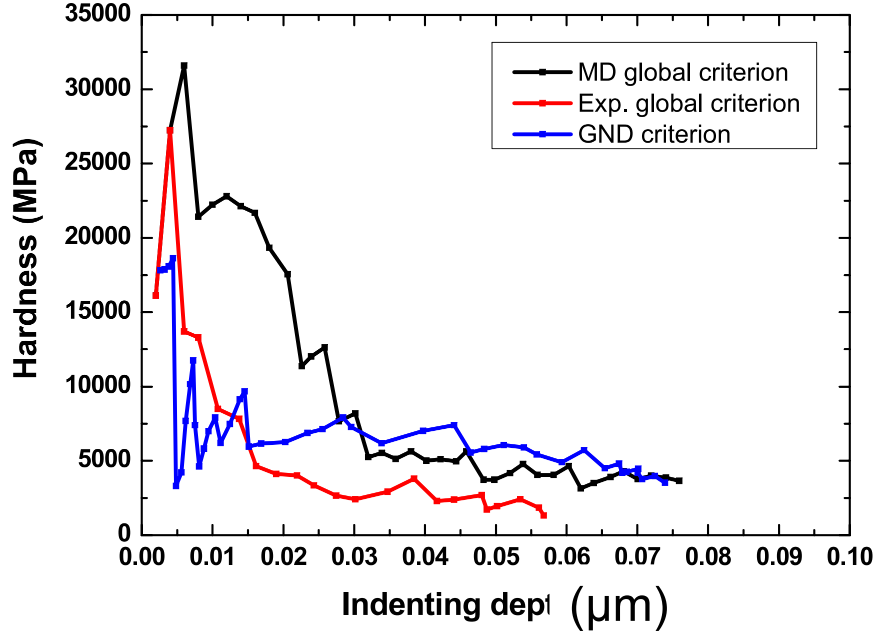
Cross-slip↑ ➔ more irreversible micro structure

(111) Conical indentation : Force-Displacement response
(exp. Nucleation crit.)

Total Force



Hardness



MD global crit.
GND crit.
} ➔Two phase behavior (linear to parabolic)

Exp. global crit. ➔ single behavior (≈ linear response)

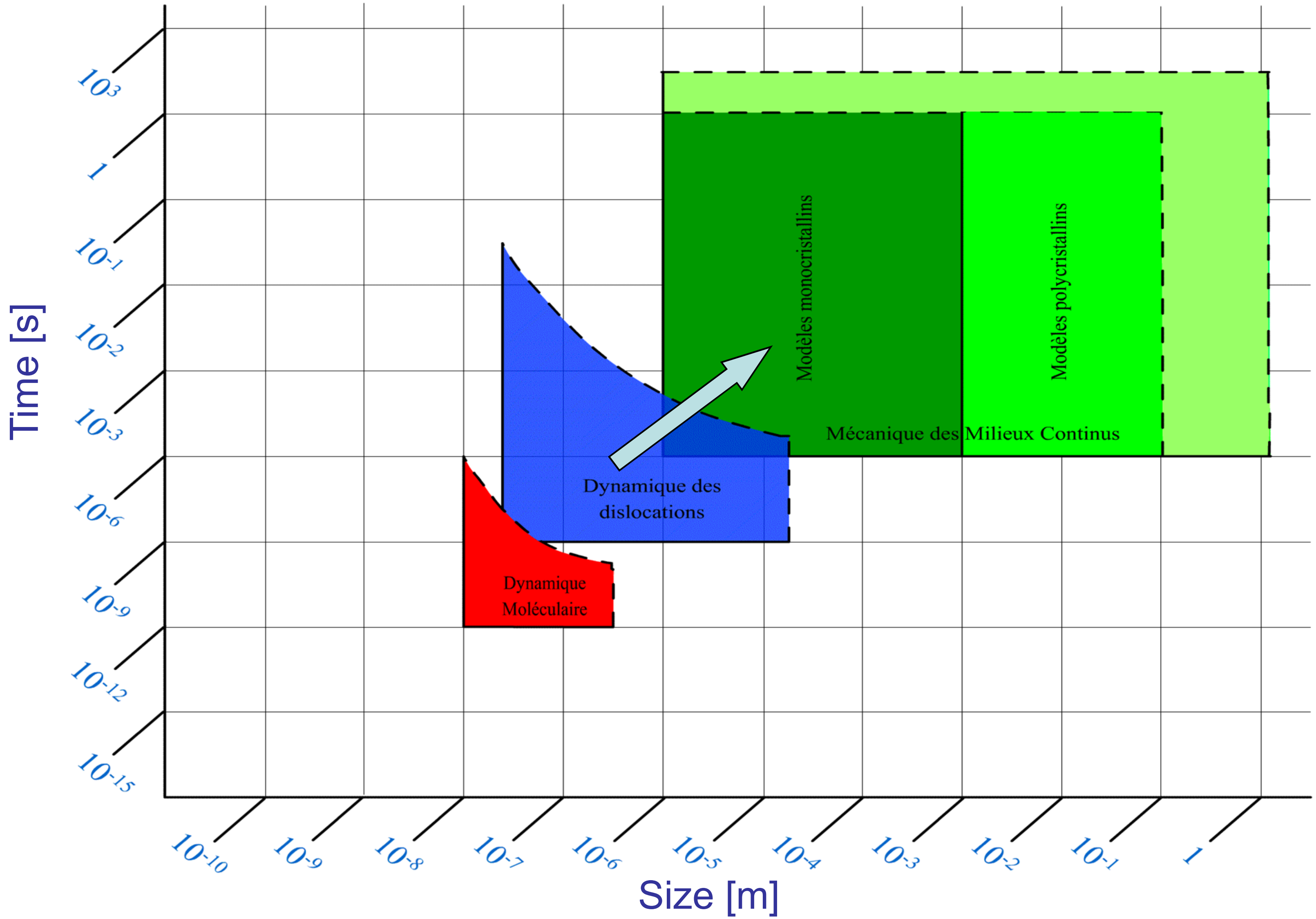
Hardness : Decreases with depth

Exp. global crit. ➔ long range decreasing

Indentation Size Effect

3D simulation of nanoindentation

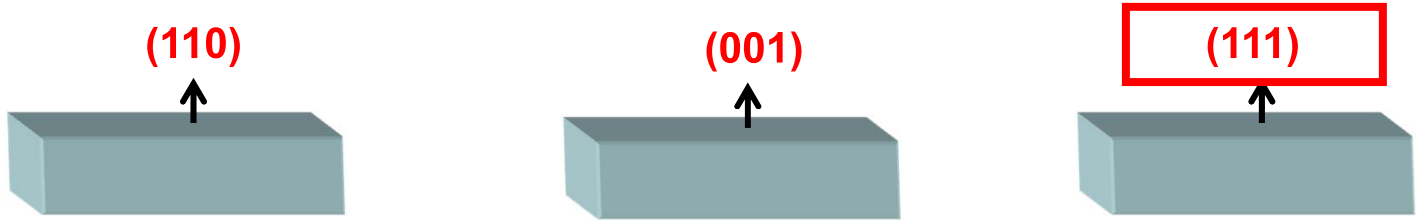
Scale Transition #2 : From Dislocation Dynamics to Continuum Mechanics



Sample preparation

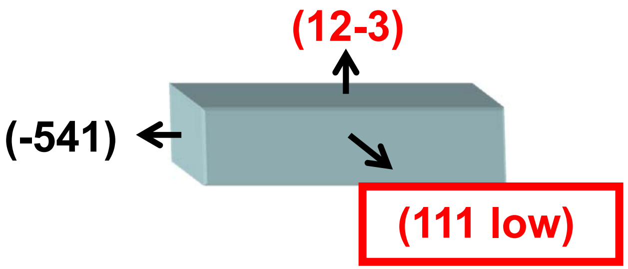
Crystal ILL : (110), (001), (111) surface orientation

Cut by spark erosion from bulk single crystal **(high ρ_{ini})**



Crystal B. : (123), (111low) surface orientation

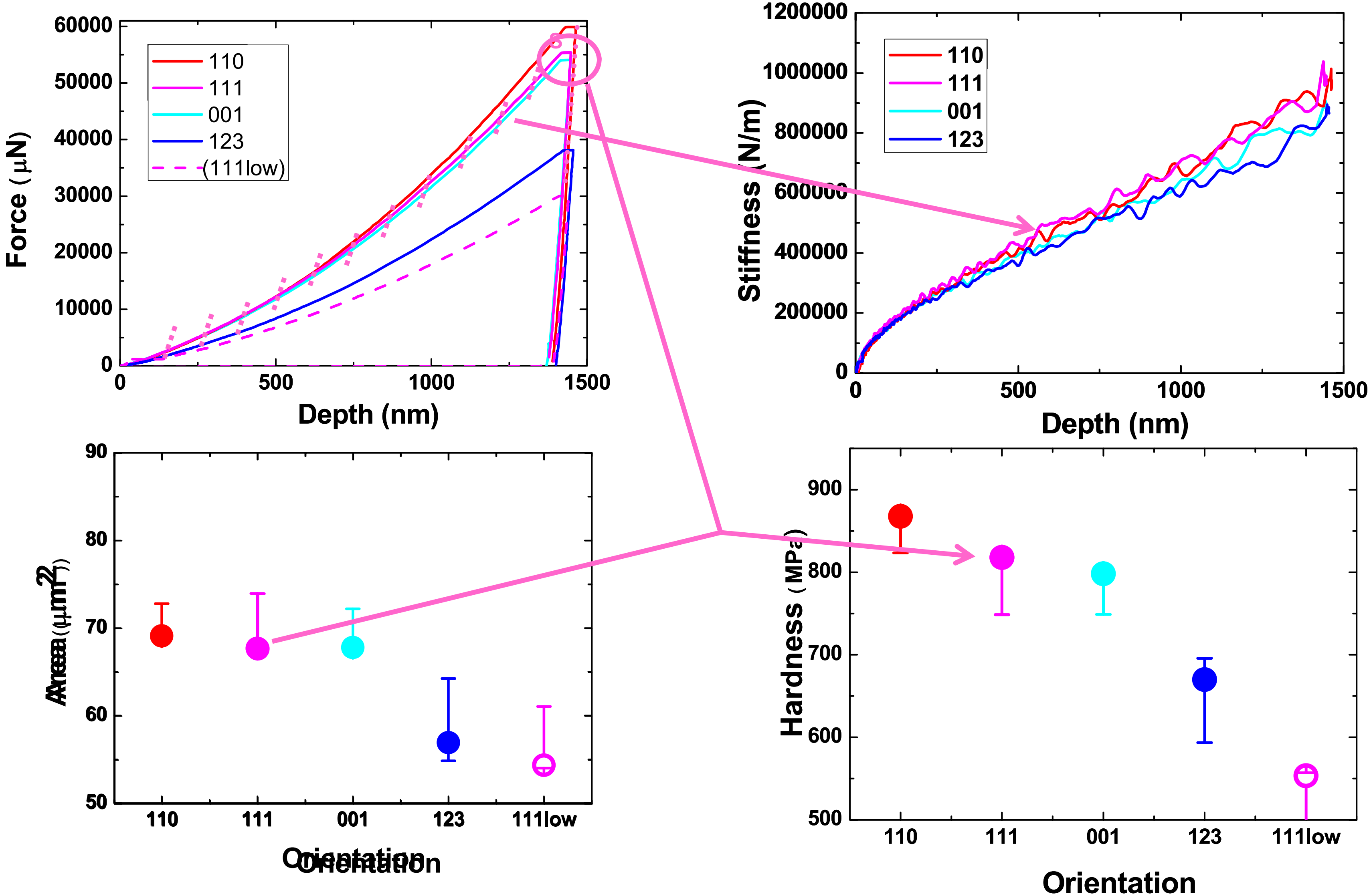
Grown from high purity Cu using Bridgman technique **(low ρ_{ini})**



- 4 surface orientations
- 2 initial dislocation densities for (111) orientation

Experimental data (conical indentation)

Indentation loading curves

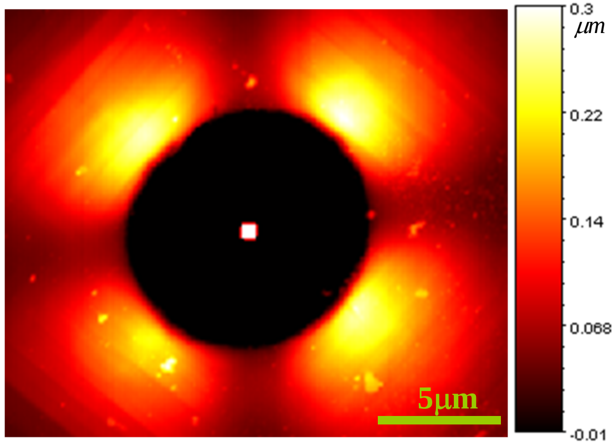


Strong effect of initial dislocation density & Weak effect of orientation

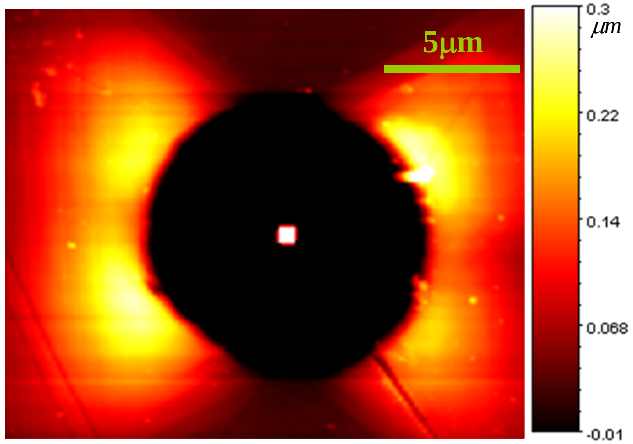
Experimental data (conical indentation)

Surface morphologies (AFM)

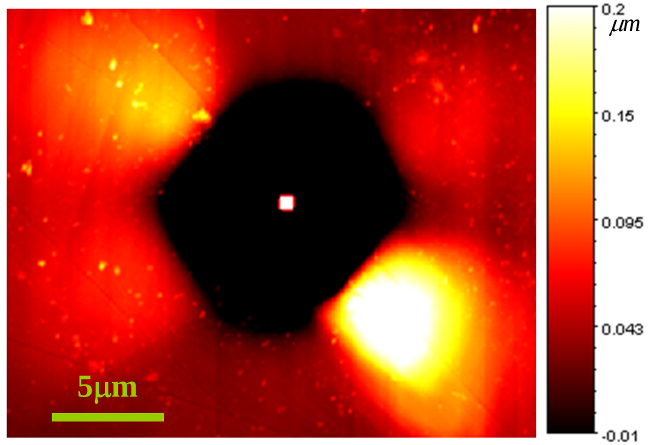
(001) Surface



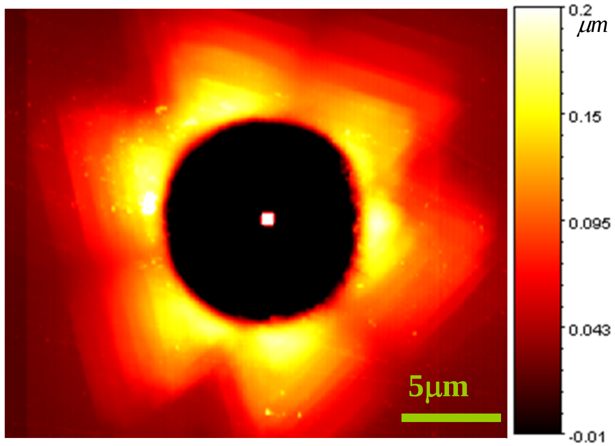
(110) Surface



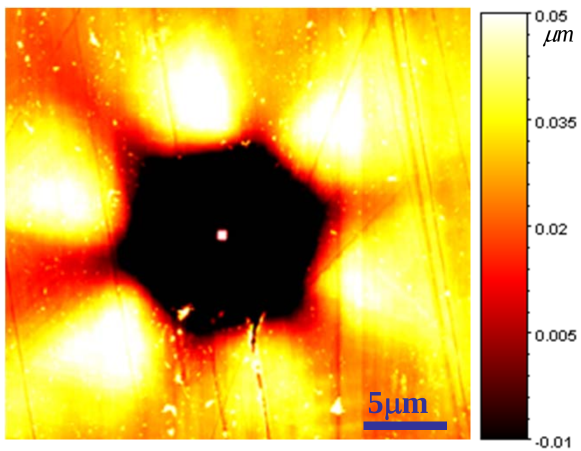
(123) Surface



(111) Surface (highρ_{ini})



(111) Surface (lowρ_{ini})



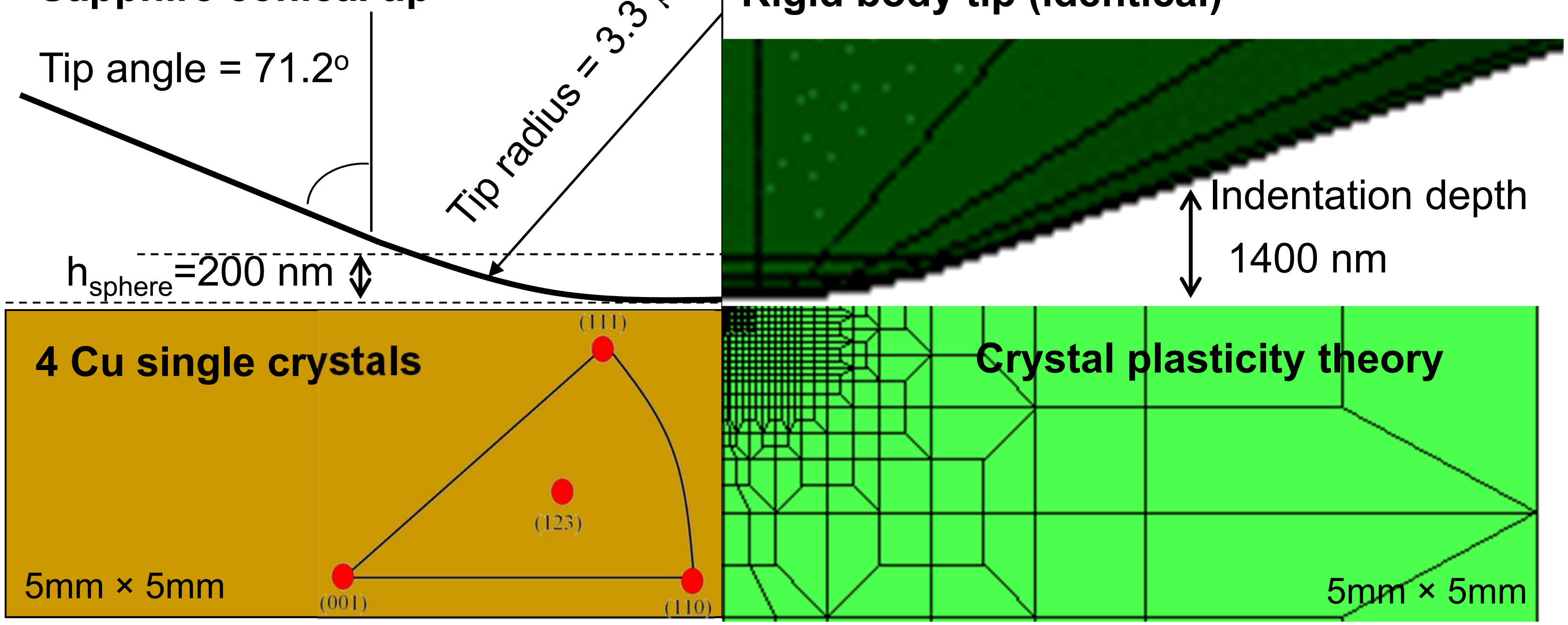
Surface morphology strongly affected by

Surface orientation

To check by FEM modelling

Nanoindentation procedure

	Experiment	**FEM**
Tip	**Sapphire conical tip**	**Rigid body tip (identical)**



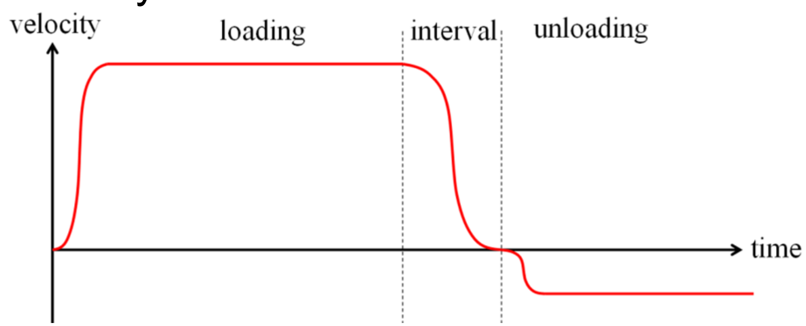
4 Specimens

Loading condition

Strain rate control

$$\dot{\varepsilon} = 5 \times 10^{-2} / \sec$$

Velocity control



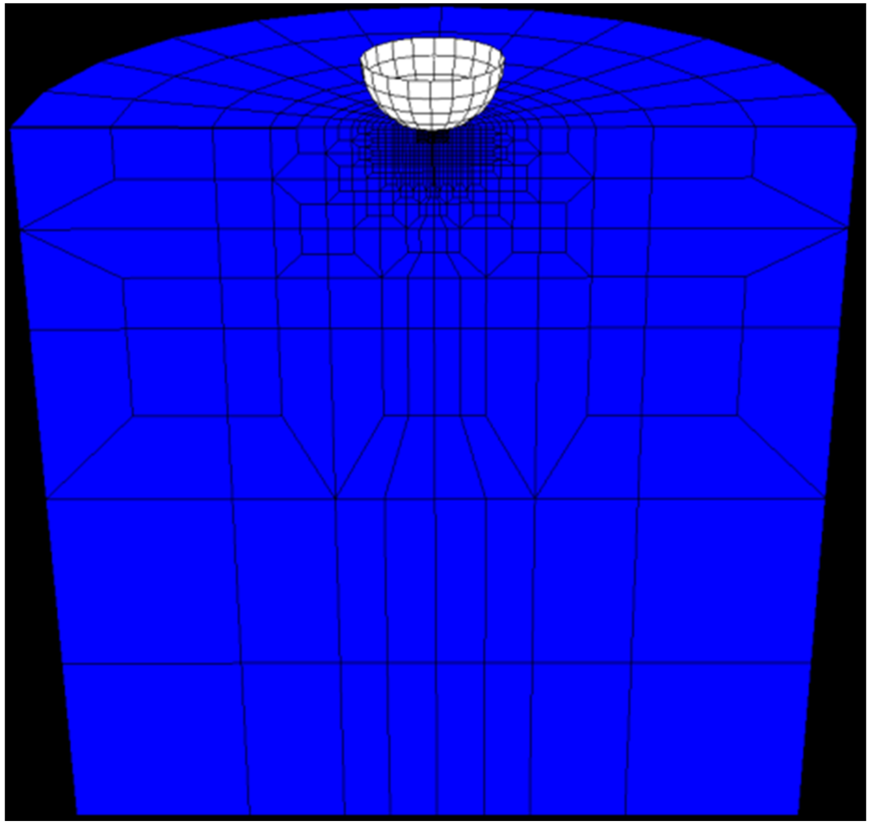
Crystal Plasticity Modeling

Dislocation density based model

$$\dot{\gamma}^{(s)} = \dot{\gamma}_0^{(s)} \left(\frac{\tau^{(s)}}{\tau_\mu^{(s)}} \right)^{1/m}$$

$$\tau_\mu^{(s)} = \mu b \sqrt{\sum_{u=1}^{12} a_{su} \rho^{(u)}}$$

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



3D ABAQUS simulations

Crystal plasticity model

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

soit

$$\boxed{\dot{\tau}_\mu^{(s)} = \sum_{u=1}^{12} h_{su} \dot{\gamma}^{(u)}}$$

Parameters used in the crystal plasticity model

Elastic properties for $\mathbf{T}^* = \mathbf{C}^E[\mathbf{E}^*]$

From text book

C_{11}	168.4 GPa
C_{12}	121.4 GPa
C_{44}	75.4 GPa

Initial dislocation density and Surface orientation

From X-ray results

Surface Orientation	FWHM (111) (θ scan °)	Relative disl. density	Initial density (total)
(011)	1.35	6 ~ 8	Unknown
(111)	0.57	3 ~ 4	
(001)	0.56	3 ~ 4	
(123)	0.2	1	
(111low)	0.08	0.2 ~ 0.3	

Hardening parameters

From DD theory

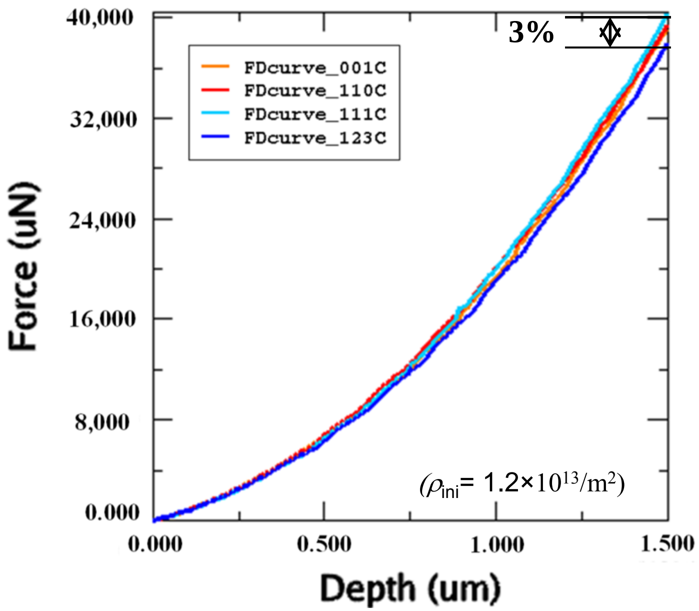
$$\tau_{\mu}^{s} = \mu b \sqrt{\sum_{p=1}^{12} \alpha^{sp} \rho^{p}}$$

$$\dot{\rho}^{s} = \frac{1}{b}\left(\frac{\sqrt{\sum_{p=1}^{12} a^{sp} \rho^{p}}}{K_g} - 2 y_c \rho^{s} \right) \left| \dot{\gamma}^{s} \right|$$

b	2.56×10^{-10} m	y_c	1.43×10^{-9} m
$\alpha_{1\sim6}$	Taylor	(0.09, 0.09, 0.09, 0.09, 0.09, 0.09)	
	Hetero	(0.122, 0.122, 0.07, 0.137, 0.122, 0.625)	
$a_{1\sim6}$ K	Normal	(0.01, 0.4, 0.4, 0.75, 1.0, 0.4), K=36	
	Same	$a_{1\text{-}6}$ same as $\alpha_{1\sim6}$, K=36	
	High K	(0.01, 0.4, 0.4, 0.75, 1.0, 0.4), K=100	

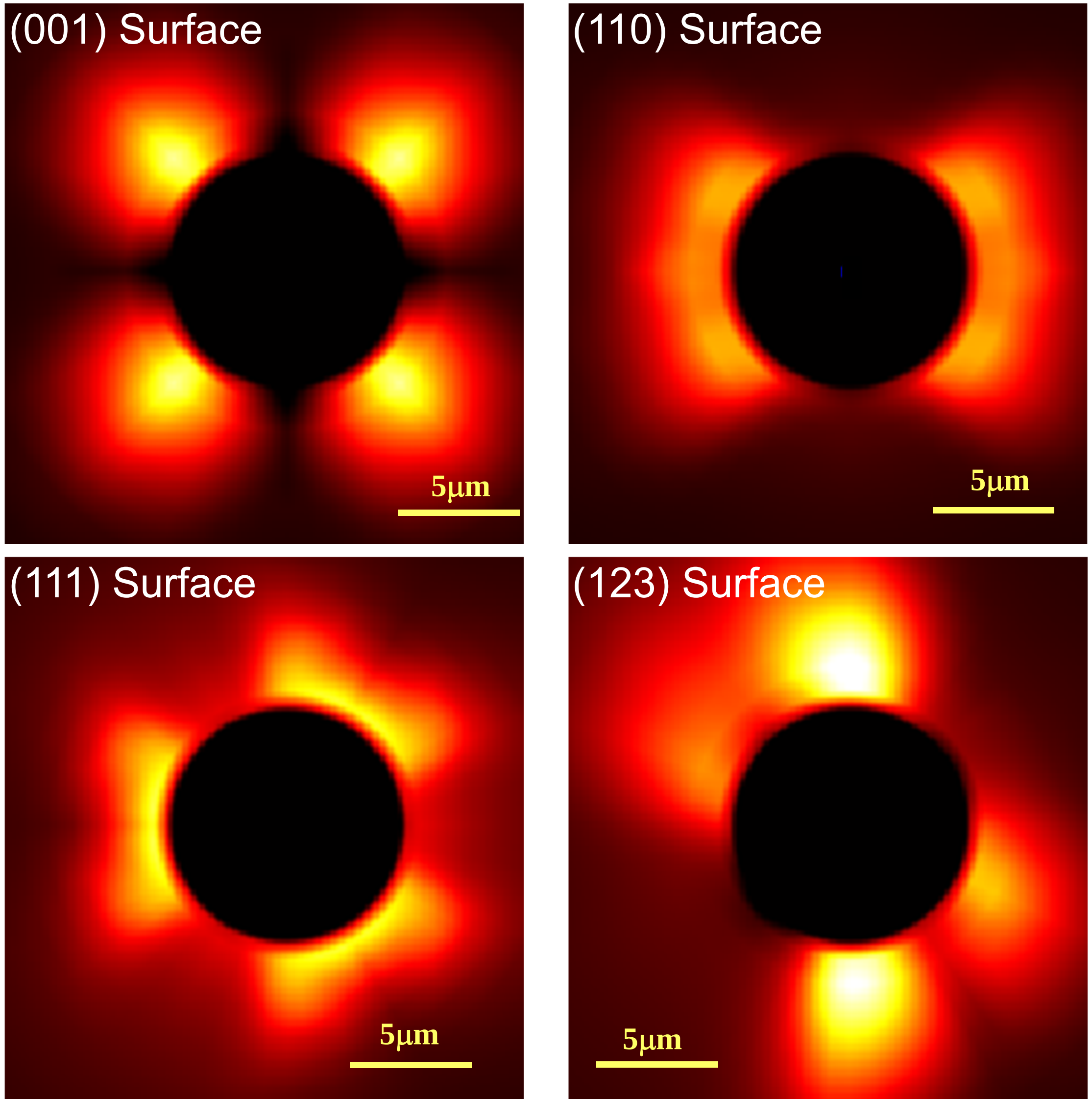
M. Fivel, PhD Thesis, (1997) L. Kubin, B. Devincre and T. Hoc, Acta Mater., (2008)

Effect of orientation



Weak effect on loading curve

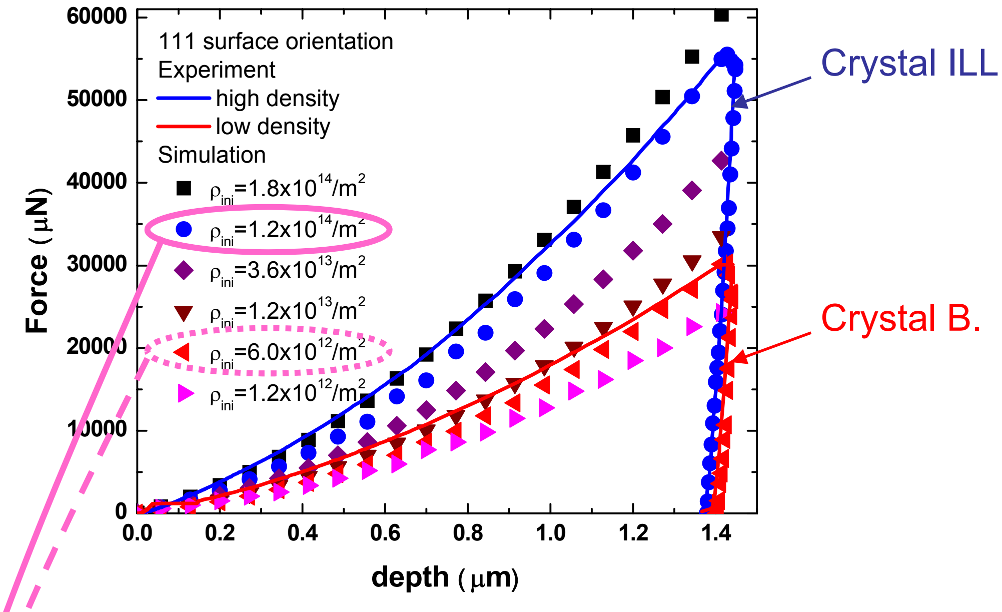
(Hetero / Same)

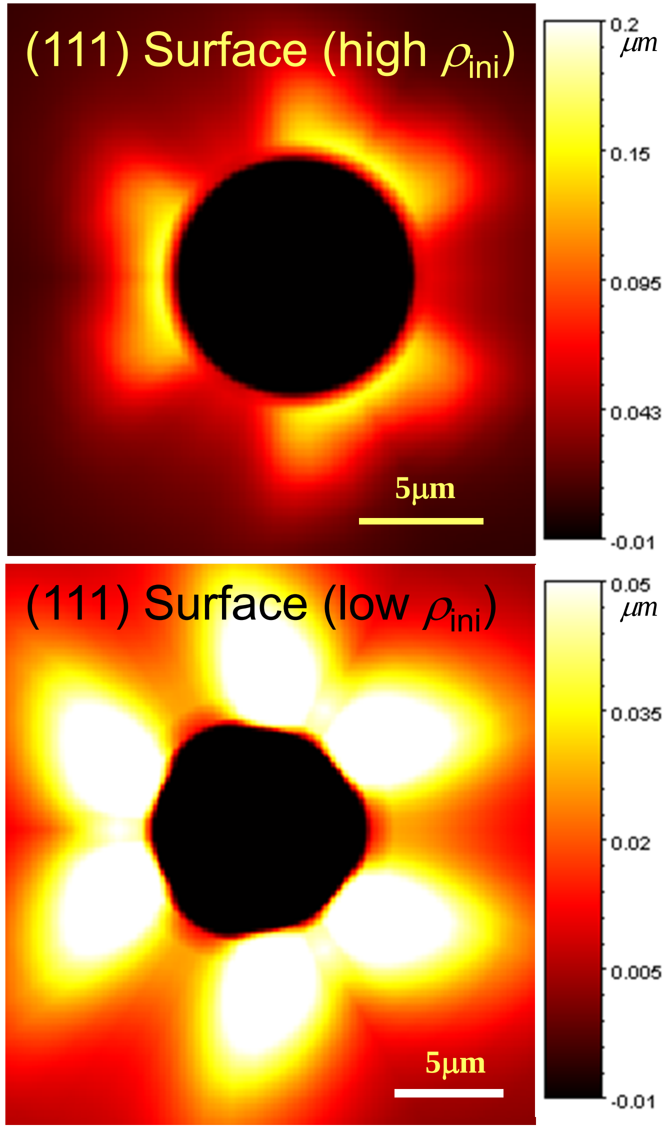


Strong effect on surface displacement

Effect of dislocation density for (111) orientation

(Hetero / Same)





Strong effect on loading curve

Optimized initial dislocation density

ρ_{ini} = 6.0×10^12/m^2 for (111low)

ρ_{ini} = 1.2×10^14/m^2 for (111high)

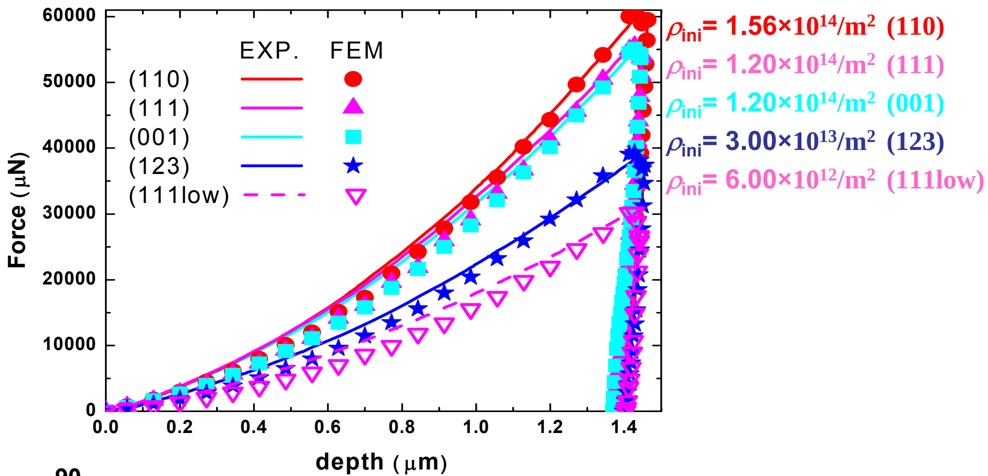
Strong effect on surface shape

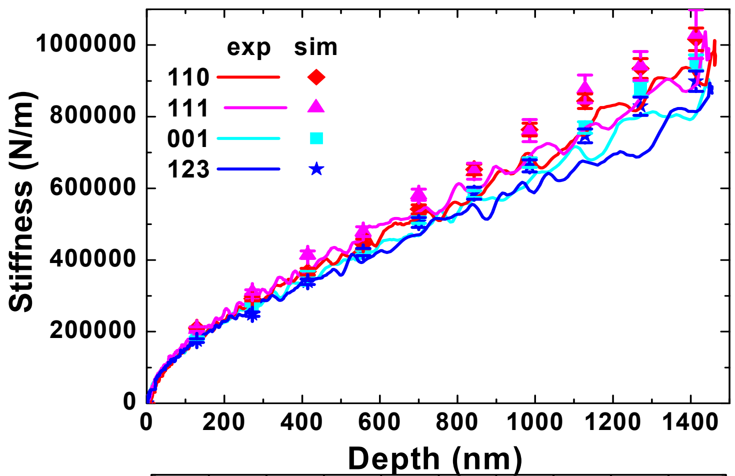
What about the other orientations ?

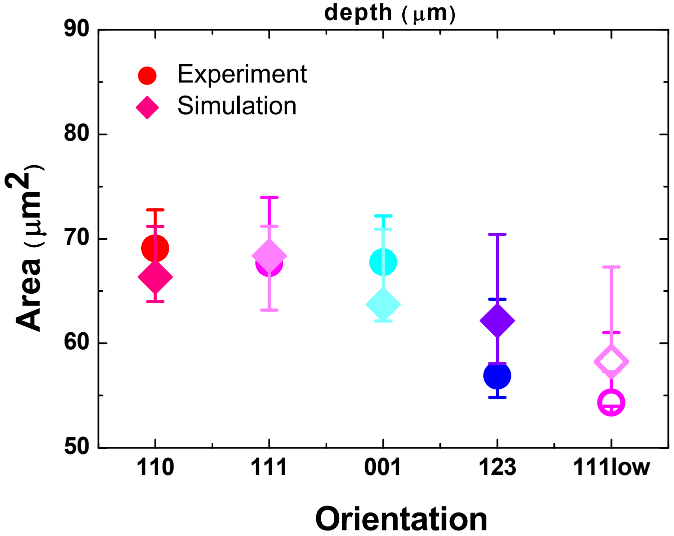
Crystal Plasticity Modeling / Comparison with experiments

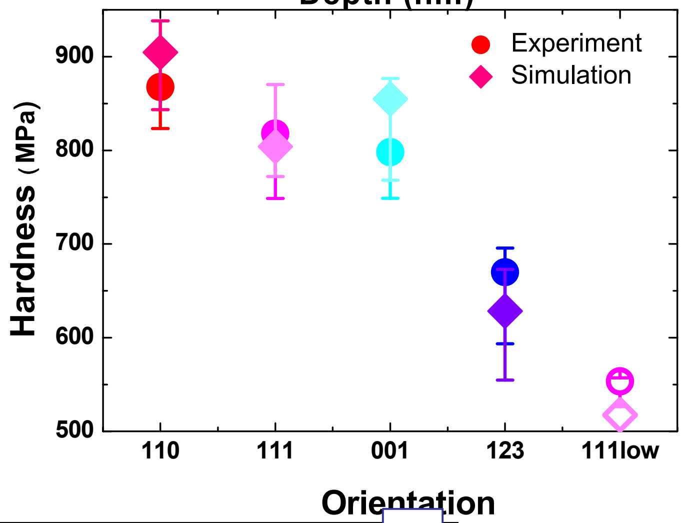
Comparison of quantitative results

(hetero / same)







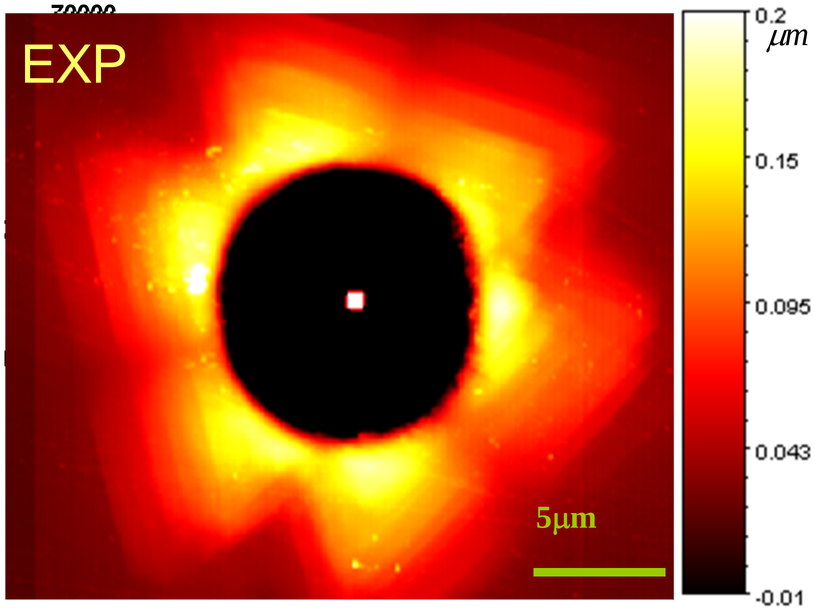


Optimized initial densities

(011)	1.56×10^{14}/... x5	(123)	3.00×10^{13}/... 1
(111)	1.20×10^{14}/... x4	(111low)	6.00×10^{12}/... x.2
(001)	1.20×10^{14}/... x4		

☑ X-Rays

Effect of hardening parameters for (111) orientation



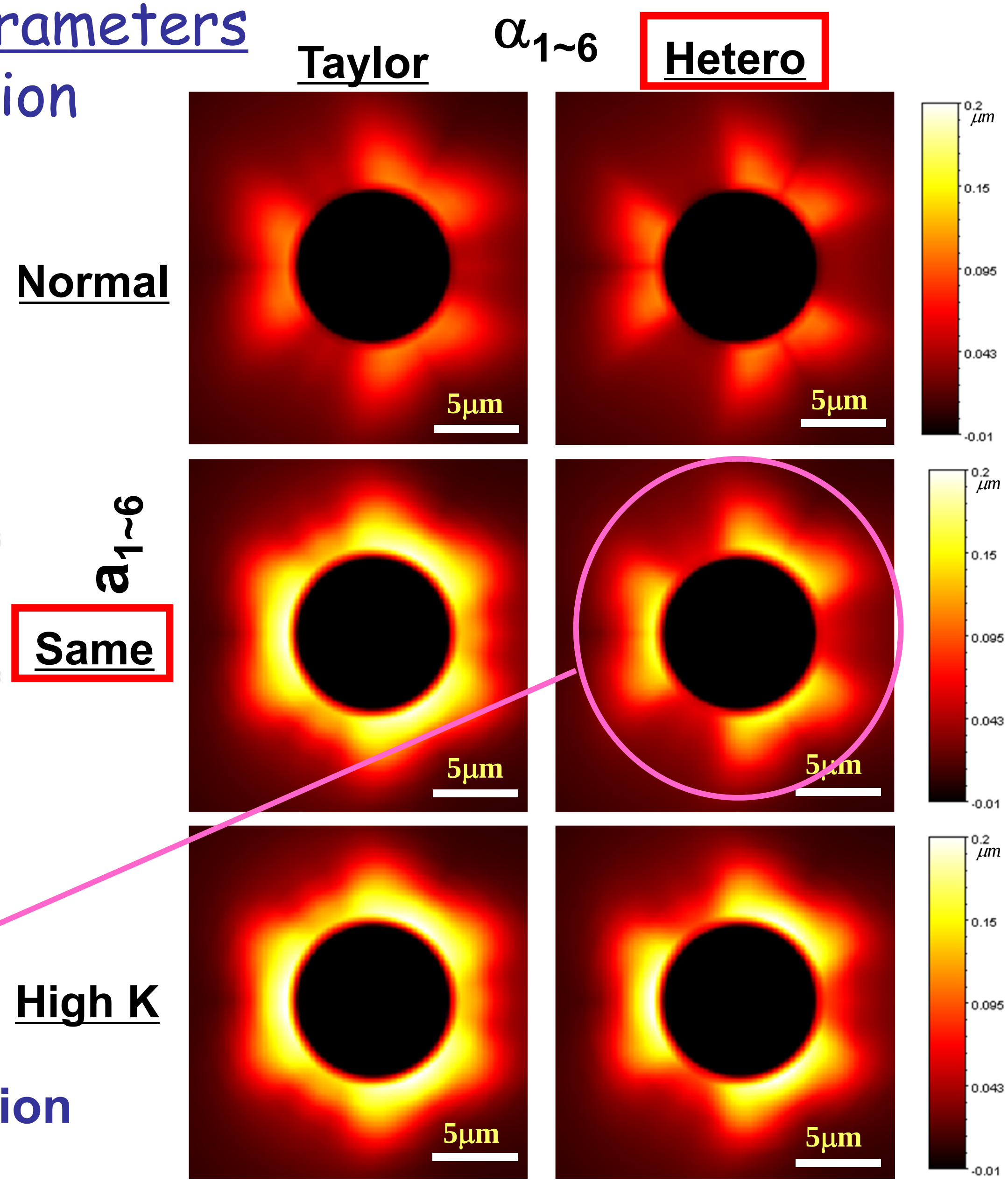
depth (μm)

Obtained hardening parameter

Weak effect on loading curve

Hetero + Same

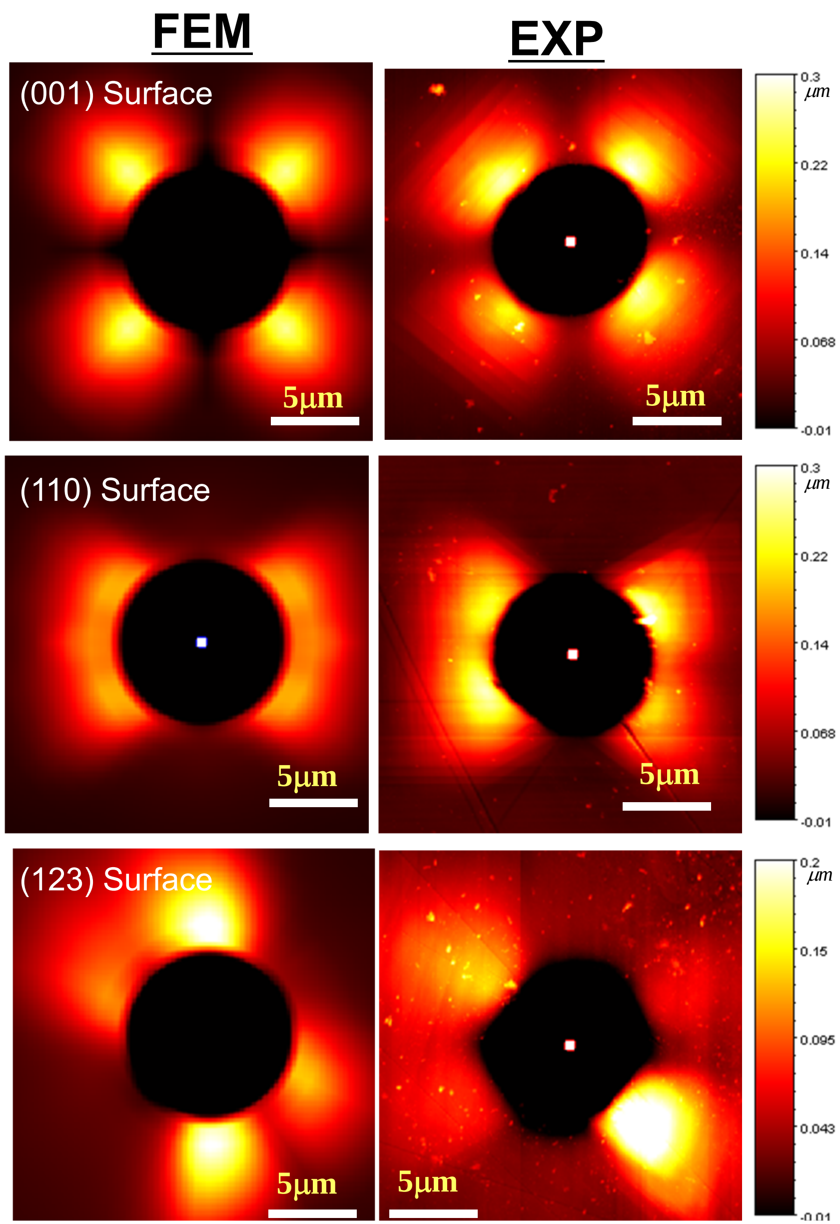
Need to check for other orientation

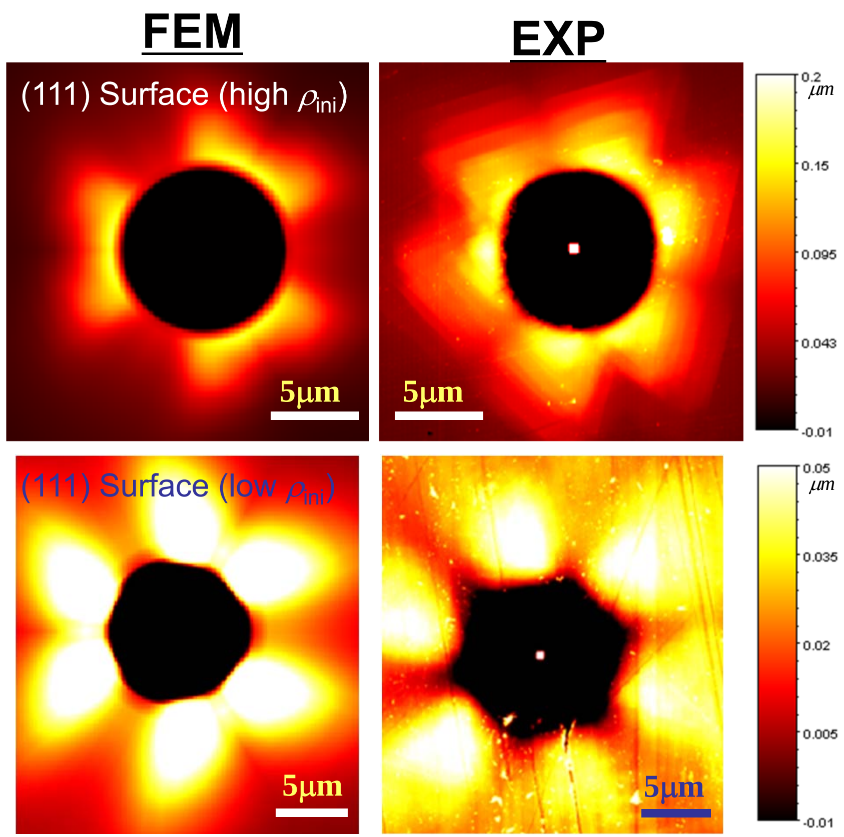


Influence surface morphology

Crystal Plasticity Modeling / Comparison with experiments

Comparison of Surface morphology (hetero / same)





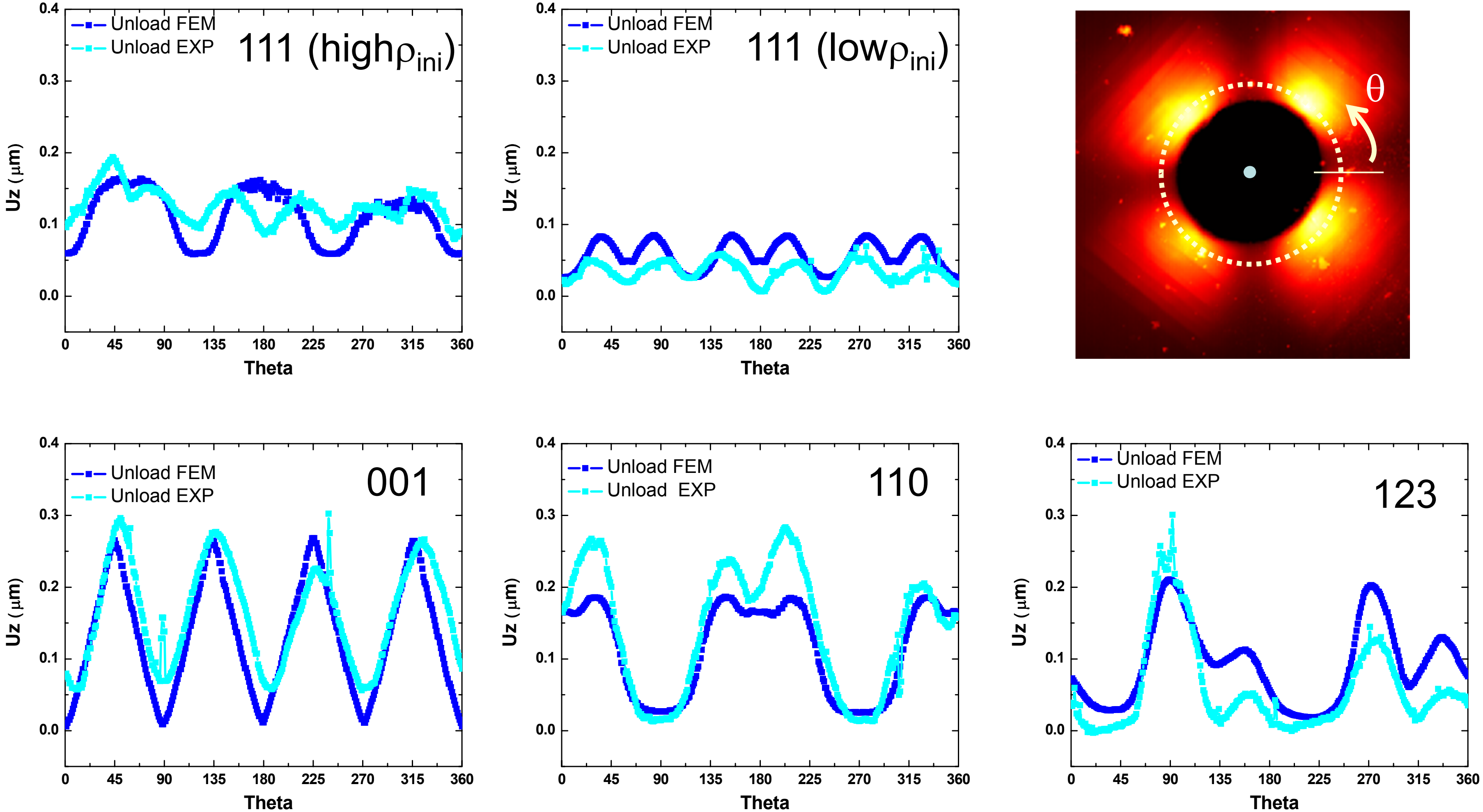
Confirmed hardening parameter

b	2.56×10^{-10} m	y_c	1.43×10^{-9} m
$\alpha_{1\sim6}$	Hetero	(0.122, 0.122, 0.07, 0.137, 0.122,0.625)	
$a_{1\sim6}$ K	Same	same as $\alpha_{1\sim6}$, K=36	

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

$$\mathbf{T}^* = \mathbf{C}^{\mathrm{E}}\left[\mathbf{E}^*\right]$$

C_{11}	168.4 GPa
C_{12}	121.4 GPa
C_{44}	75.4 GPa

Initial dislocation density and Surface orientation

Surface Orientation	Relative disl. density	Initial density (total)
(011)	6 ~ 8	$1.56\times10^{14}/m^2$
(111)	3 ~ 4	$1.20\times10^{14}/m^2$
(001)	3 ~ 4	$1.20\times10^{14}/m^2$
(123)	1	$3.00\times10^{13}/m^2$
(111low)	0.2 ~ 0.3	$6.00\times10^{12}/m^2$

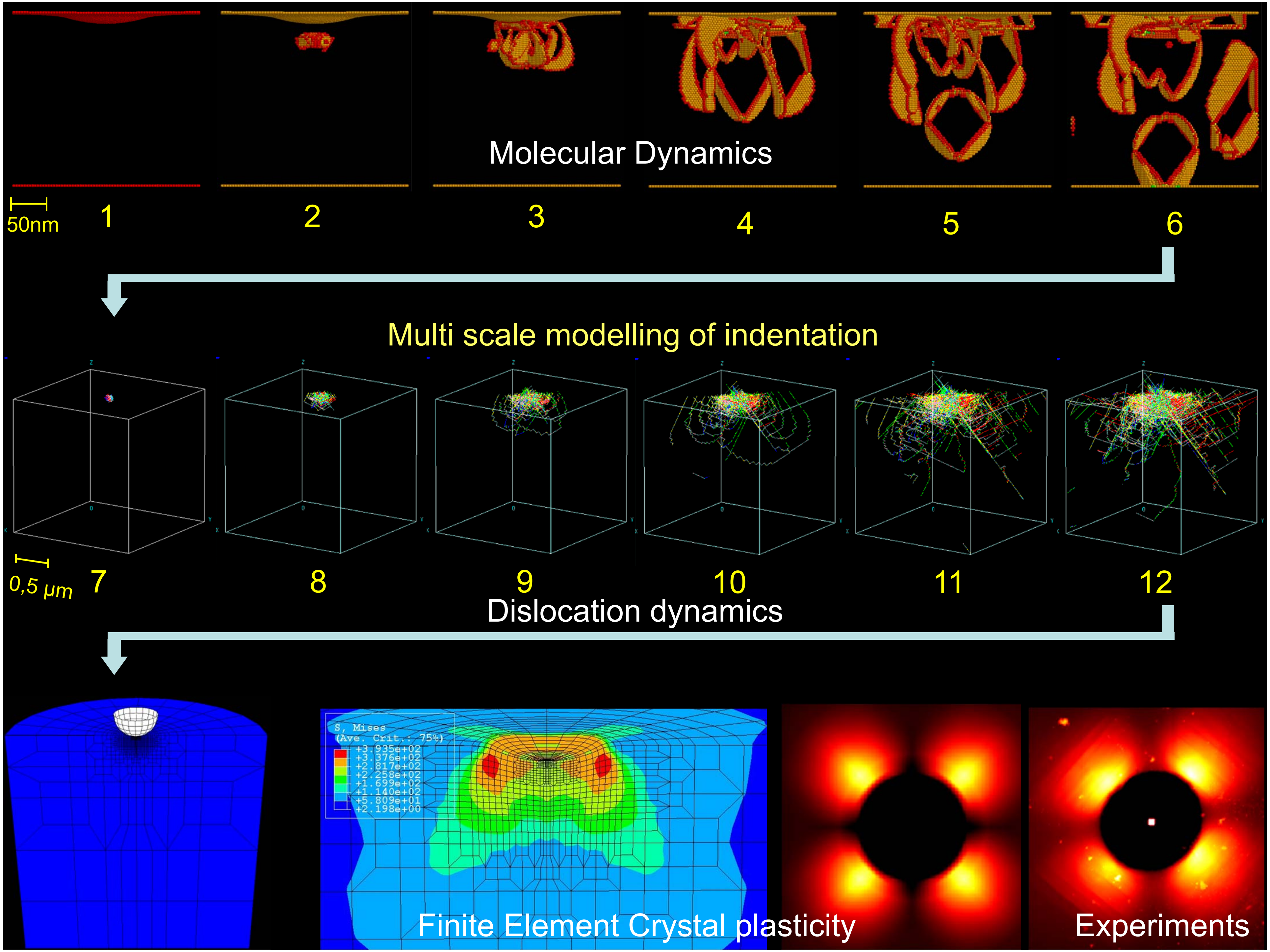
Hardening

$$\tau_{\mu}^{s} = \mu b \sqrt{\sum_{p=1}^{12} \alpha^{sp} \rho^{p}}$$

$$\dot{\rho}^{s} = \frac{1}{b}\left(\frac{\sqrt{\sum_{p=1}^{12} a^{sp} \rho^{p}}}{K_g} - 2 y_c \rho^{s}\right)\left|\dot{\gamma}^{s}\right|$$

b	2.56×10^{-10} m	y_c	1.43×10^{-9} m
$\alpha_{1\sim6}$	Hetero	(0.122, 0.122, 0.07, 0.137, 0.122,0.625)	
$a_{1\sim6}$ K	Same	same as $a_{1\sim6}$, K=36	

L. Kubin, B. Devincre and T. Hoc, Acta Mater., (2008)



Molecular Dynamics
50nm
1
2
3
4
5
6
Multi scale modelling of indentation
0,5 µm
7
8
9
10
11
12
Dislocation dynamics
S, Mises
(Ave. Crit.: 75%)
+3.935e+02
+3.376e+02
+2.817e+02
+2.258e+02
+1.699e+02
+1.140e+02
+5.809e+01
+2.198e+00
Finite Element Crystal plasticity
Experiments

Challenge & Perspectives

Challenge	Perspectives
Too large computation time - Limited cumulated strain	Parallel computing - ParaDis, Paranoid, Tridis, Numodis,..
Large deformation, large rotations - jogs, …	Updating Schmid factor Updating dislocation positions, slip planes
Polycrystal plasticity - Static and dynamic interfaces	Accounting for grain boundary
Taking into account climb	Coupling with diffusion theory Dealing with heterogeneous time steps
Dislocation core effect	Rules to be defined by MD or TEM
Real materials impurities, solutes, etc..)	Rules needed from experiments