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DE LA RECHERCHE À L'INDUSTRIE



# PREDICTION OF INTERGRANULAR MICRO-CRACK INITIATION INDUCED BY THE IMPINGEMENT OF PERSISTENT SLIP BANDS ON GRAIN BOUNDARIES

**Jérôme HAZAN, Maxime SAUZAY**

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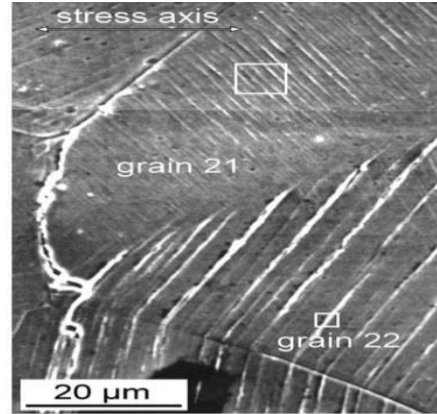
TMS 2018 - MARS 12TH 2018

- **CONTEXT & GOALS**
- METHODS
- RESULTS
- CONCLUSIONS & WORK IN PROGRESS

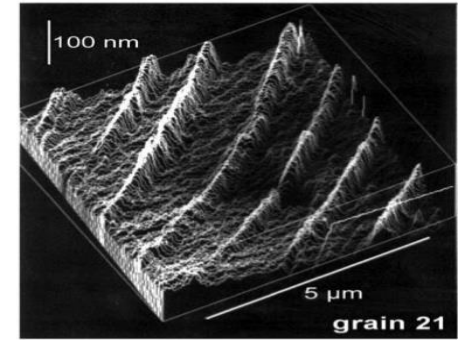
## Cyclic deformation induces localization of plastic slip within Persistent Slip Bands (PSBs) for grains oriented for single slip

⇒ Formation of a two phase microstructure (if  $|\tau_p| = \tau_{PSB}$ ) :

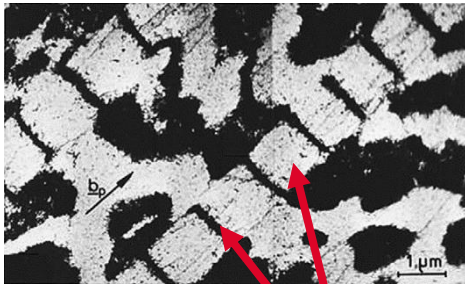
- Elastic matrix
- Elastic-plastic bands (PSBs)



[Man et al. 2002]



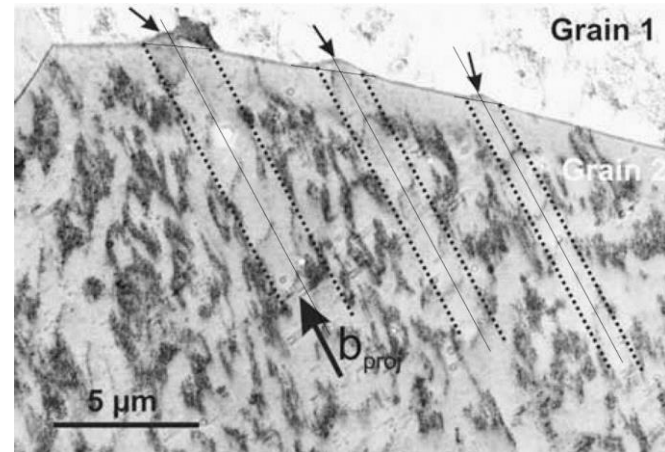
316L SS polycrystal



Copper single crystal

[Mughrabi 1979]

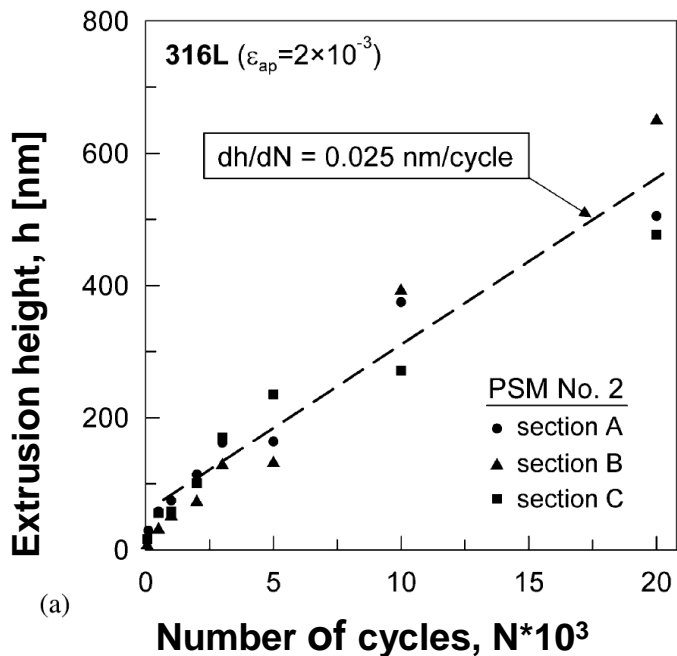
Poor channels ( $\sim 10^{13} \text{ m}^{-2}$ )  
 rich walls ( $\sim 10^{15} \text{ m}^{-2}$ ) :  
 Ladder like structure



Nickel polycrystal

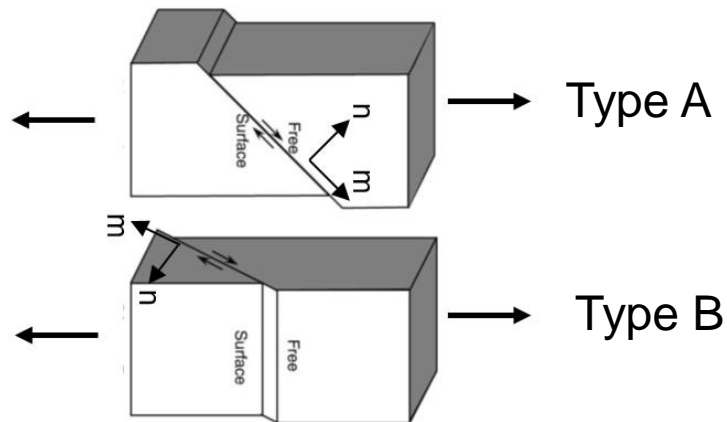
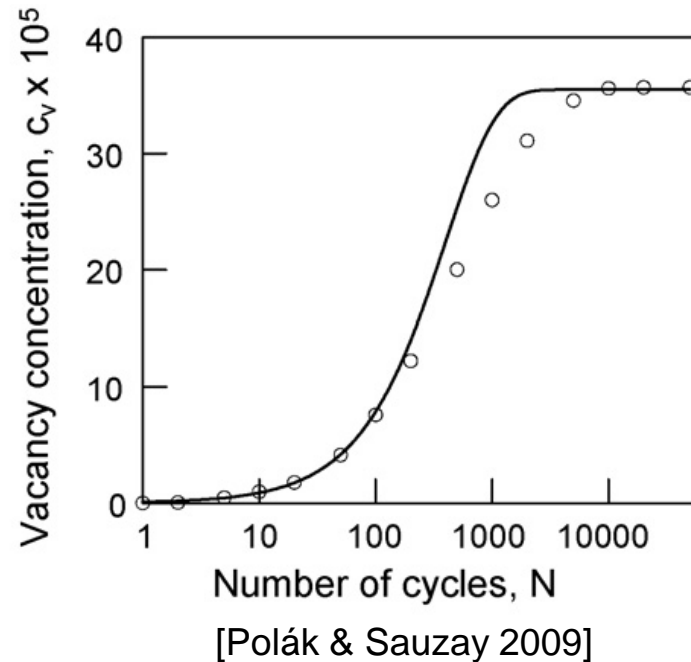
[Weidner et al. 2010]

The extrusion of PSBs is due to the production of vacancies during cyclic deformation



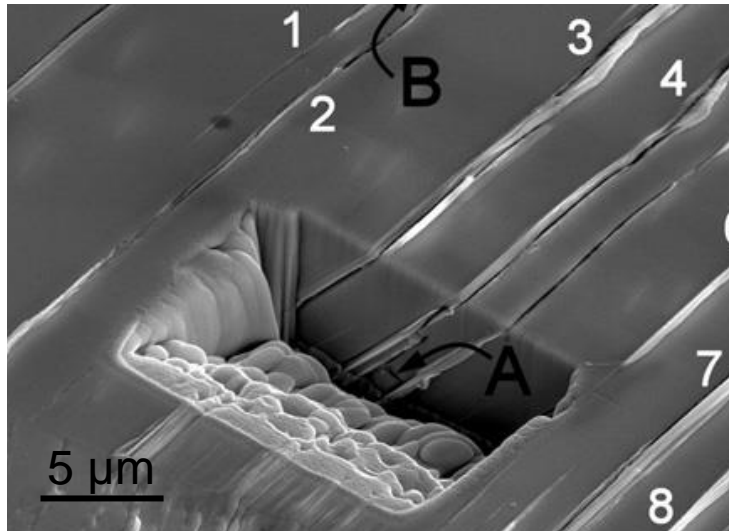
[Man et al. 2003]

Almost constant growth rate of PSBs during cycling



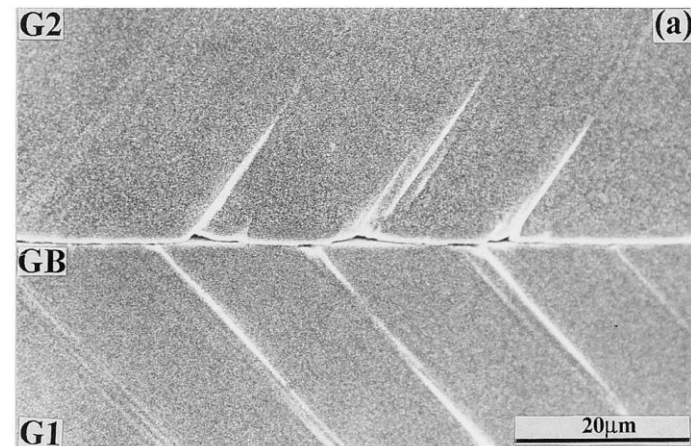
Slip localization in PSBs leads to microcrack initiation (in LCF):

Transgranular (type B):



[Polák et al. 2009]

Grain Boundaries (type A):



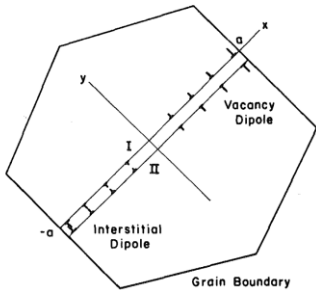
[Zhang et al. 1999]

Aim of the present work: Predicting micro-cracks initiation due to the impingement of PSBs on grain boundaries

- Prediction of GB extrusions and GB stress fields  
Transgranular initiation treated by [Liu & Sauzay 2014]

Reference models mostly based on dislocations pile-up at GB :

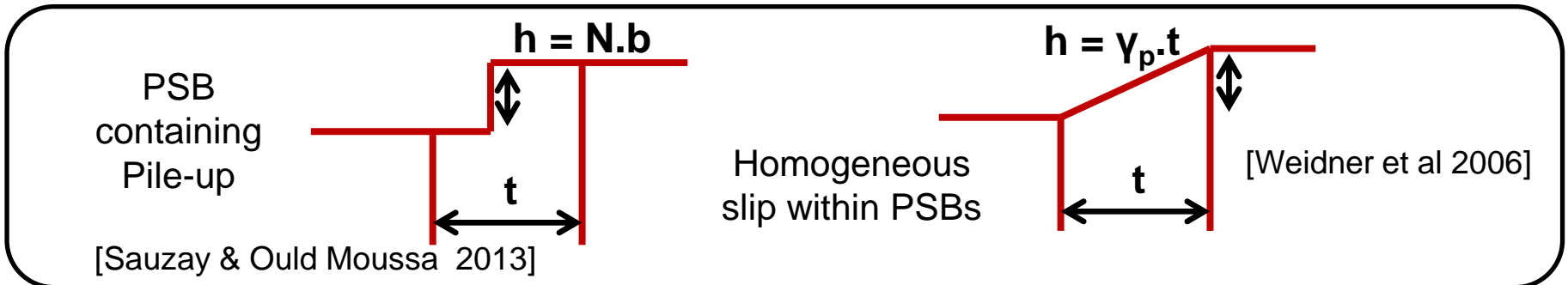
- Tanaka & Mura 1981



$$Ni = \frac{8 \mu \gamma_{eff}}{2 \pi (1 - \nu) a (\Delta\tau - 2\tau_f)^2}$$

Cyclic deformation causes ratcheting of dislocations at grain boundaries

- Sangid et al. 2011 (Molecular Dynamics input for dislocation absorption and nucleation at GB)



**Our aim: Possibility of predicting GB micro-crack initiation through PSB cyclic plasticity and vacancy production ?**

- CONTEXT & GOAL
- **METHODS**
  - **Elastic-plastic model and behavior**
  - Cohesive zone model
- RESULTS
- CONCLUSIONS & WORK IN PROGRESS



## Finite Element Calculations based on:

### ① Mixture rule of Winter:

$$\gamma_{cryst}^p = \gamma_{Mat}^p f_{v_{Mat}} + \gamma_{PSB}^p f_{v_{PSB}}$$

$$\gamma_{Mat}^p \approx 1/100 \gamma_{PSB}^p$$

$$\Rightarrow \gamma_{cryst}^p = \gamma_{PSB}^p f_{v_{PSB}}$$

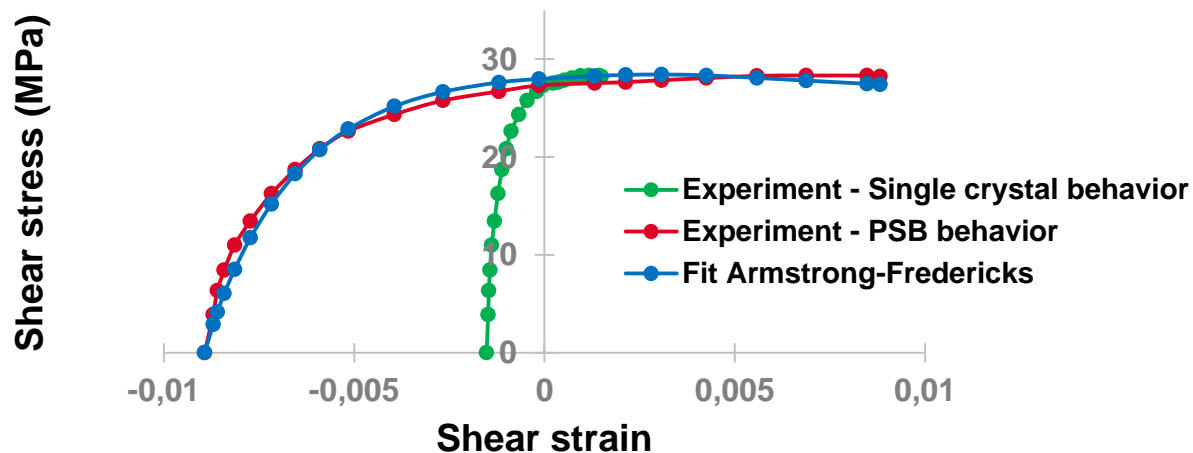
$\Rightarrow$  Localisation of slip in PSBs

### ② Elastic-Plastic behavior for PSBs

$\Rightarrow$  Armstrong-Fredericks non-linear kinematic hardening

$$\delta \chi_i = C \left( \frac{2}{3} A \delta \gamma_i^p - \chi_i \delta \gamma_{cum,i}^p \right)$$

$\Rightarrow$  Plateau behavior



## Finite Element Calculations based on:

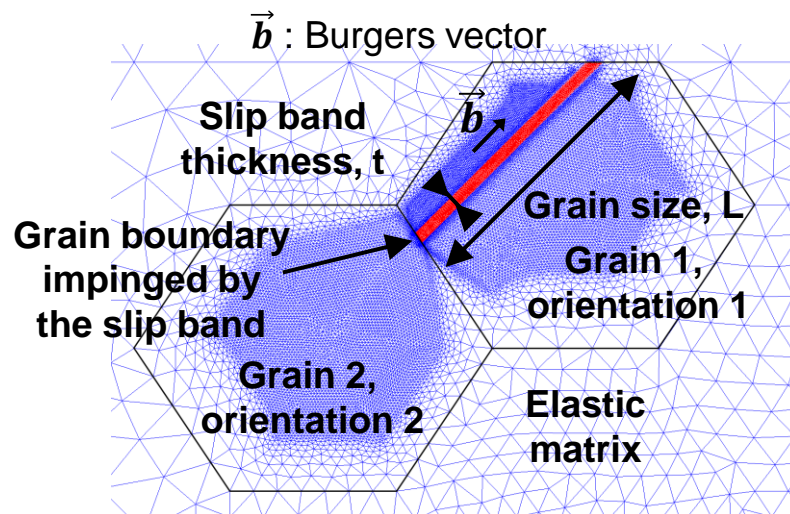
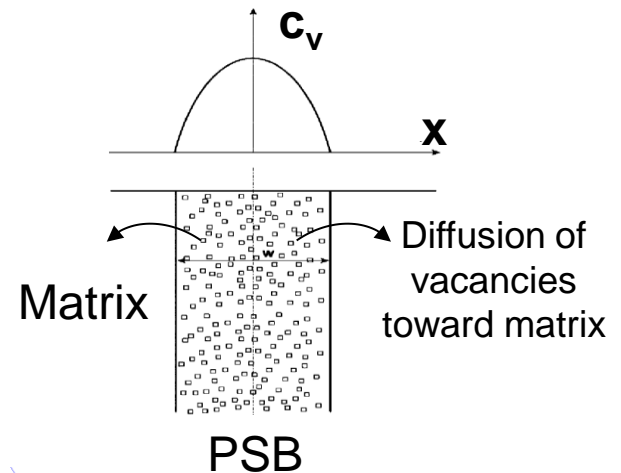
### ③ Production of vacancies inducing the free dilatation of persistent slip bands

⇒ Resistivity measurements on copper single crystals cycled at 4K [Polák 1987]

⇒ Determination of the vacancy production term [Polák & Sauzay 2009]

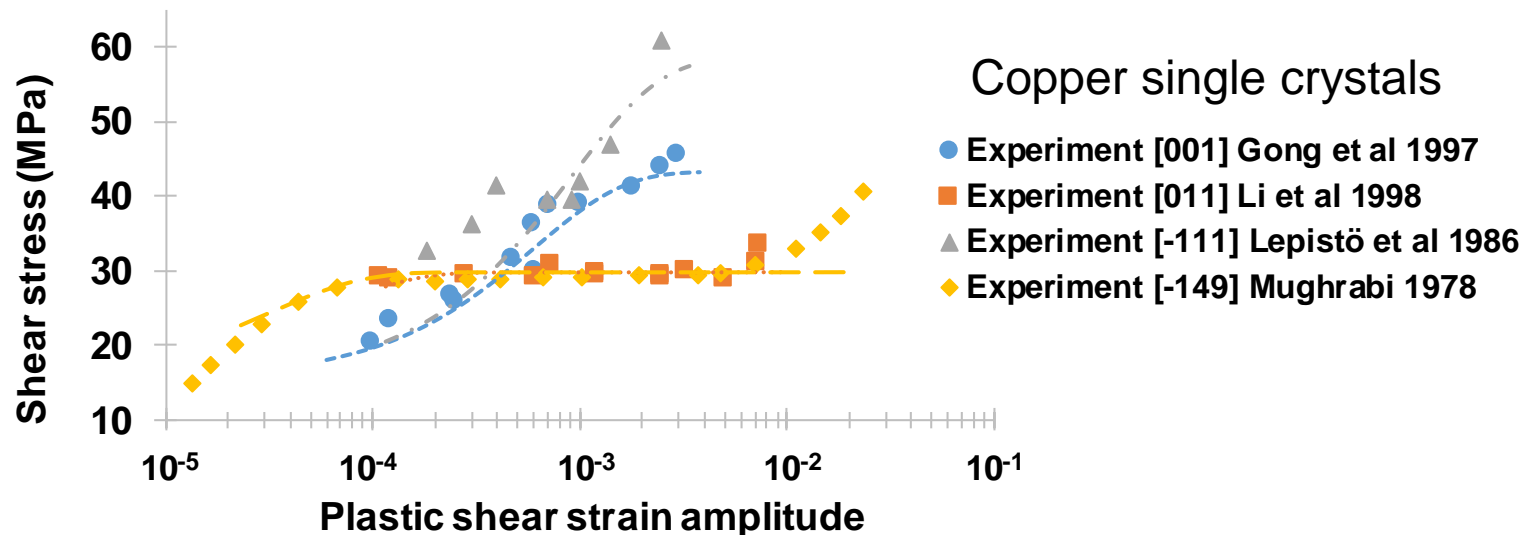
$p = 3.1 \cdot 10^{-7}$  for Copper

$$\varepsilon_{vacancy}^* = N_{cycles} * p$$



## Finite Element Calculations based on:

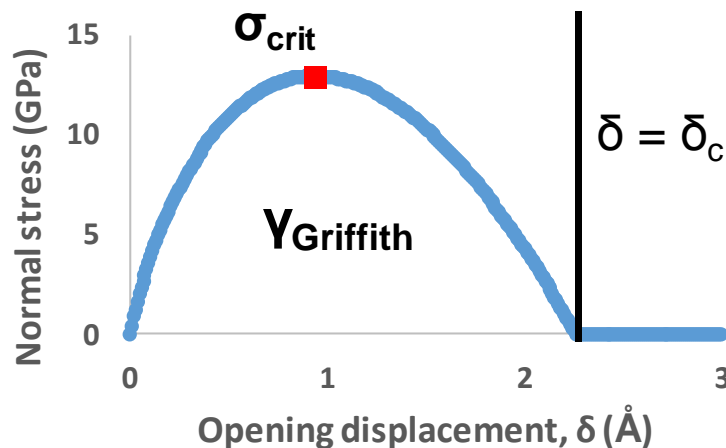
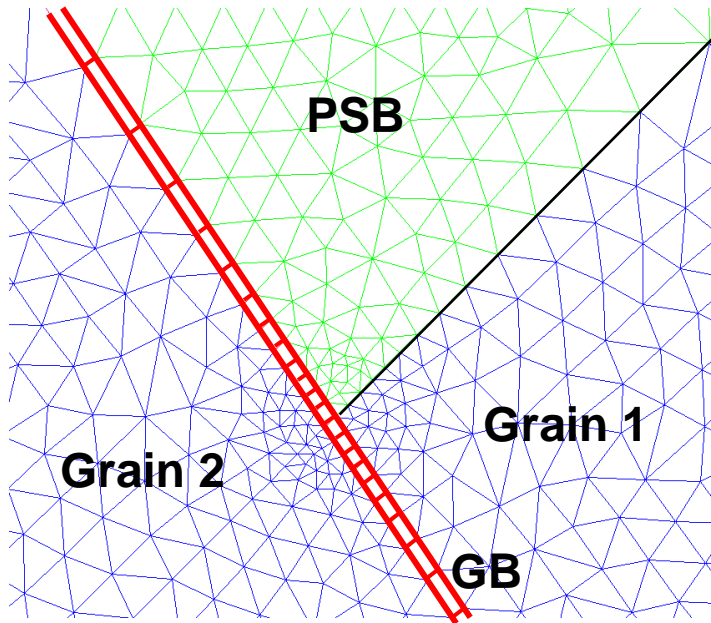
### ④ Elastic-plastic behavior of neighbor grain impinged by the PSB



### Assumptions for the calculations:

- ⇒ Elastic-Plastic behavior of PSBs & production, annihilation of vacancies within PSBs and diffusion toward the matrix
- ⇒ Elastic-Plastic behavior of neighbor grain
- ⇒ Elastic matrix

- **CONTEXT & GOAL**
- **METHODS**
  - Elastic-plastic model and behavior
  - **Cohesive zone model**
- **RESULTS**
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## GB obeys a non linear cohesive law:

2 criteria for crack initiation :

- Critical stress (UBER model)  
[Rice & Wang, 1989] [Rose et al. 1981]
- Critical energy released by the cracked interface [Griffith]

Evaluation of three parameters:

- GB Young modulus  $E_{GB}$
- Fracture energy of the interface

$$\gamma_{fract} = 2\gamma_s - \gamma_{GB}$$

- Critical stress

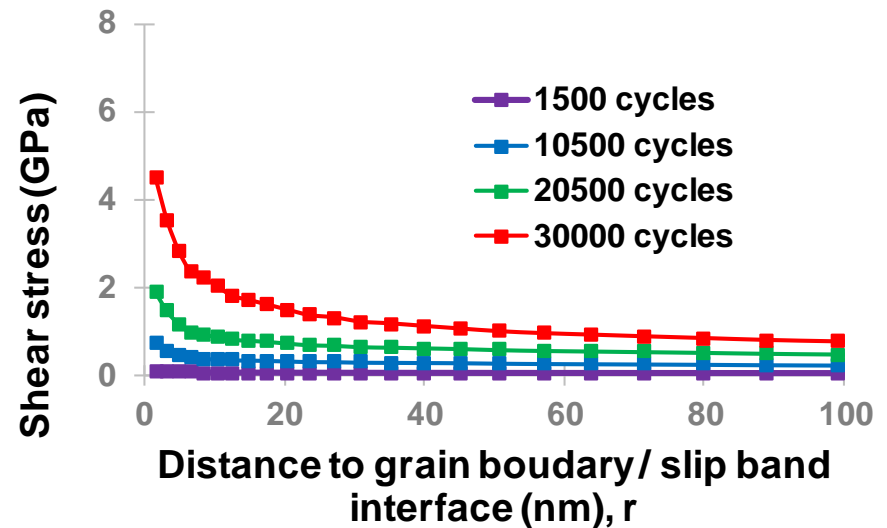
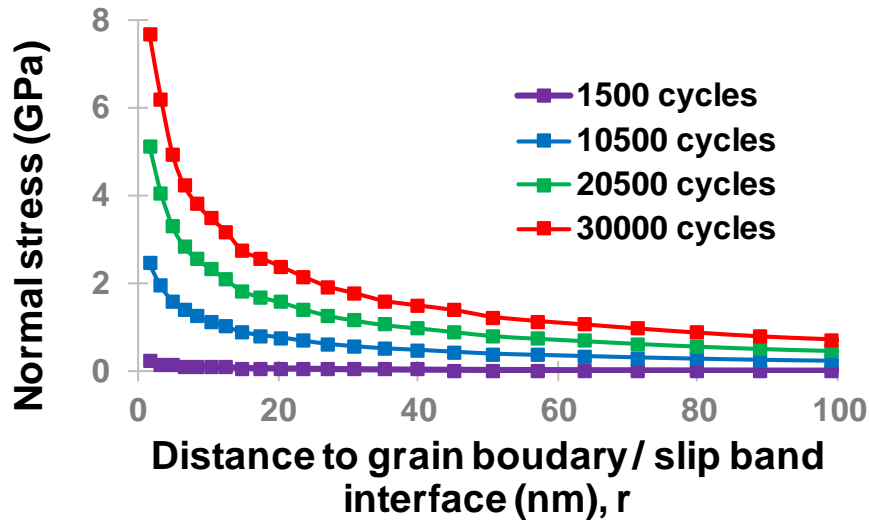
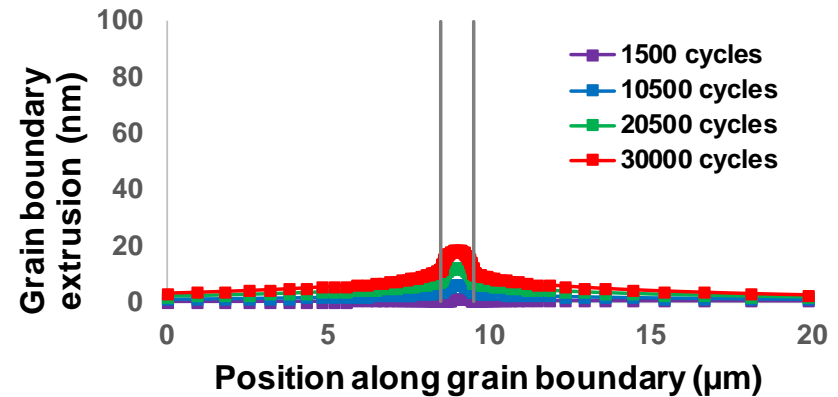
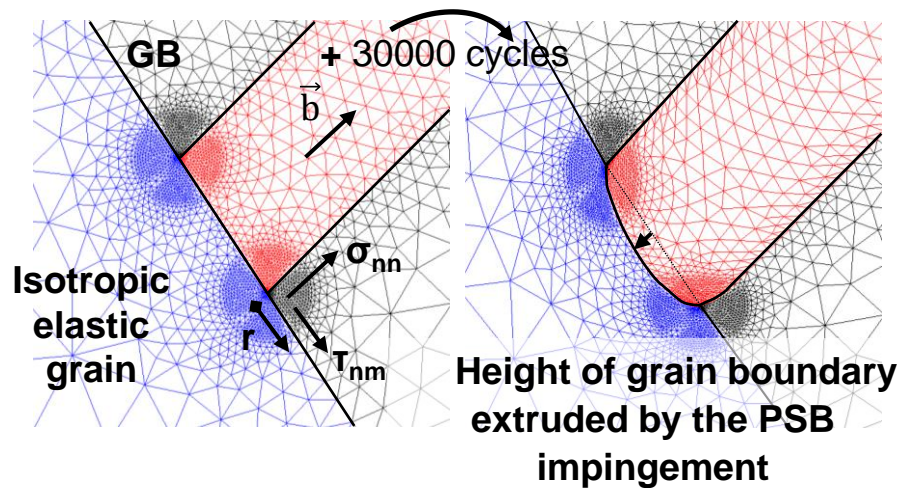
$$\sigma_{crit} = \frac{\sqrt{E/d_{GB} * \gamma_{fract}}}{e} \quad \text{See [Barbé et al 2018]}$$

Output: Opening of the interface,  $\delta$   
 $\Rightarrow \delta/\delta_c = 1$  : Complete separation

- **CONTEXT & GOAL**
- **METHODS**
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  - **GB extrusions and stress-fields**
  - **Prediction of crack initiation**
- **CONCLUSIONS & WORK IN PROGRESS**

# RESULTS : PREDICTION OF MECHANICAL FIELDS

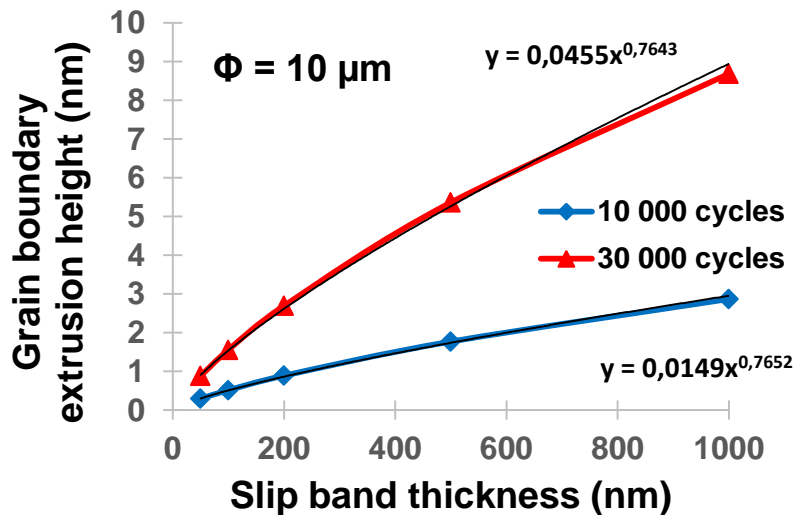
Copper | PSB thickness = 1  $\mu\text{m}$  | Grain size = 50  $\mu\text{m}$  | 30 000 cycles



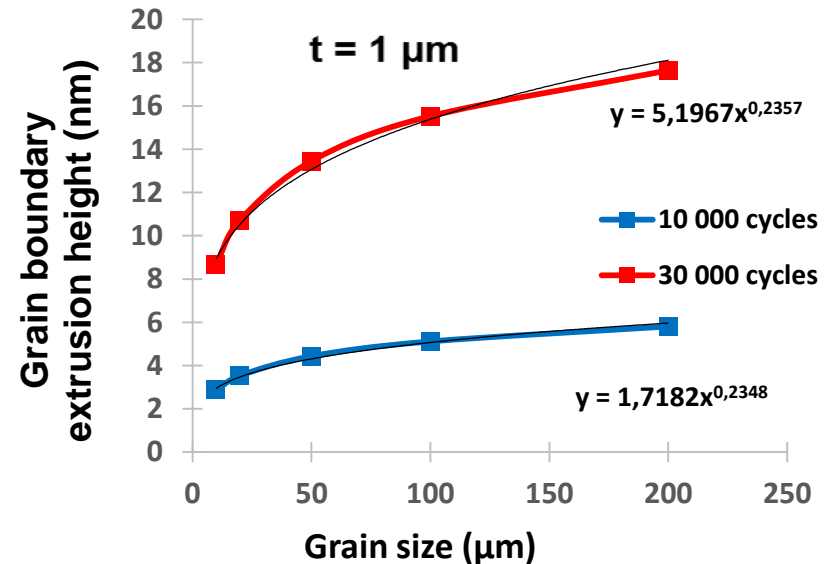
# RESULTS: PREDICTION OF MECHANICAL FIELDS

Influence of the persistent slip band characteristic lengths:  
=> **grain boundary extrusion**

Influence of slip band thickness,  $t$



Influence of grain size,  $L$



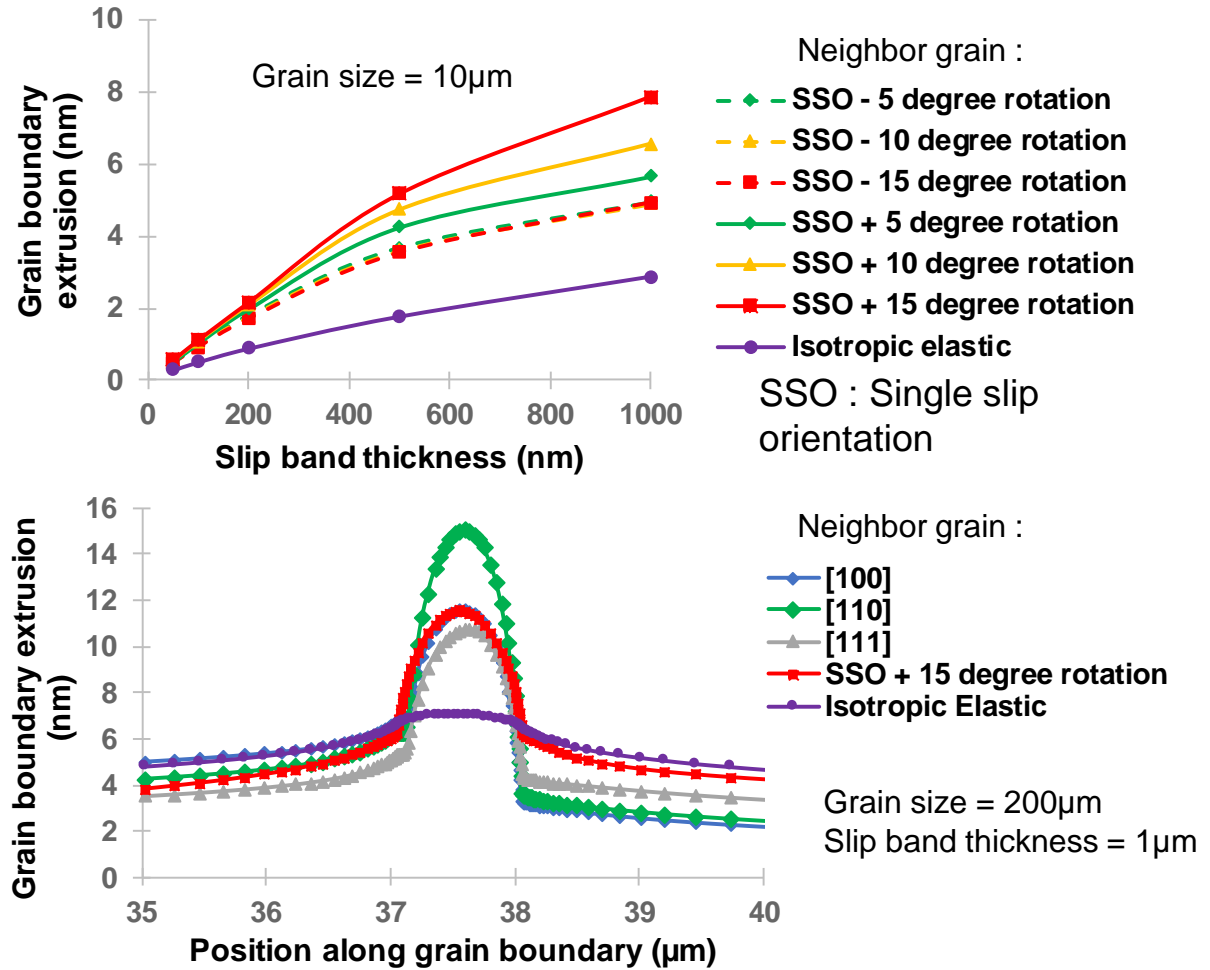
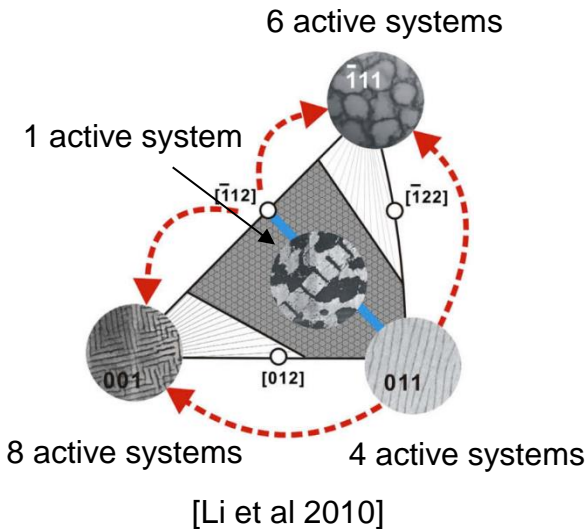
$$h(N) = 0,56 \cdot p \cdot N \cdot t^{0,77} * L^{(1-0,77)}$$

**Combined effect of the slip band thickness and grain size on the grain boundary extrusion : Higher damage expected**



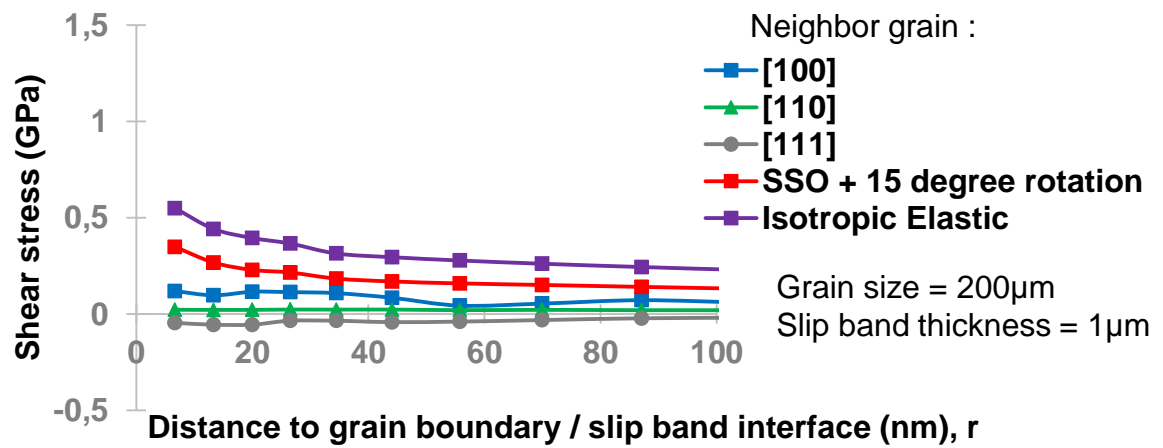
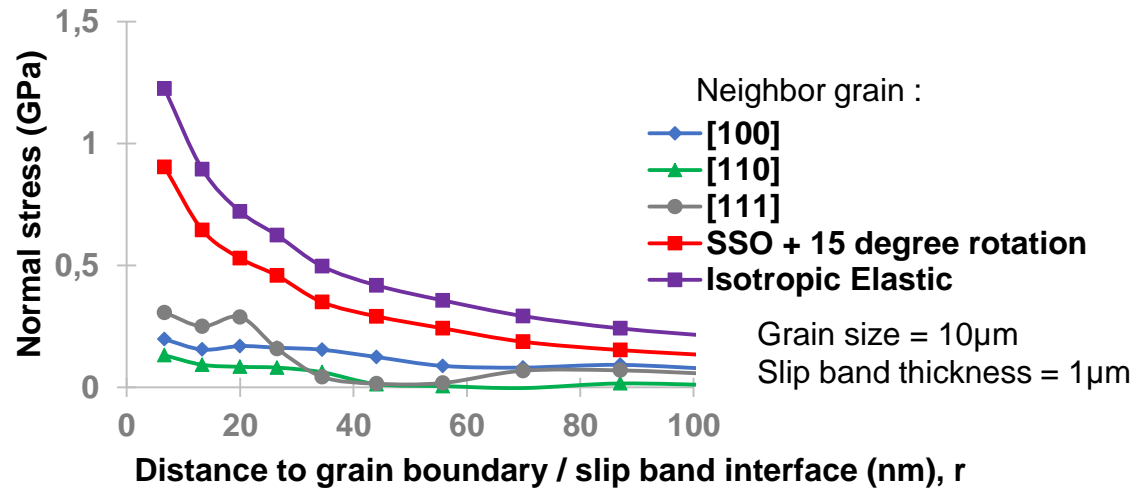
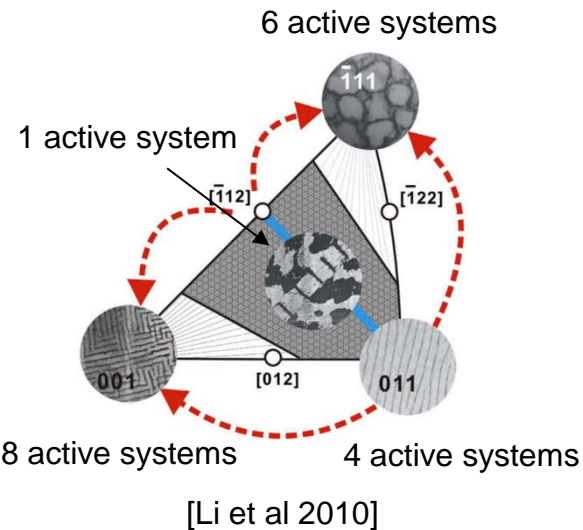
## Influence of neighbor grain crystallographic orientation ?

10000 cycles



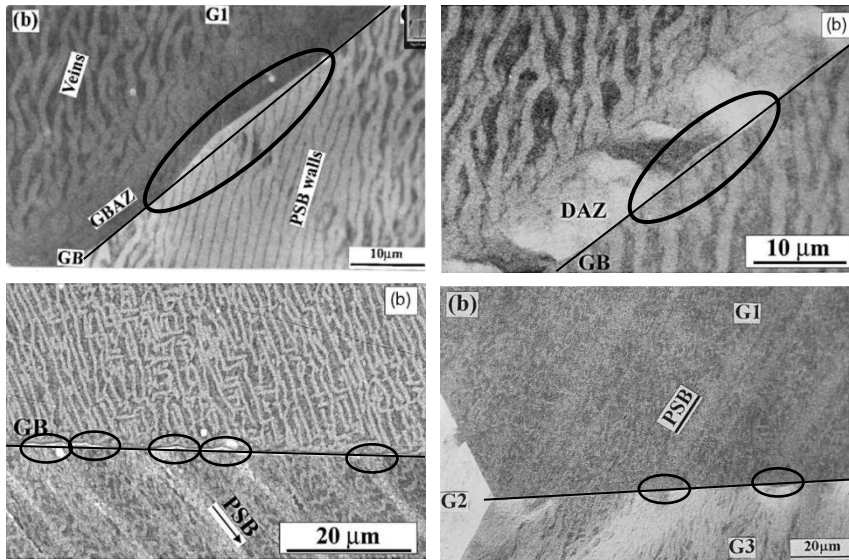
**High increase in the grain boundary extrusion due to plasticity in the neighbor grain**

## Influence of neighbor grain crystallographic orientation ?

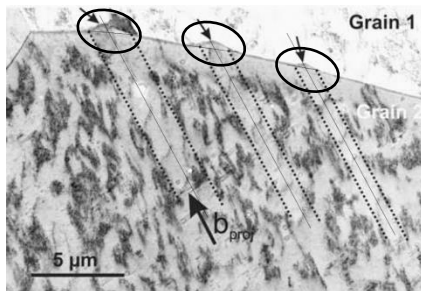


**Expected decrease of GB stress fields due to plasticity in the neighbor grain**

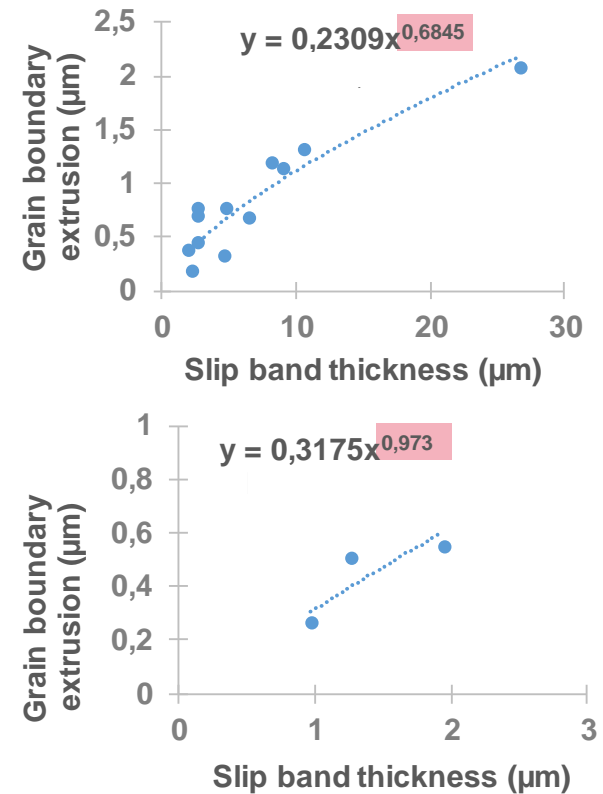
Comparison of the prediction to experimental data from literature :  
Impact of PSB thickness on GB extrusion height ?



[Zhang & Wang]



[Weidner et al. 2010]

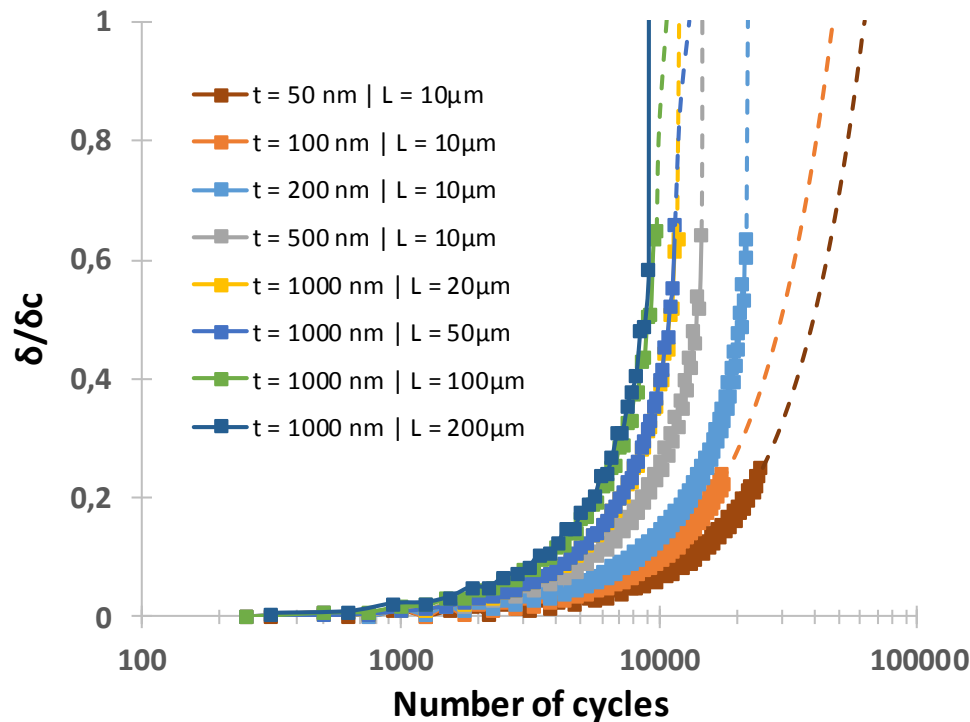


**Exponents adjusted using experimental data in reasonable agreement with the exponents provided by the FE computations ~0.7**

- CONTEXT & GOAL
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# RESULTS: PREDICTION OF MICRO-CRACK INITIATION

Preliminary results: influence of PSBs characteristic lengths on GB micro-crack initiation : Copper, elastic neighbor



t (nm)	L ( $\mu\text{m}$ )	Ni (cycles)
50	10	60k
100	10	45k
200	10	25k
500	10	15k
1000	10	13k
1000	20	13k
1000	50	11k
1000	100	10k
1000	200	9k

Prediction: Stronger influence of PSB thickness than grain size  
Order of magnitude in agreement with experimental observation ?

# RESULTS: PREDICTION OF MICRO-CRACK INITIATION

Observations of intergranular initiation published in literature (RT, air environment):

Material	$\Delta\epsilon_p/2$	t ( $\mu\text{m}$ )	L ( $\mu\text{m}$ )	Ni	Reference
316L - polycristal	$10^{-3}$	$\approx 0,45 \mu\text{m}$	<30>	<5000 (20%Nr)	[Mineur et al. 2000]
316L - polycristal	$10^{-3}$	$\approx 0,45 \mu\text{m}$	<47>	<10000 (20%Nr)	[Blochwitz et Richter 1999]
316L - polycristal	$2.5 \cdot 10^{-4}$	$\approx 0,45 \mu\text{m}$	<47>	<40000 (20%Nr)	[Blochwitz et Richter 1999]
Ni - polycristal	$2.5 \cdot 10^{-4}$	$\approx 1 \mu\text{m}$	<24>	<145000 (66% Nr)	[Morrison et Moosbrugger 1997]
Ni - polycristal	$2.5 \cdot 10^{-3}$	$\approx 1 \mu\text{m}$	<290>	<200 (4% Nr)	[Morrison et Moosbrugger 1997]
Ni - polycristal	$2.5 \cdot 10^{-4}$	$\approx 1 \mu\text{m}$	<290>	<17000	[Morrison et Moosbrugger 1997]
Ni - polycristal	$2.5 \cdot 10^{-3}$	$\approx 1 \mu\text{m}$	<24>	<1200 (19% Nr)	[Morrison et Moosbrugger 1997]
Ni - polycristal	$3 \cdot 10^{-4}$	$\approx 1 \mu\text{m}$	<150>	18000	[Dorr & Blochwitz 1987]
Cu - polycristal	$10^{-3}$	$\approx 1 \mu\text{m}$	<100>	<10000 (25%Nr)	[Liu et al 1992]
Cu - bicystal	$2 \cdot 10^{-3}$	$\approx 1 \mu\text{m}$	$\sim 5 \text{ mm}$	<10000	[Zhang et Wang 2002]
Cu - bicystal	$5 \cdot 10^{-4}$	$\approx 1 \mu\text{m}$	$\sim 5 \text{ mm}$	<20000	[Zhang Wang Hu 1999]

First prediction are in the good order of magnitude

=> Precise microstructure needed for more precise comparison

- CONTEXT & GOAL
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## Conclusions :

- Simulation based on basic physical assumptions
- Prediction of stress-fields induced by impingement of PSBs at GB for different crystallographic orientations of the neighbor grains
- Analytical formulas of GB extrusion heights (elastic neighbor)

## Work in progress :

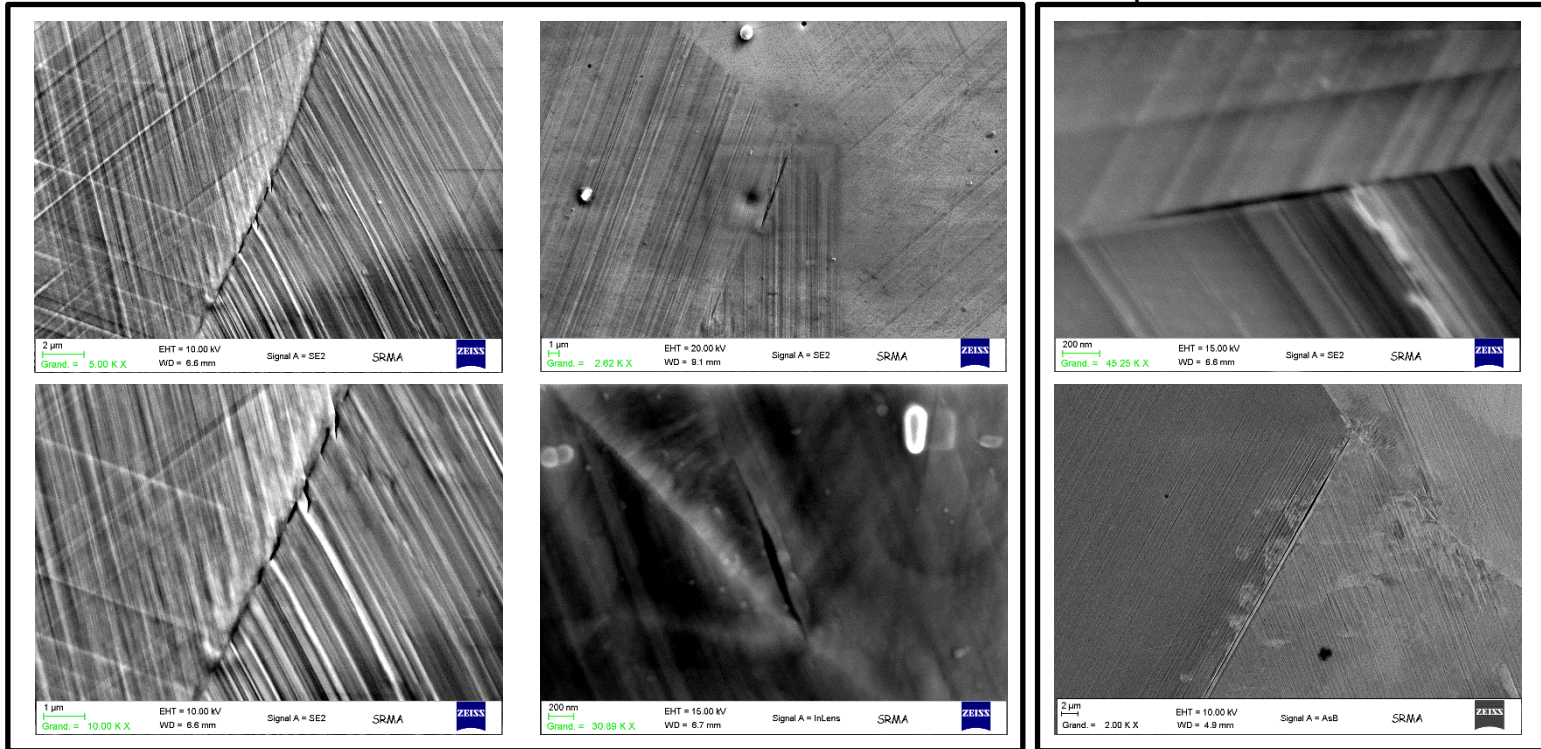
- Prediction of intergranular initiation introducing atomistic considerations in the calculations as M.Sangid did [Sangid et al. 2011]
    - GB type, environment, material, etc.
  - Interrupted fatigue test carried out on two 316L SS containing (i) very large grains and (ii) small grains
    - EBSD scan + SEM observations of crack-initiations
- ⇒ Comparison of predictions to real cases microstructures
- Analytical model for the prediction of intergranular, transgranular and twin boundaries microcrack initiation



Interrupted fatigue test :

316L SS, 2000 cycles,  $<200 \mu\text{m}>$ ,  $\Delta\varepsilon_p/2 = 10^{-3}$

Intergranular initiation



Twin boundary initiation

**=> Microstructure informed FE computations based on EBSD data and post-FIB cutting (3D information)**



Many thanks for your attention  
Any question ?

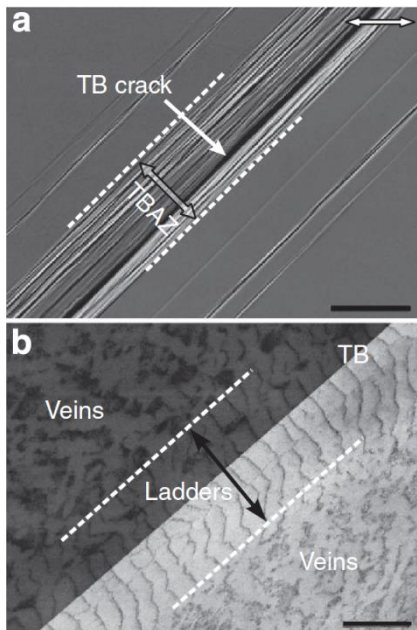
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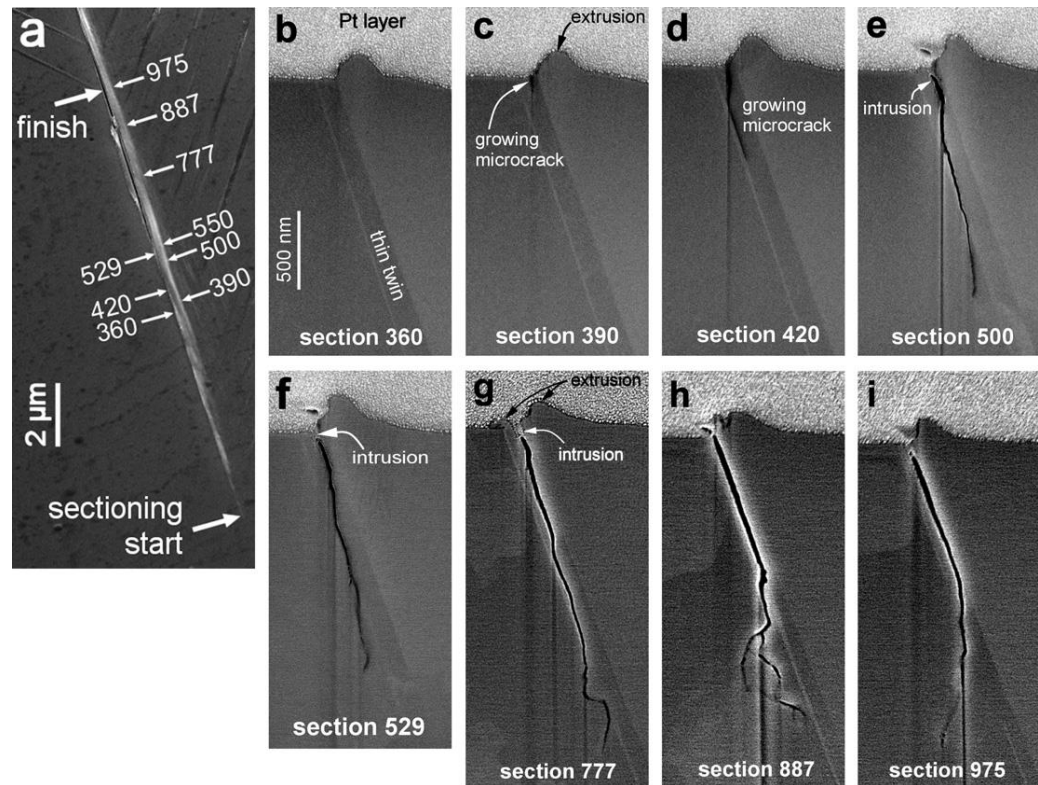
Nuclear Energy Division  
Nuclear Material Department  
Section for Applied Metallurgy Research  
Materials Mechanical Analysis Laboratory

=> Case of HCF & VHCF

Same methodology applicable for twin boundary cracking



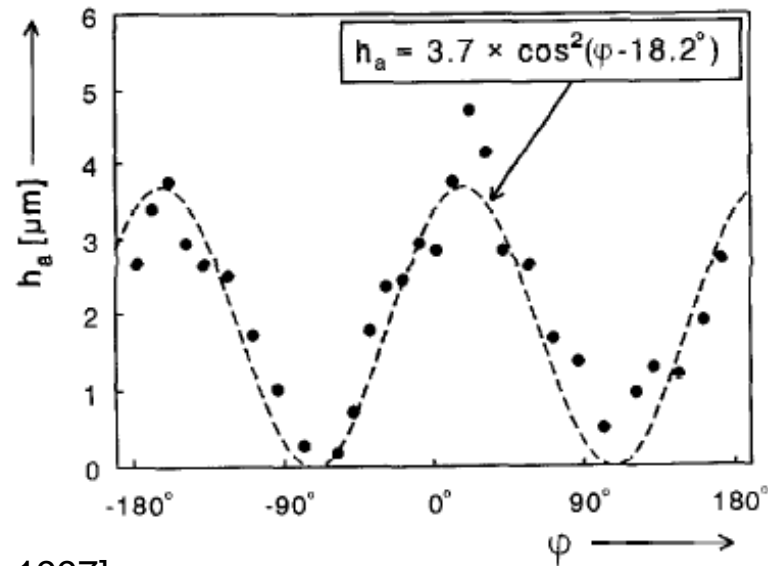
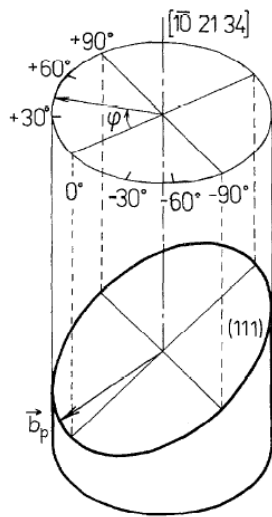
[Li et al. 2014]



[Man et al. 2012]

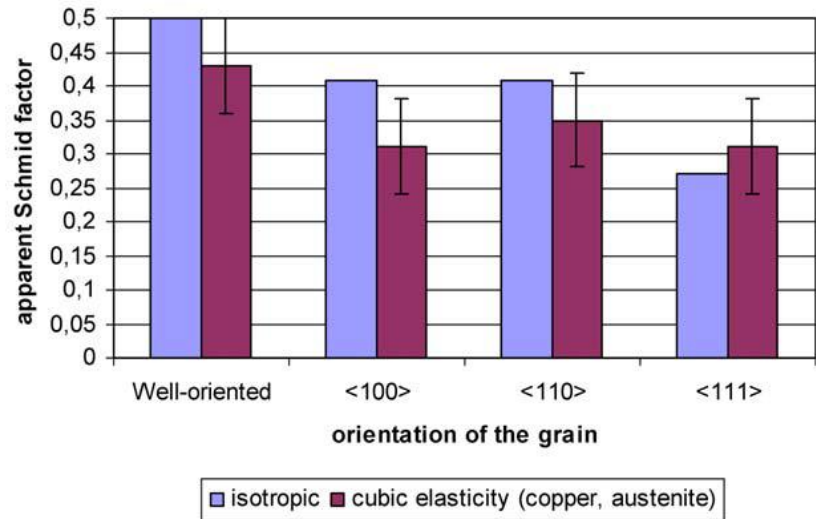
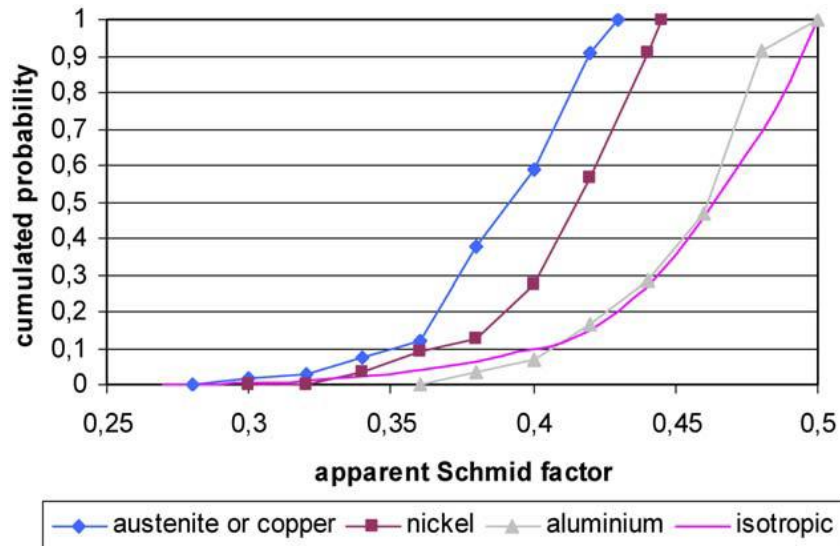
Cylindrical Copper single crystal cyclically deformed :

- Each peak is offset by 180°
- => Preferential direction of slip



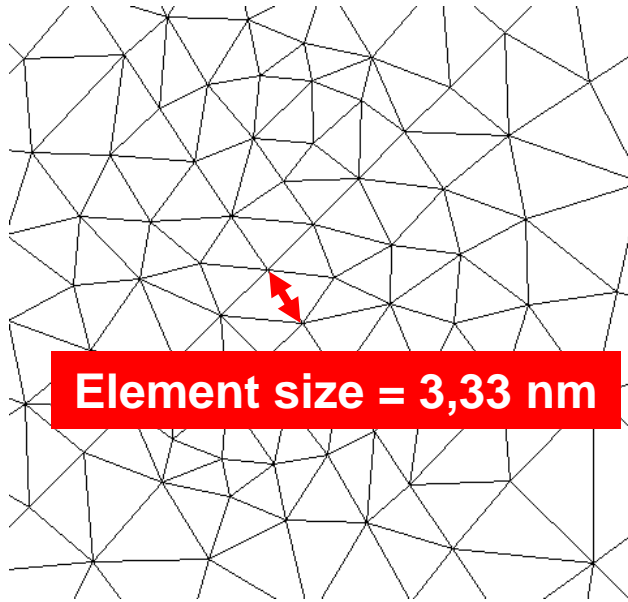
[Obtlik et al, 1997]

# NUMBER OF GRAINS CONTAINING PSBs



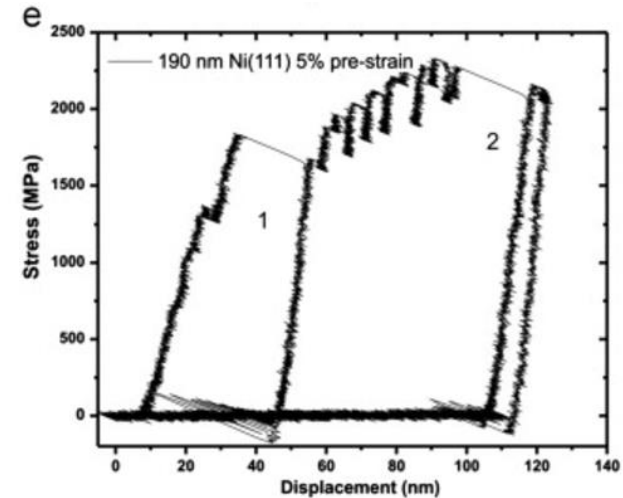
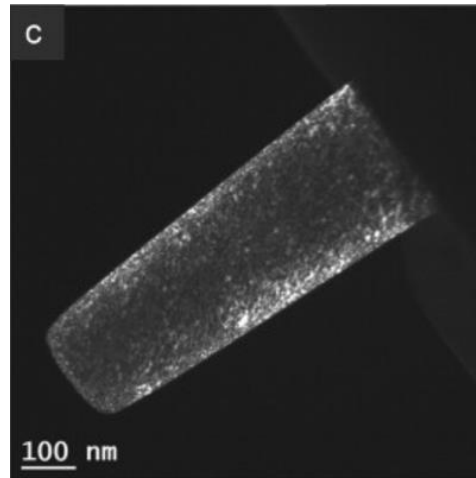
[Sauzay 2006]

Why matrix is supposed to be elastic ?



**Element size = 3,33 nm**

Compression test on Ni micropillar [Legros 2014]

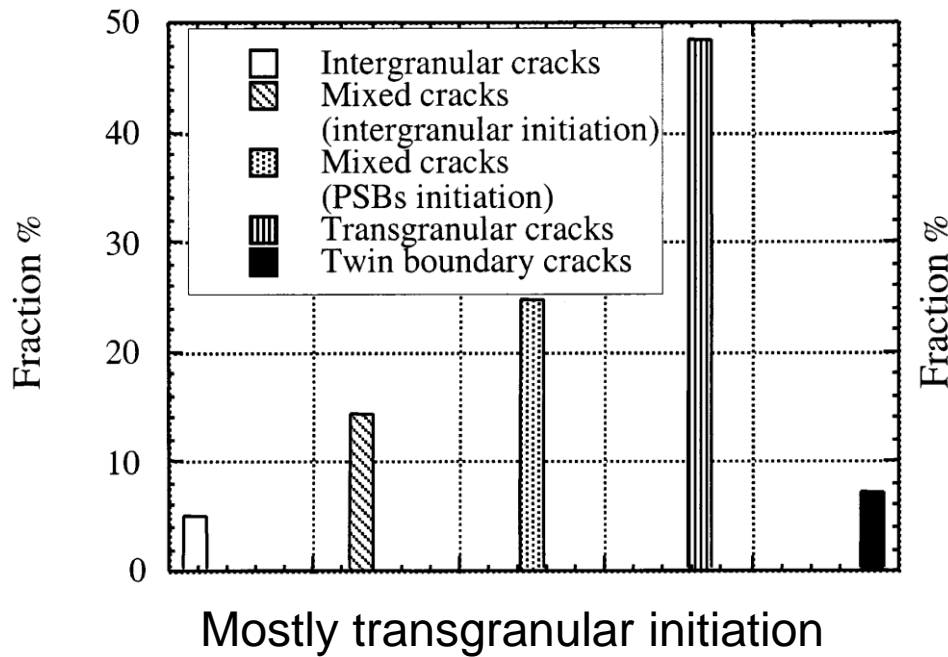


$$10^{13} \text{ m}^{-2} < \rho_{\text{Matrix}} < 10^{15} \text{ m}^{-2}$$

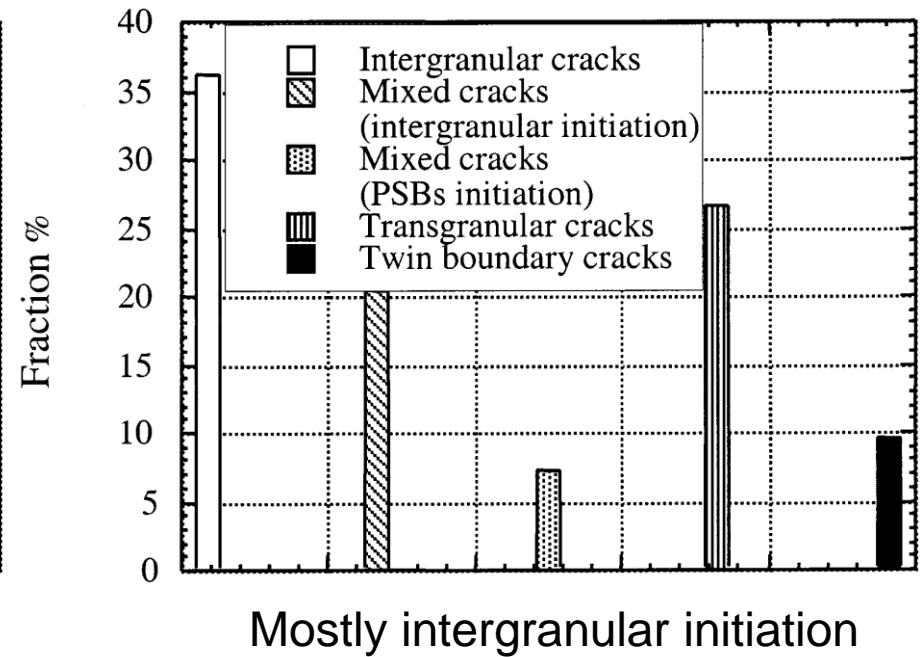
$$N_{\text{dislocation, max}} = 3.33 \cdot 10^{-10} \times 3.33 \cdot 10^{-10} \times 10^{15} = 1.1 \cdot 10^{-4} \approx 0 \text{ dislocation}$$

# ENVIRONMENT EFFECT ON MICRO-CRACK INITIATION

Air, RT,  $\Delta\epsilon_p/2 = 2.10^{-3}$



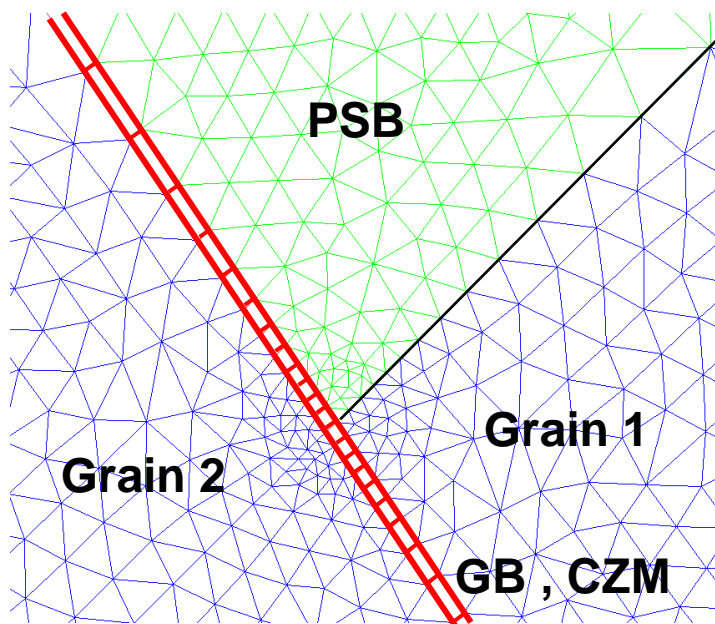
Vacuum, RT,  $\Delta\epsilon_p/2 = 2.10^{-3}$



[Mineur et al, 2000]

## METHOD : COHESIVE ZONE MODEL

$$\sigma_{crit} = \frac{\sqrt{E/d_{GB} * \gamma_{fract}}}{e}$$



	Copper	Nickel	316 SS
Young modulus (Pa)	1.3 10 <sup>11</sup>	1.8 10 <sup>11</sup>	1.9 10 <sup>11</sup>
E <sub>GB</sub> min (Pa)	5.9 10 <sup>10</sup>	8.1 10 <sup>10</sup>	8.6 10 <sup>10</sup>
E <sub>GB</sub> max (Pa)	1.3 10 <sup>11</sup>	1.8 10 <sup>11</sup>	1.9 10 <sup>11</sup>
d <sub>GB</sub> min (Å)	3	3	3
d <sub>GB</sub> max (Å)	7	7	7
γ <sub>surf</sub> min (J/m <sup>2</sup> )	1.9	2	2
γ <sub>surf</sub> max (J/m <sup>2</sup> )	2.2	2.4	3
γ <sub>GB</sub> min (J/m <sup>2</sup> )	0.3	0.45	0.48
γ <sub>GB</sub> max (J/m <sup>2</sup> )	1	1.4	1.6
<b>γ<sub>frac</sub> (J/m<sup>2</sup>) min</b>	<b>2.8</b>	<b>2.6</b>	<b>2.4</b>
<b>γ<sub>frac</sub> (J/m<sup>2</sup>) max</b>	<b>4.1</b>	<b>4.4</b>	<b>5.5</b>
<b>σ<sub>c</sub> min (GPa)</b>	<b>5.6</b>	<b>6.4</b>	<b>6.3</b>
<b>σ<sub>c</sub> max (GPa)</b>	<b>15</b>	<b>19</b>	<b>22</b>

References : [Latapie & Farkas 2003] [Shen et al 1994], [Barbé et al 2018] [Tschopp & McDowell 2007] [Vitos 1998], [Holm et al 2010]



Many experimental and simulation efforts have been carried out to better understand grain boundaries role :

[Lim & Raj 1984]

Influence of the  
Coincident Site  
Lattice

Grains  
misorientation  
and GB  
characteristics

[Shenyang group]  
[Liu et al 1992]

[Tschopp & McDowell 2007]  
[Yamakov et al 2006]

GB energy, GB  
thickness

Influence of  
Grain Size

[Morrison & Moosbrugger  
1997]  
[Taira et al 1979]

[Mineur et al 2000]

Influence of  
environment