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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

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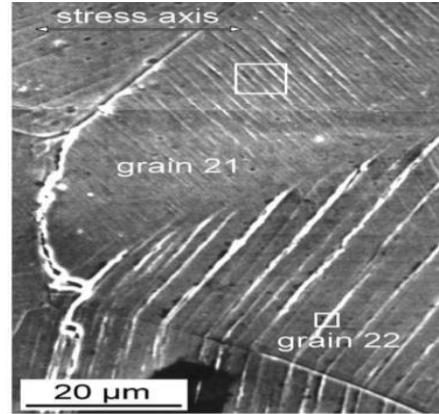
FATIGUE 2018 - MAY 29TH 2018

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

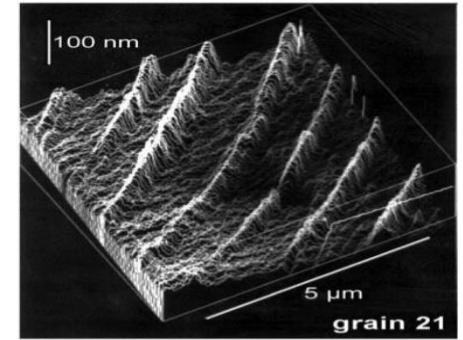
Cyclic deformation induces localization of plastic slip within Persistent Slip Bands (PSBs) for grains oriented for single slip

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

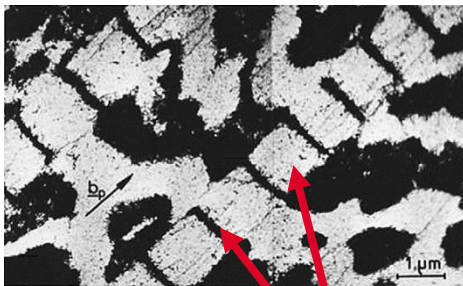
- Elastic matrix
- Elastic-plastic bands (PSBs)



[Man et al. 2002]



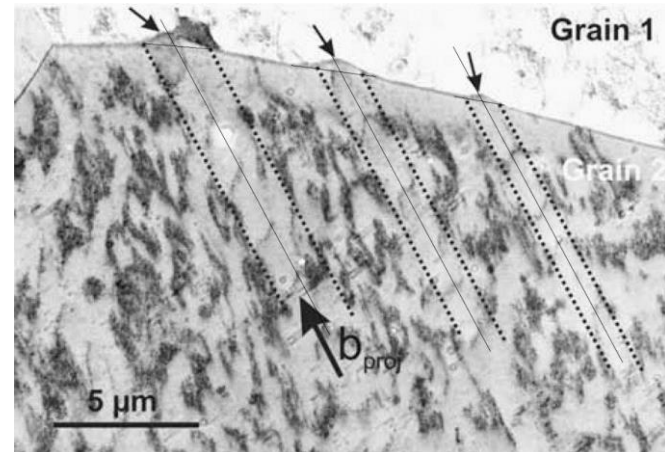
316L SS polycrystal



Copper single crystal

[Mughrabi 1979]

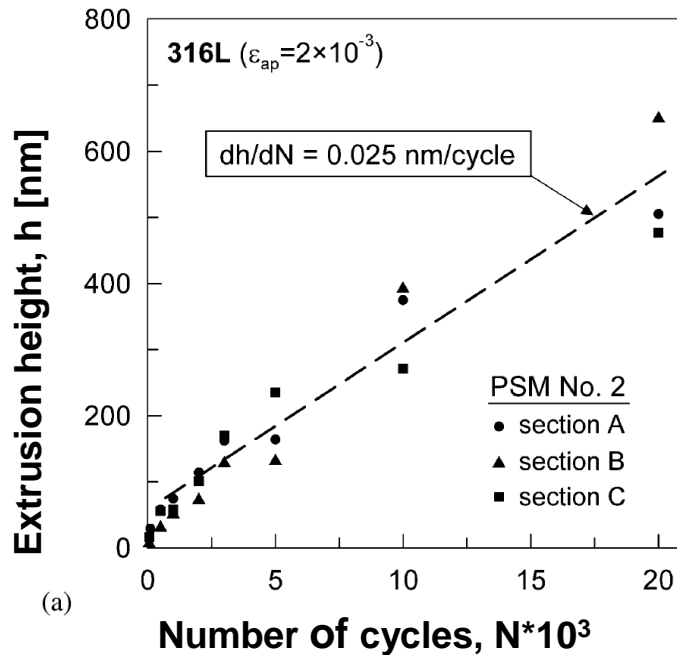
Poor channels ($\sim 10^{13} \text{ m}^{-2}$)
 rich walls ($\sim 10^{15} \text{ m}^{-2}$) :
 Ladder like structure



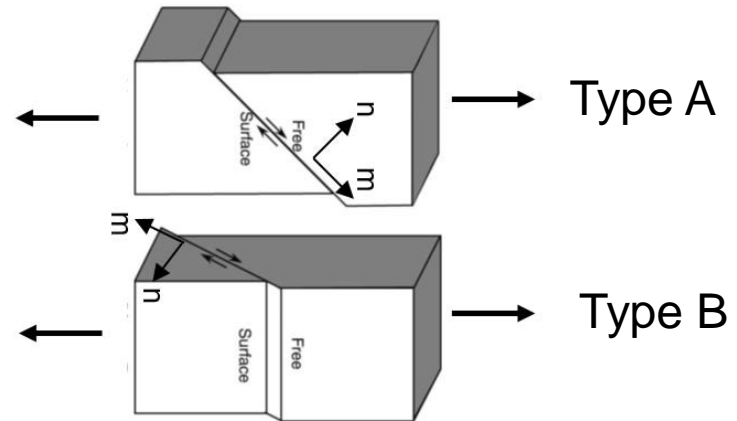
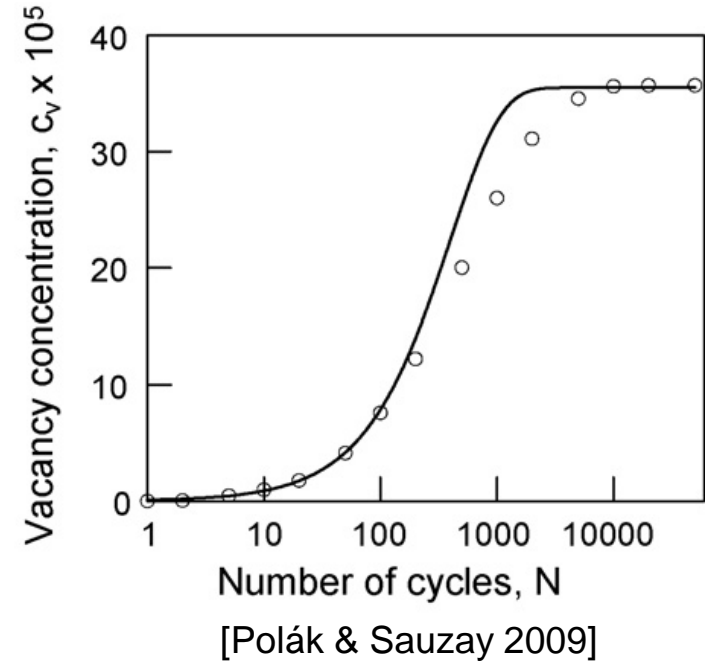
Nickel polycrystal

[Weidner et al. 2010]

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



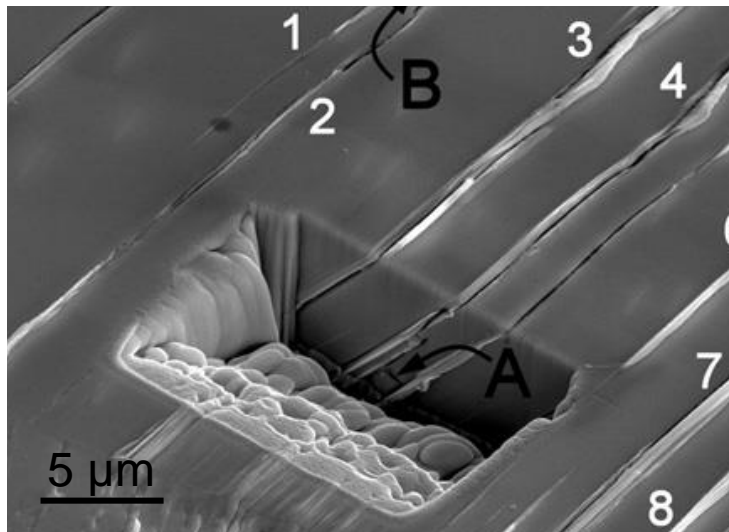
Almost constant growth rate of PSBs during cycling



[Man et al. 2003]

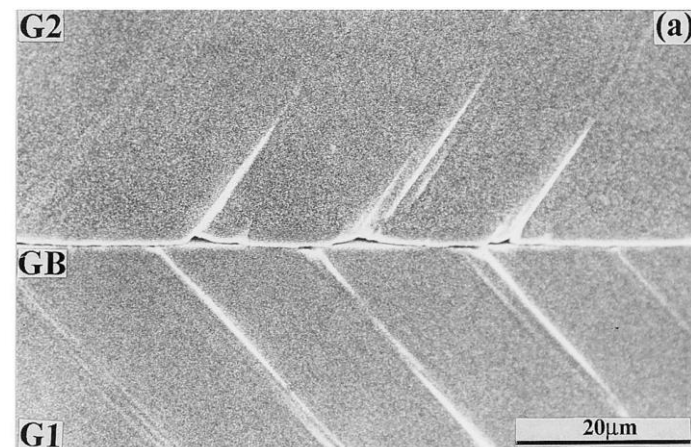
Slip localization in PSBs leads to microcrack initiation (in LCF):

Transgranular (type B):



[Polák et al. 2009]

Grain Boundaries (type A):



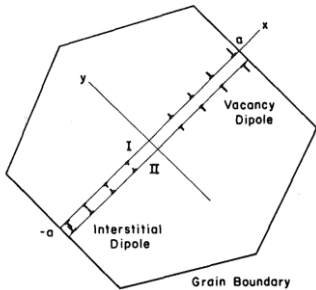
[Zhang et al. 1999]

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 :

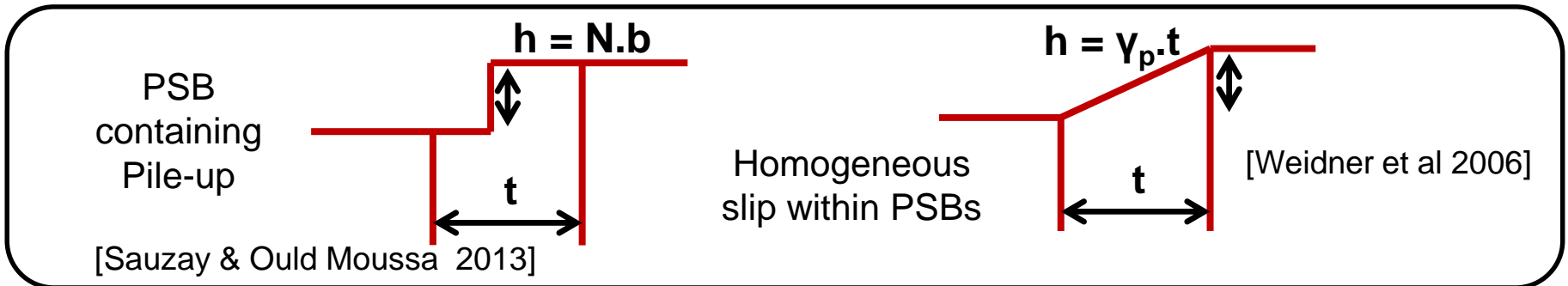
- Tanaka & Mura 1981



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

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:

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

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

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

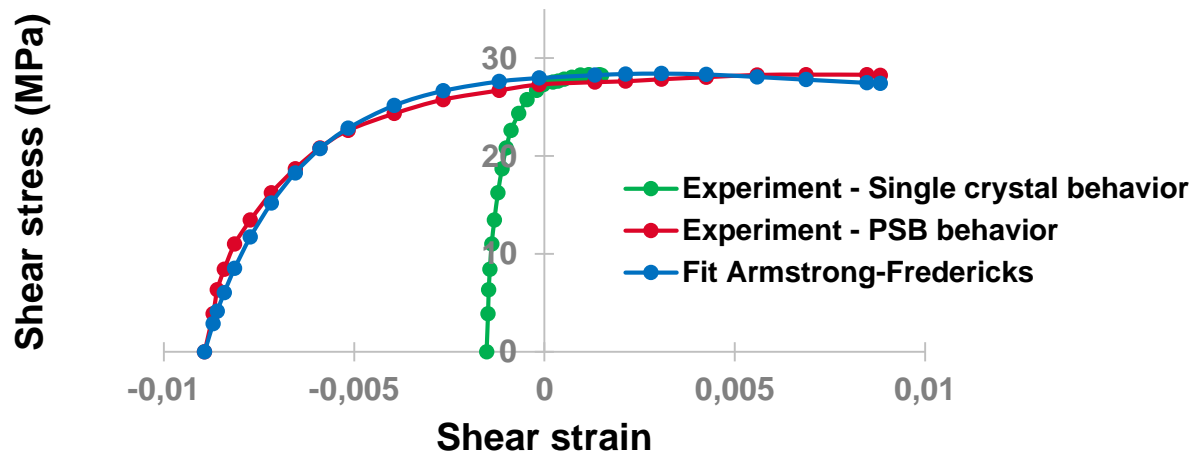
\Rightarrow Localisation of slip in PSBs

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:

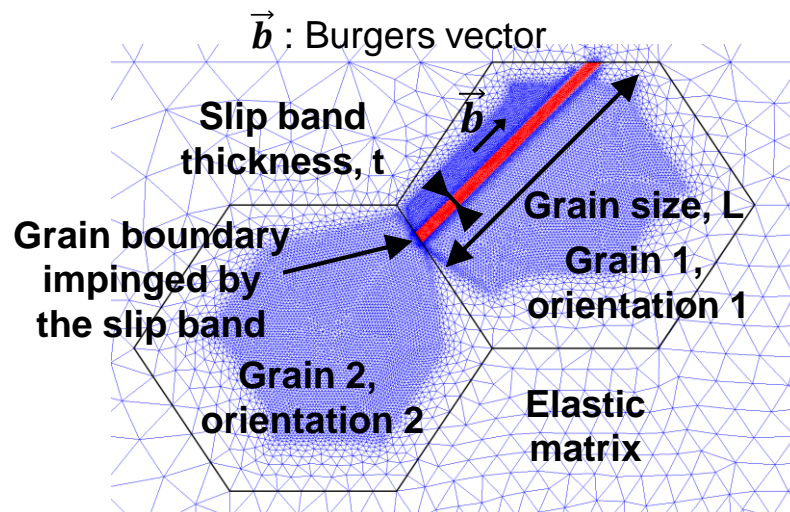
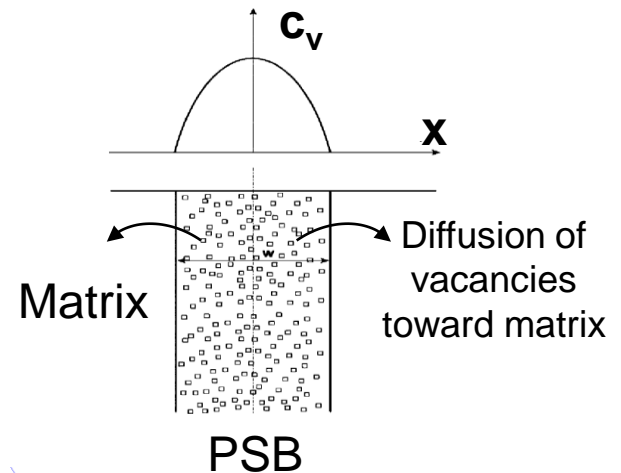
③ Production of vacancies inducing the free dilatation of persistent slip bands

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

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

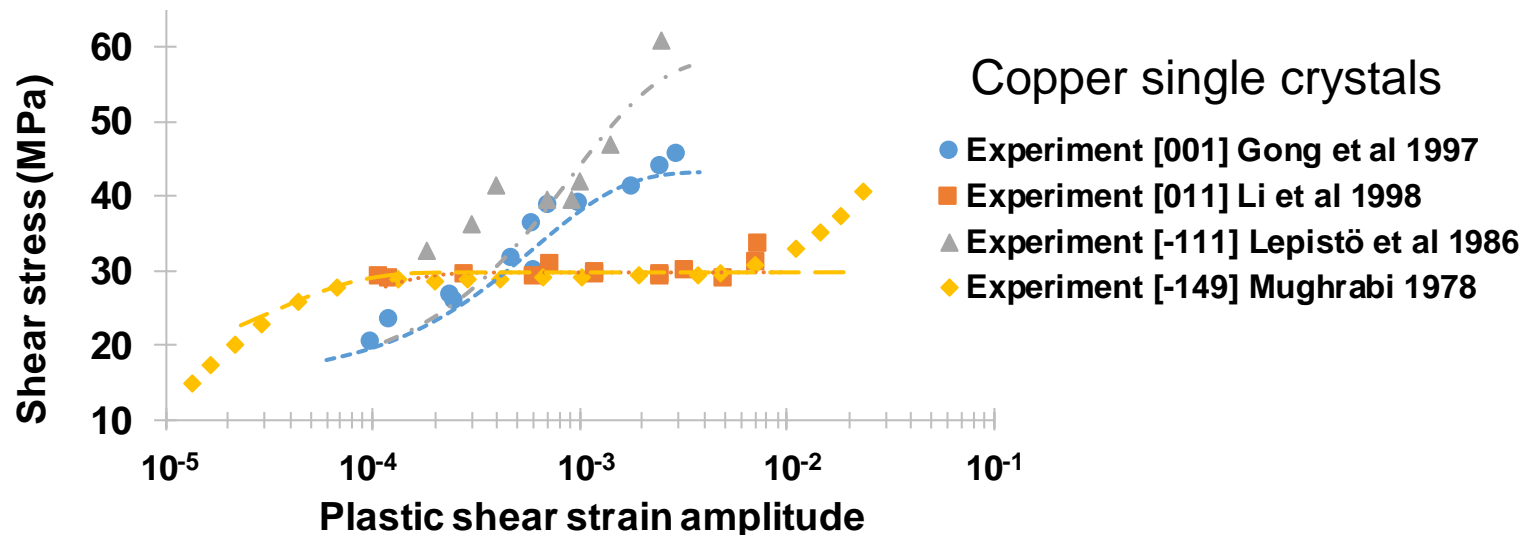
$p = 3.1 \cdot 10^{-7}$ for Copper

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



Finite Element Calculations based on:

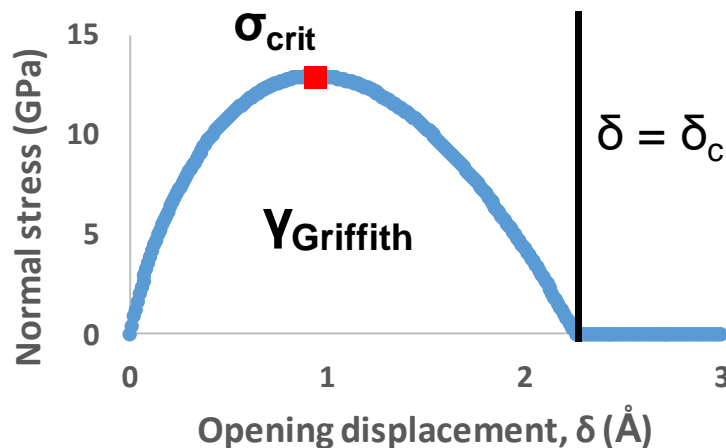
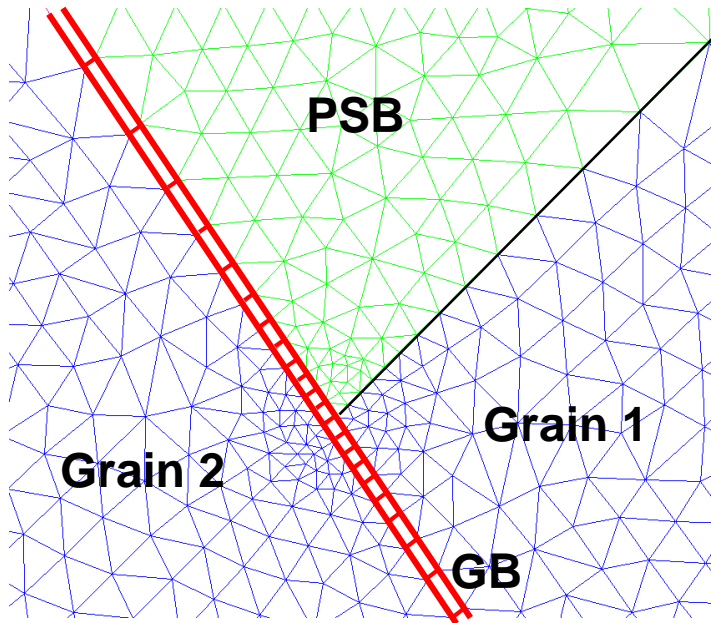
④ Elastic-plastic behavior of neighbor grain impinged by the PSB



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**
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 - **Cohesive zone model**
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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

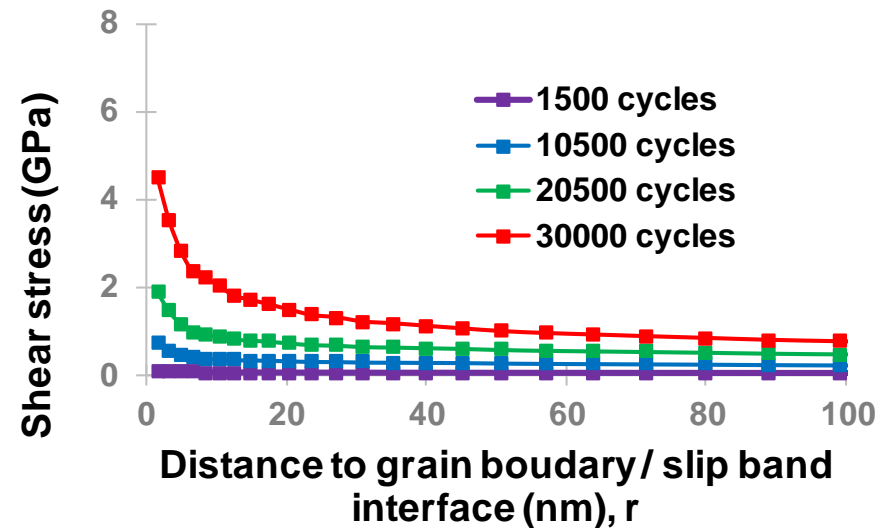
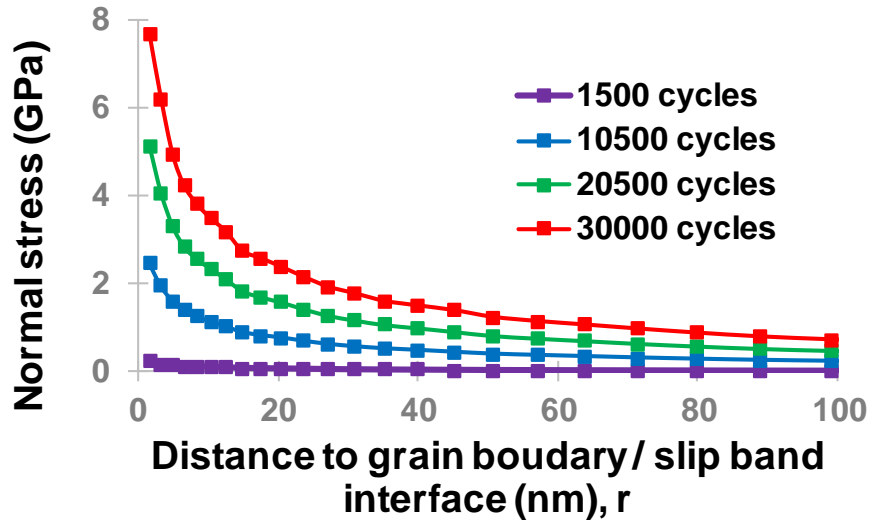
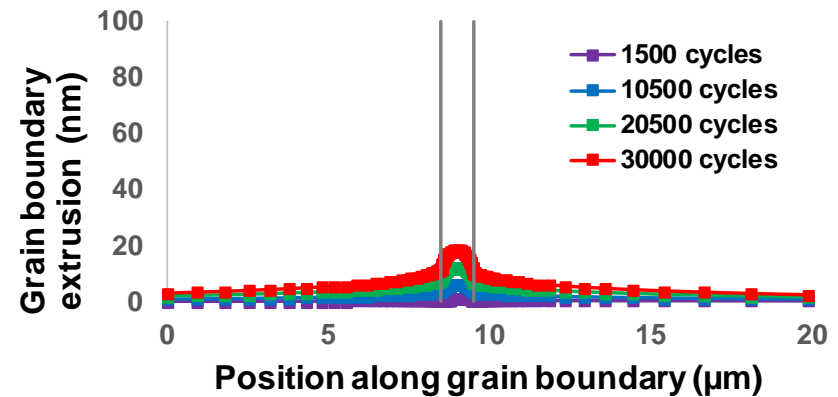
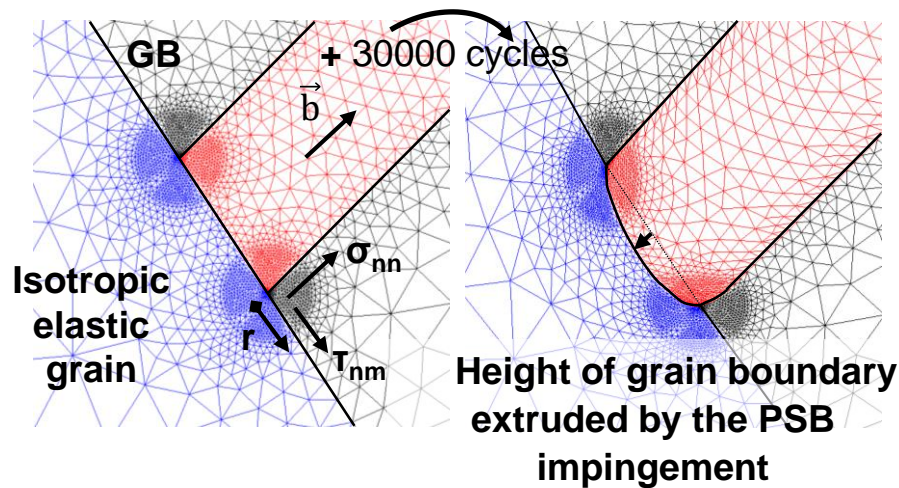
$$\sigma_{crit} = \frac{\sqrt{E/d_{GB} * \gamma_{fract}}}{e} \quad \text{See [Barbé et al 2018]}$$

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

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

RESULTS : PREDICTION OF MECHANICAL FIELDS

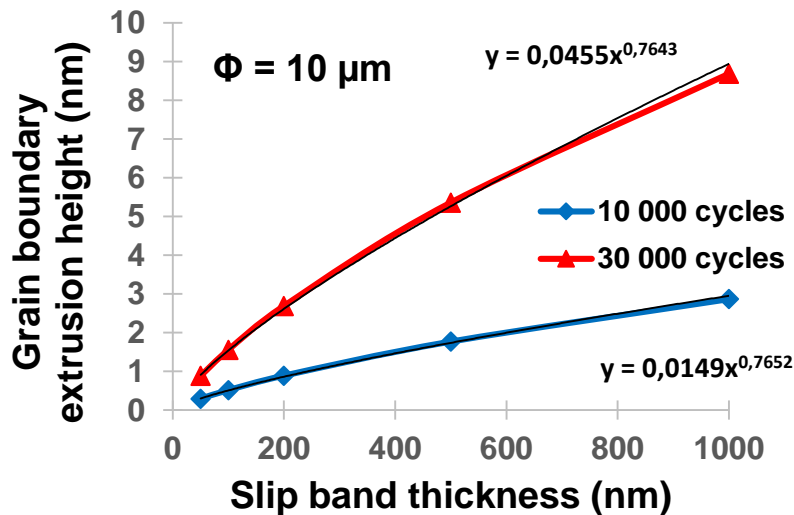
Copper | PSB thickness = 1 μm | Grain size = 50 μm | 30 000 cycles



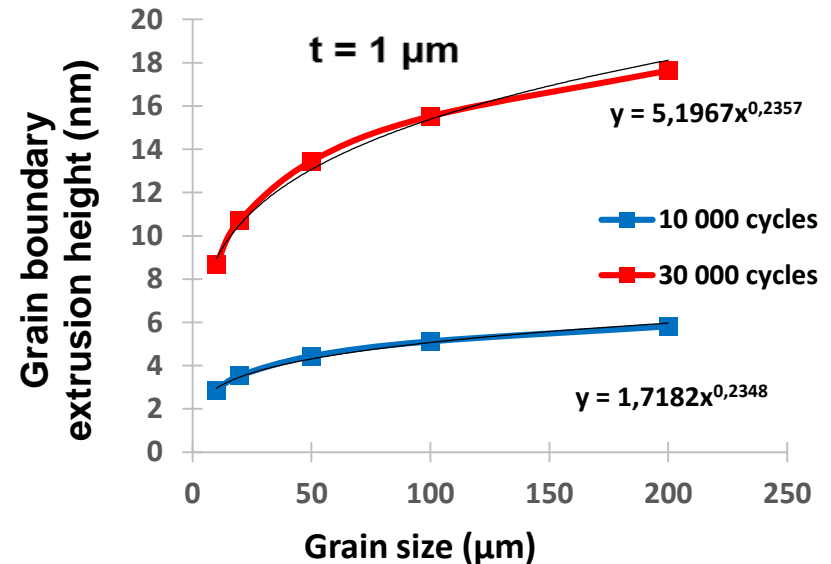
RESULTS: PREDICTION OF MECHANICAL FIELDS

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

Influence of slip band thickness, t



Influence of grain size, L

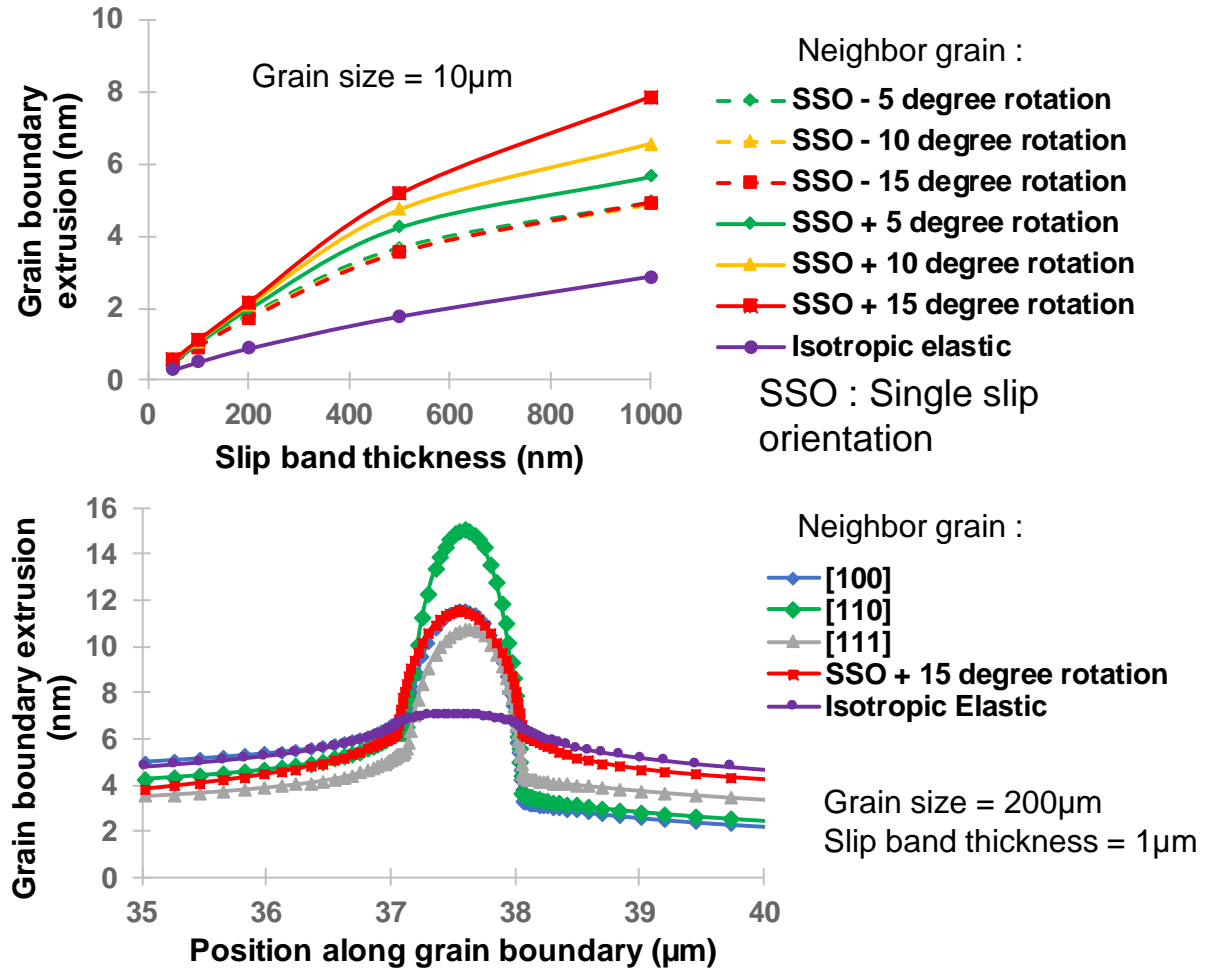
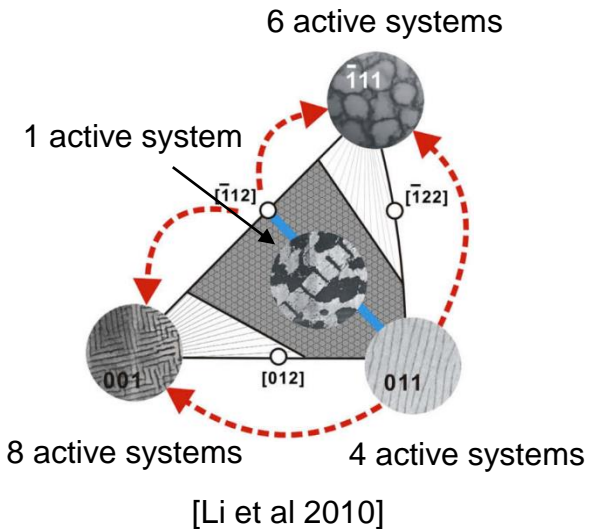


$$h(N) = 0,56 \cdot p \cdot N \cdot t^{0,77} * L^{(1-0,77)}$$

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

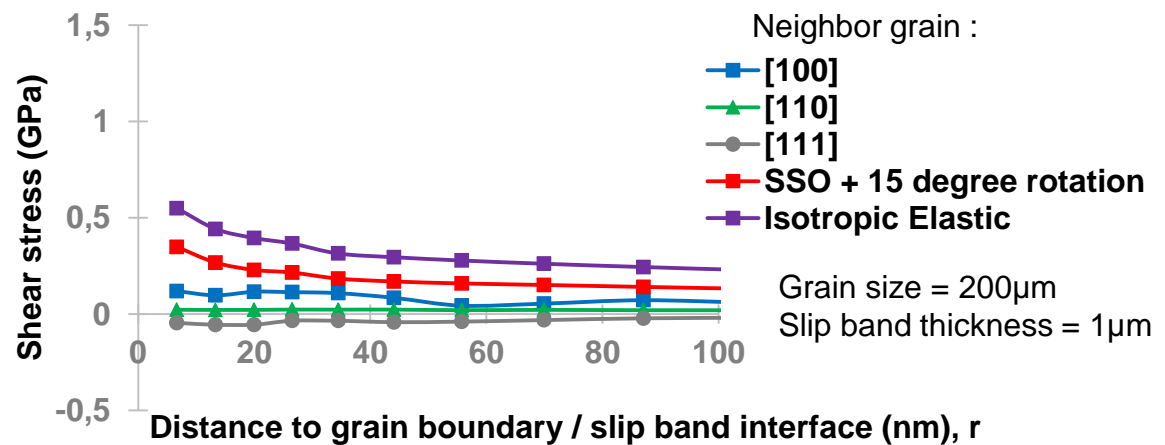
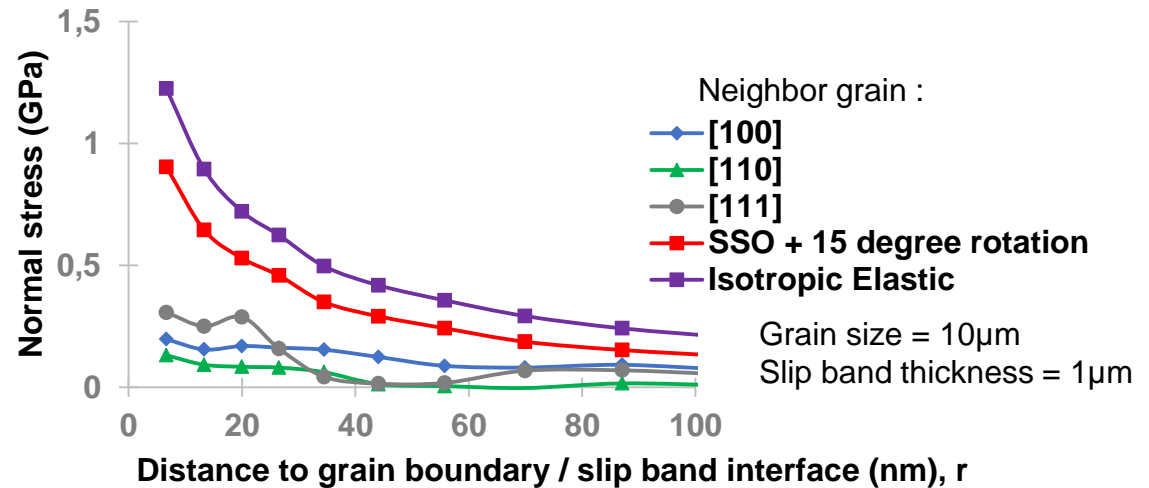
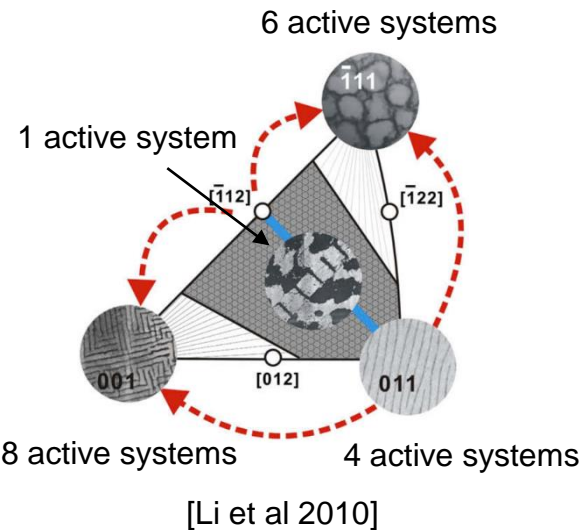
Influence of neighbor grain crystallographic orientation ?

10000 cycles



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

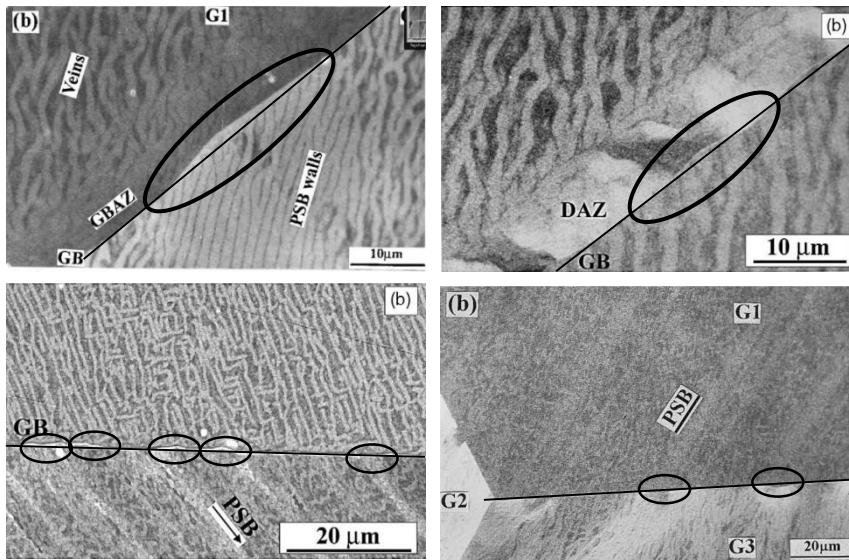
Influence of neighbor grain crystallographic orientation ?



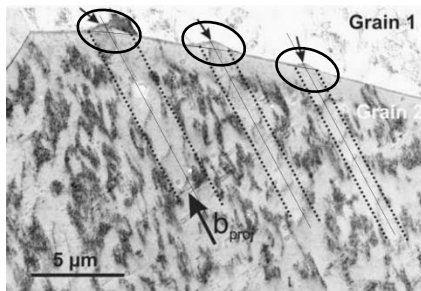
Expected decrease of GB stress fields due to plasticity in the neighbor grain

RESULTS: PREDICTION OF MECHANICAL FIELDS

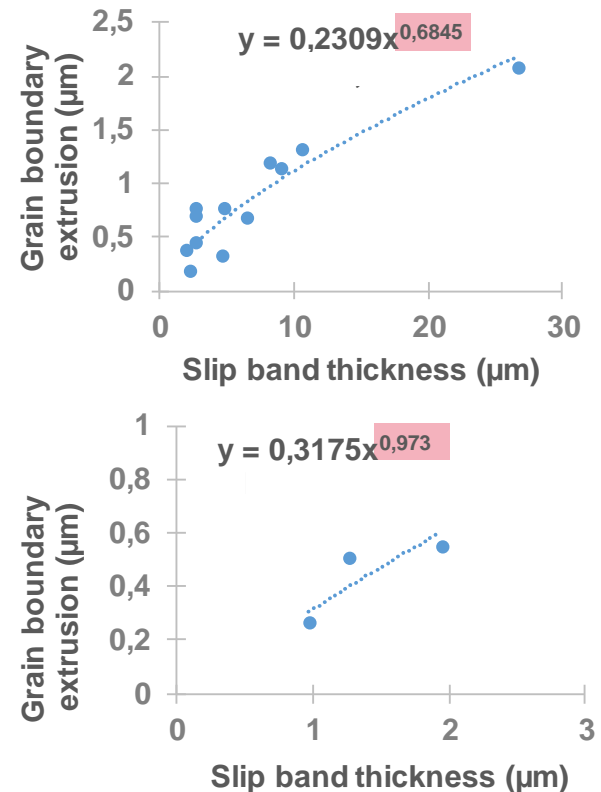
Comparison of the prediction to experimental data from literature :
Impact of PSB thickness on GB extrusion height ?



[Zhang & Wang]



[Weidner et al. 2010]

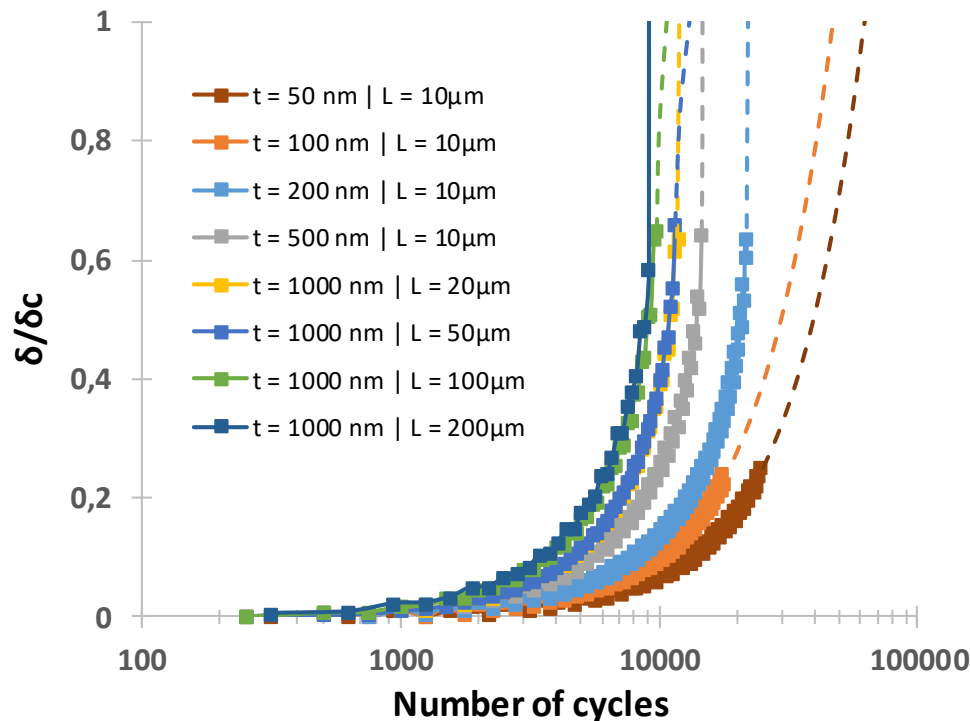


Exponents adjusted using experimental data in reasonable agreement with the exponents provided by the FE computations ~0.7

- CONTEXT & GOAL
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 - **Prediction of crack initiation**
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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 (μm)	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 (μm)	L (μm)	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)

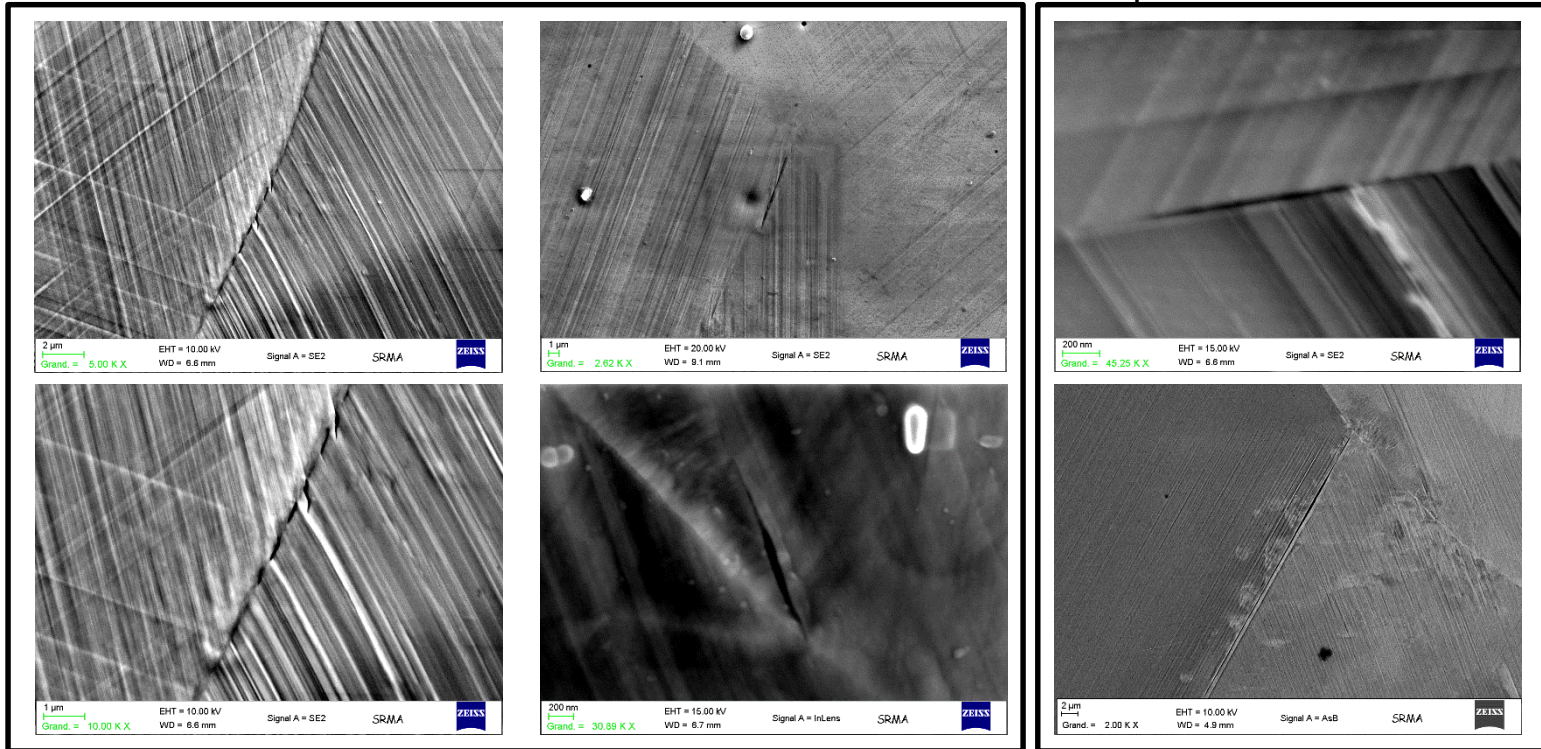
Work in progress :

- 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 ?**

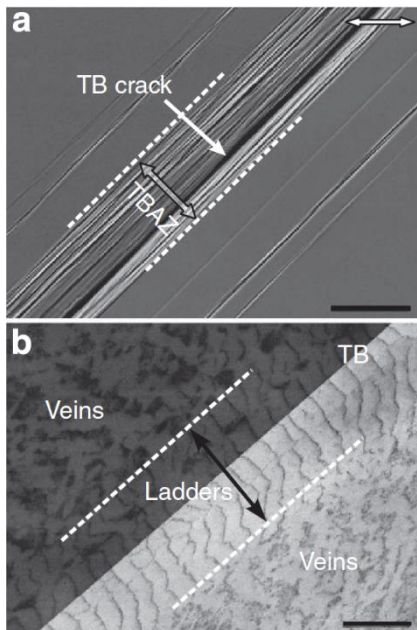
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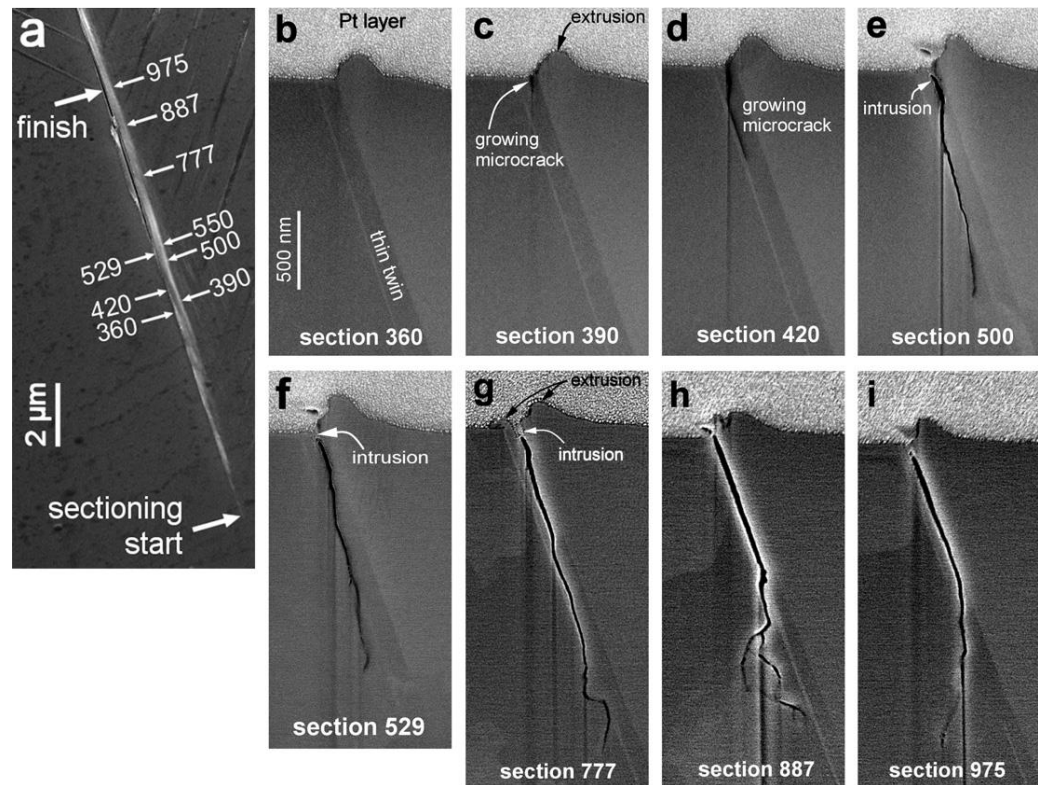
Nuclear Energy Division
Nuclear Material Department
Section for Applied Metallurgy Research
Materials Mechanical Analysis Laboratory

=> Case of HCF & VHCF

Same methodology applicable for twin boundary cracking



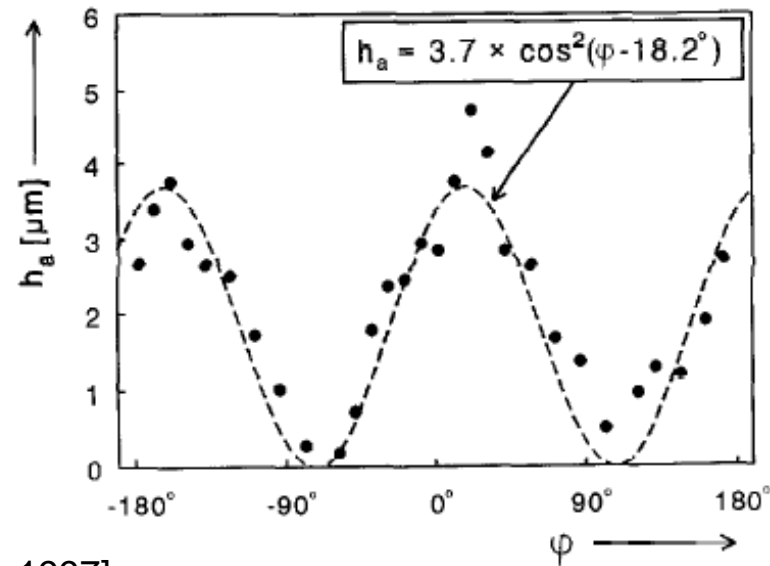
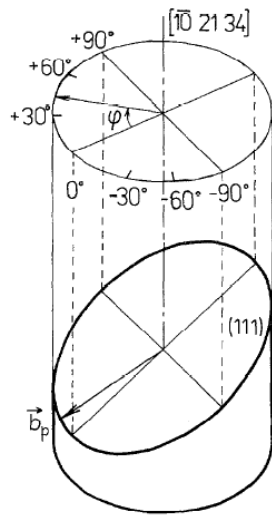
[Li et al. 2014]



[Man et al. 2012]

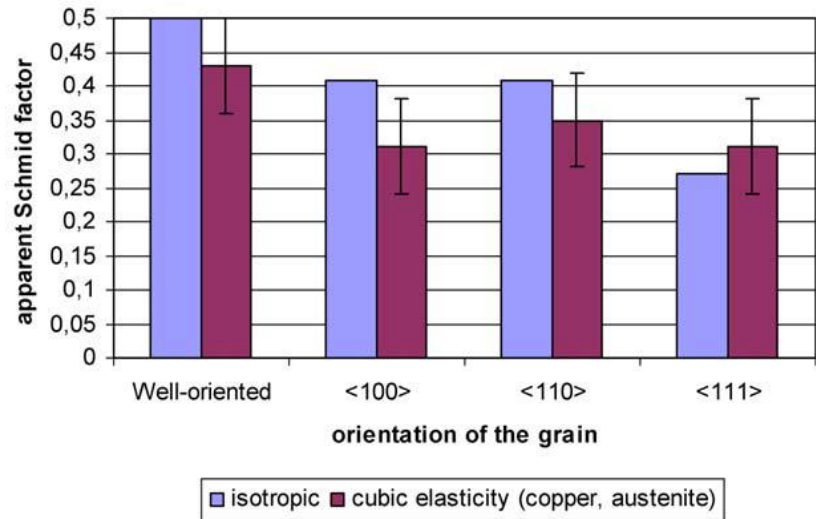
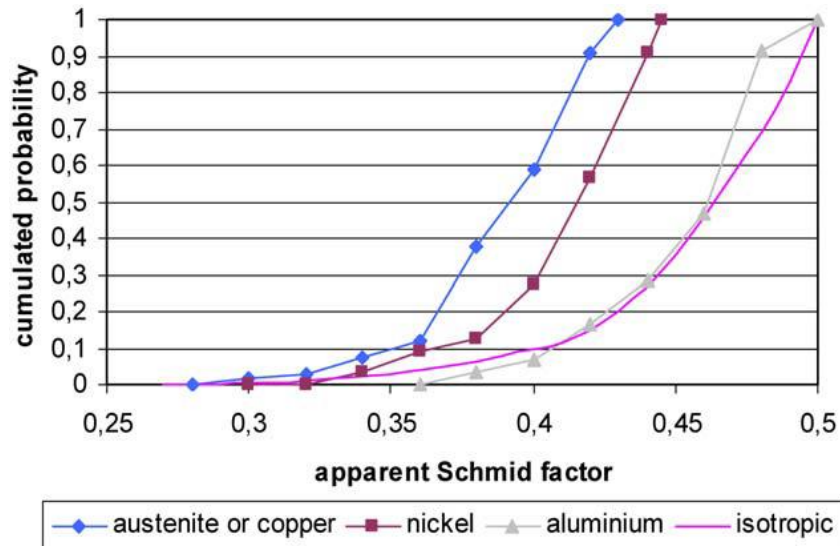
Cylindrical Copper single crystal cyclically deformed :

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



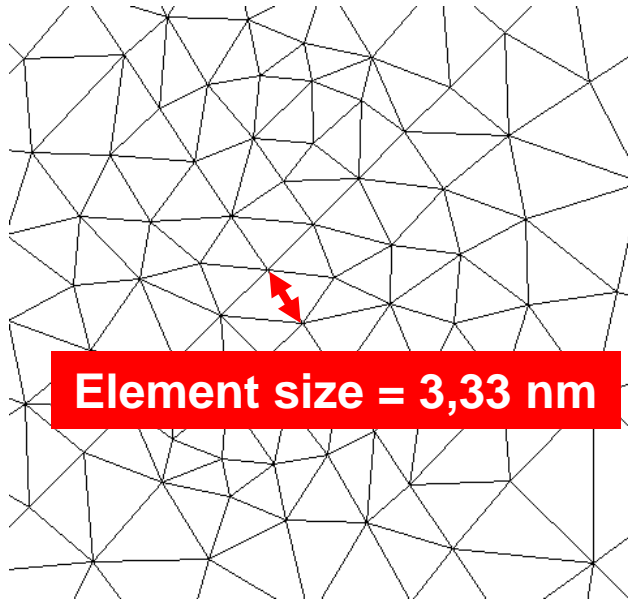
[Obtlik et al, 1997]

NUMBER OF GRAINS CONTAINING PSBs



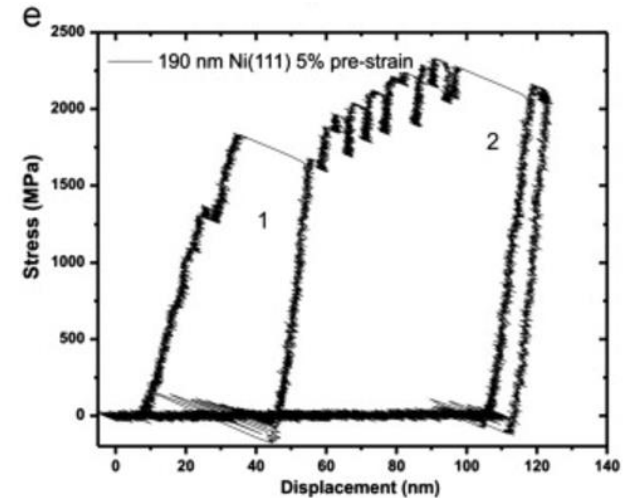
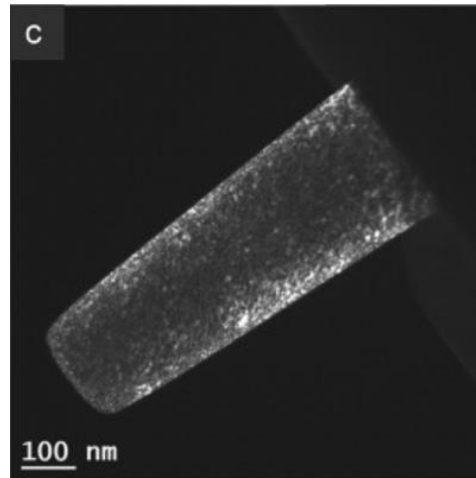
[Sauzay 2006]

Why matrix is supposed to be elastic ?



Element size = 3,33 nm

Compression test on Ni micropillar [Legros 2014]

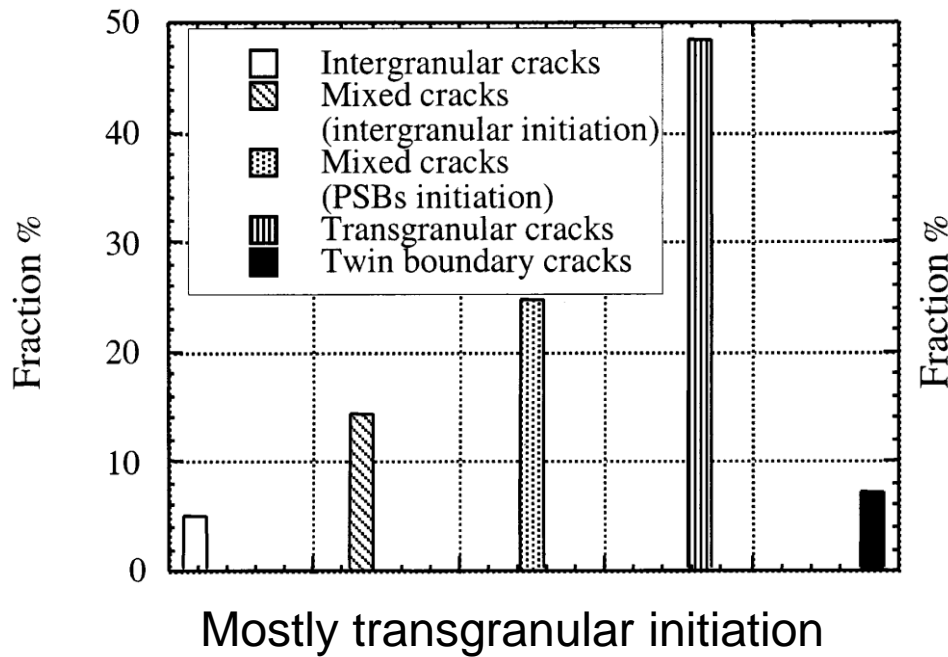


$$10^{13} \text{ m}^{-2} < \rho_{\text{Matrix}} < 10^{15} \text{ m}^{-2}$$

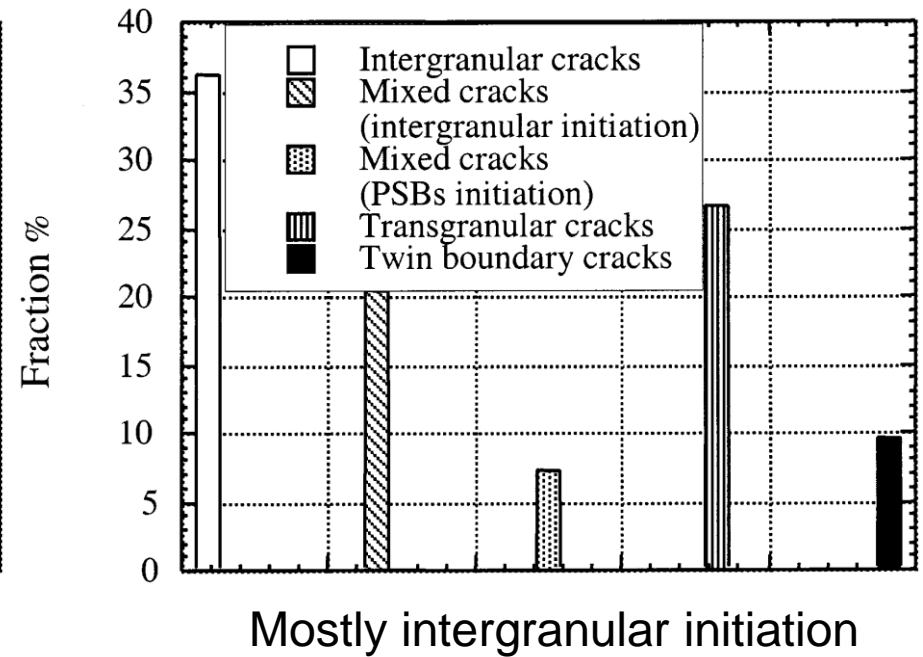
$$N_{\text{dislocation, max}} = 3.33 \cdot 10^{-10} \times 3.33 \cdot 10^{-10} \times 10^{15} = 1.1 \cdot 10^{-4} \approx 0 \text{ dislocation}$$

ENVIRONMENT EFFECT ON MICRO-CRACK INITIATION

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



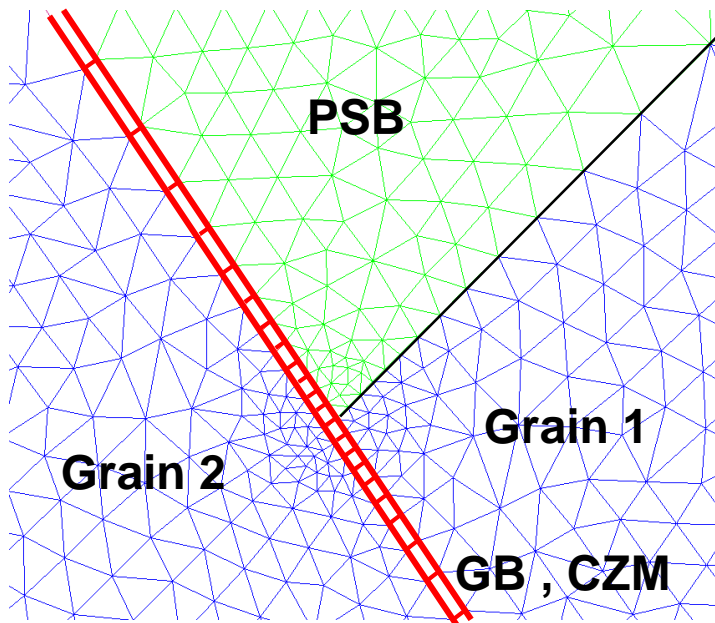
Vacuum, RT, $\Delta\epsilon_p/2 = 2.10^{-3}$



[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 ¹¹	1.8 10 ¹¹	1.9 10 ¹¹
E _{GB} min (Pa)	5.9 10 ¹⁰	8.1 10 ¹⁰	8.6 10 ¹⁰
E _{GB} max (Pa)	1.3 10 ¹¹	1.8 10 ¹¹	1.9 10 ¹¹
d _{GB} min (Å)	3	3	3
d _{GB} max (Å)	7	7	7
γ _{surf} min (J/m ²)	1.9	2	2
γ _{surf} max (J/m ²)	2.2	2.4	3
γ _{GB} min (J/m ²)	0.3	0.45	0.48
γ _{GB} max (J/m ²)	1	1.4	1.6
γ_{frac} (J/m²) min	2.8	2.6	2.4
γ_{frac} (J/m²) max	4.1	4.4	5.5
σ_c min (GPa)	5.6	6.4	6.3
σ_c max (GPa)	15	19	22

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