Prediction of intergranular micro-cracks initiation induced by the impingement of persistent slip bands on grain boundaries

J. Hazan, M. Sauzay

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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CONTENTS

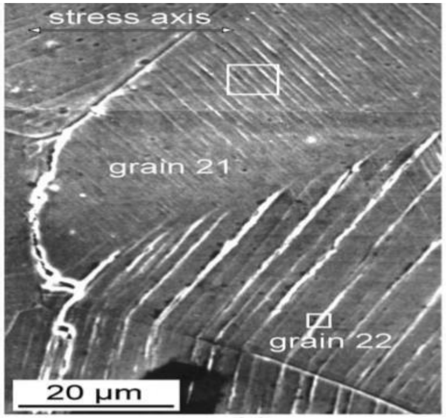
CONTEXT

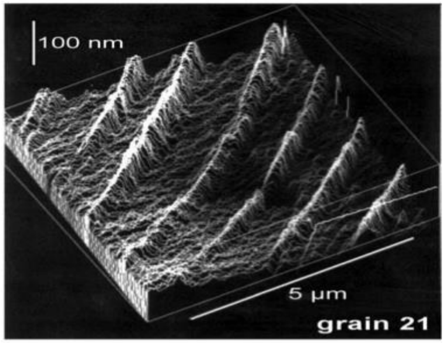
Cyclic deformation induces localization of plastic slip within Persistent Slip Bands (PSBs) for grains oriented for single slip

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

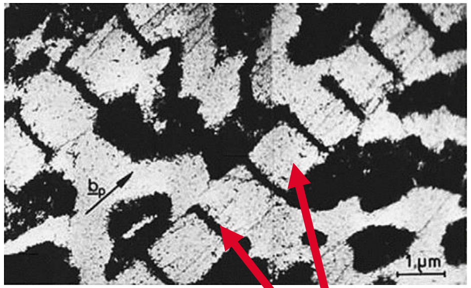
- Elastic matrix
- Elastic-plastic bands (PSBs)

[Man et al. 2002]





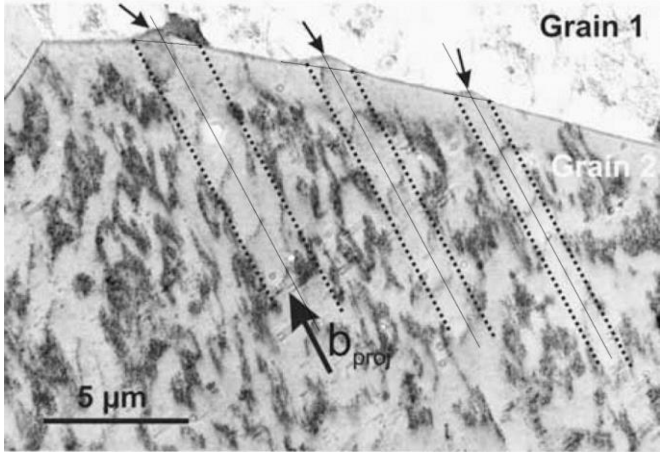
316L SS polycrystal



Copper single crystal

[Mughrabi 1979]

Poor channels(~10^{13} m^{-2}) rich walls(~10^{15} m^{-2}) : Ladder like structure

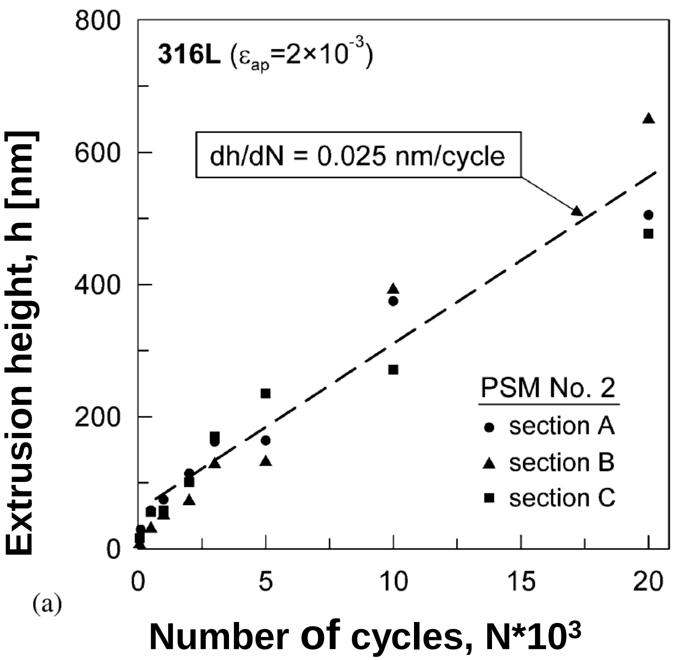


Nickel polycrystal

[Weidner et al. 2010]

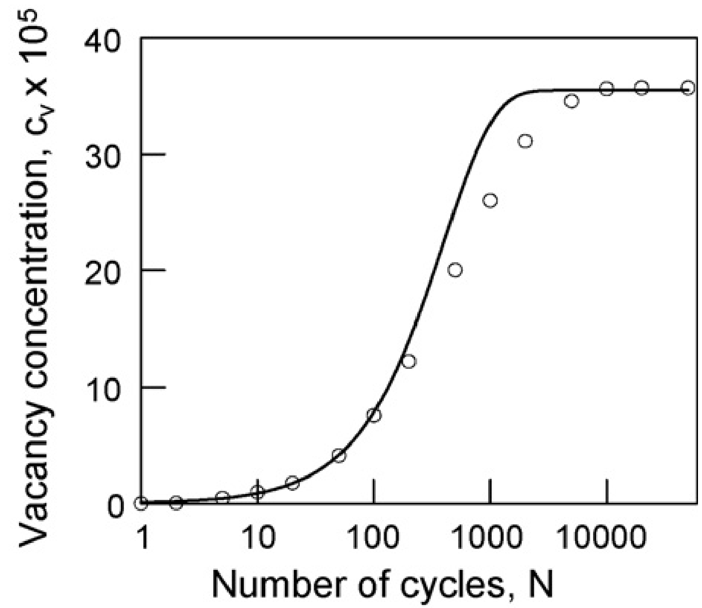
CONTEXT

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

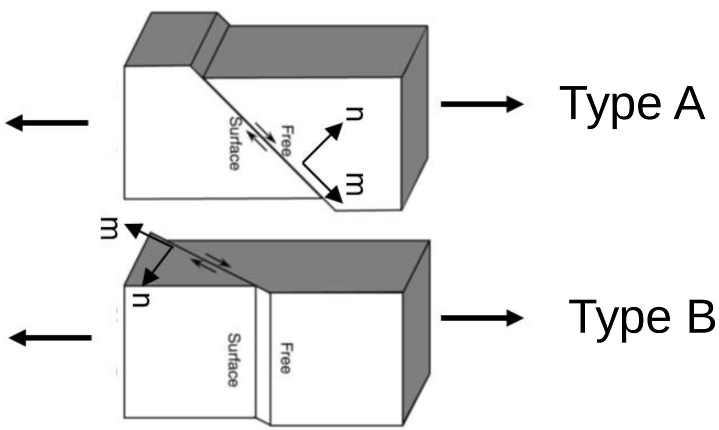


[Man et al. 2003]

Almost constant growth rate of PSBs during cycling



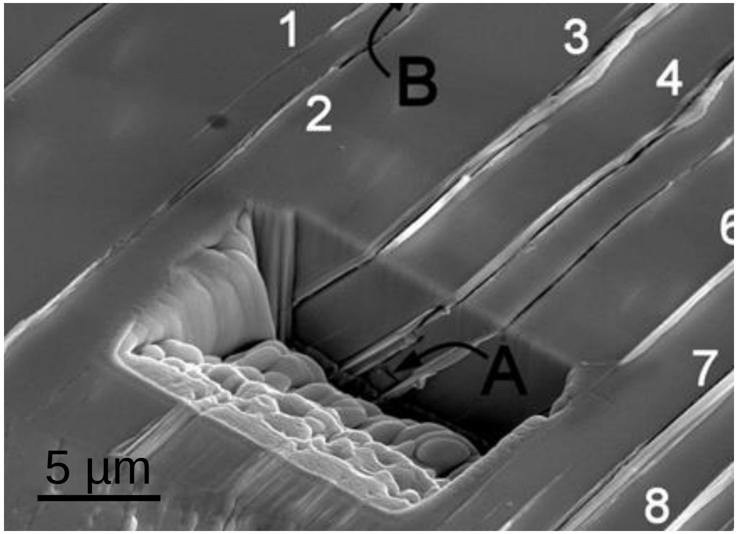
[Polák & Sauzay 2009]



CONTEXT

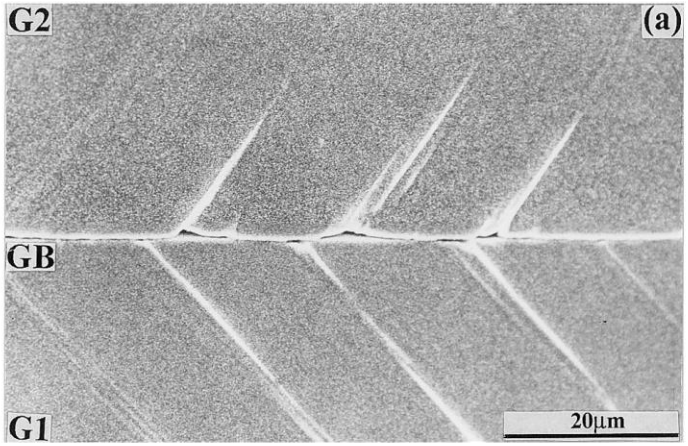
Slip localization in PSBs leads to microcrack initiation (in LCF):

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

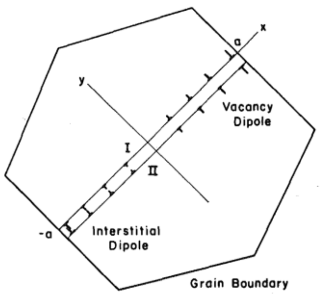
- ➢ Prediction of GB extrusions and GB stress fields

Transgranular initiation treated by [Liu & Sauzay 2014]

CONTEXT: EXISTING MODELS

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

- Tanaka & Mura 1981

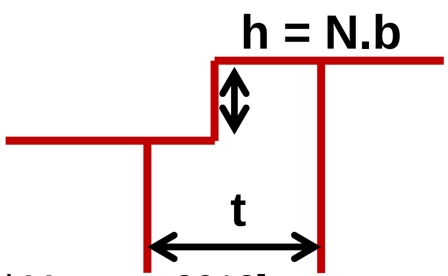


$$Ni = \frac{8\,\mu\,\gamma_{eff}}{2\,\pi\,(1-\nu)\,a\,(\Delta\tau\ - 2\tau_f)^2}$$

Cyclic deformation causes ratcheting of dislocations at grain boundaries

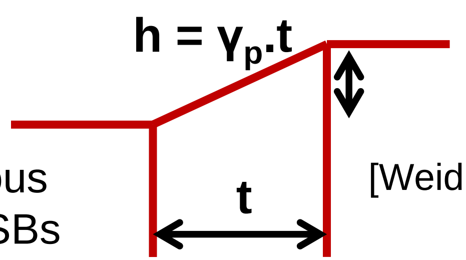
- Sangid et al. 2011 (Molecular Dynamics input for dislocation absorption and nucleation at GB)

PSB containing Pile-up



[Sauzay & Ould Moussa 2013]

Homogeneous slip within PSBs



[Weidner et al 2006]

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

CONTENTS

METHOD : ELASTIC-PLASTIC MODEL AND BEHAVIOR

Finite Element Calculations based on:

① Mixture rule of Winter:

$$\gamma^p_{cryst} = \gamma^p_{Mat}\, f_{v_{Mat}} + \gamma^p_{PSB}\, f_{v_{PSB}}$$

$$\gamma^p_{Mat} \approx {}^1\!/_{100}\ \gamma^p_{PSB}$$

$$\Rightarrow \gamma^p_{cryst} = \gamma^p_{PSB}\, f_{v_{PSB}}$$

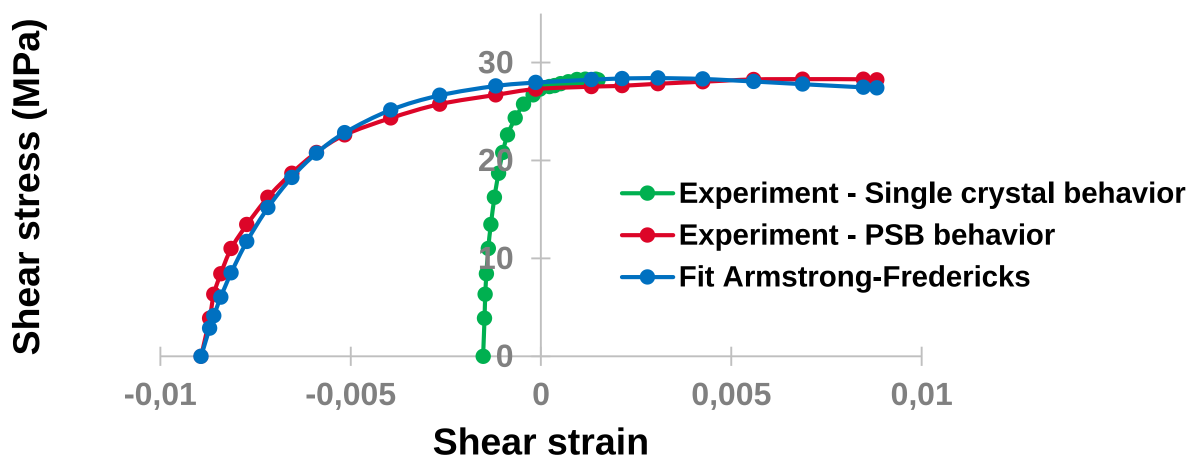
$\Rightarrow$ Localisation of slip in PSBs

② Elastic-Plastic behavior for PSBs

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

$$\delta\chi_i = C\left(\frac{2}{3}A\delta\gamma^p_i - \chi_i\delta\gamma^p_{cum,i}\right)$$

$\Rightarrow$ Plateau behavior



[Mughrabi 1978]

METHOD

Finite Element Calculations based on:

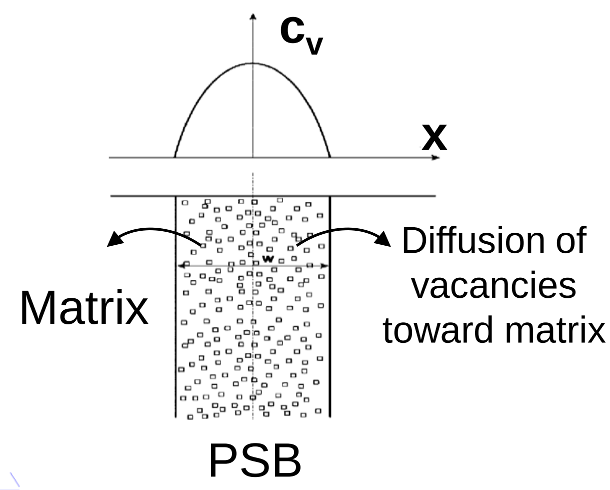
3 Production of vacancies inducing the free dilatation of persistent slip bands

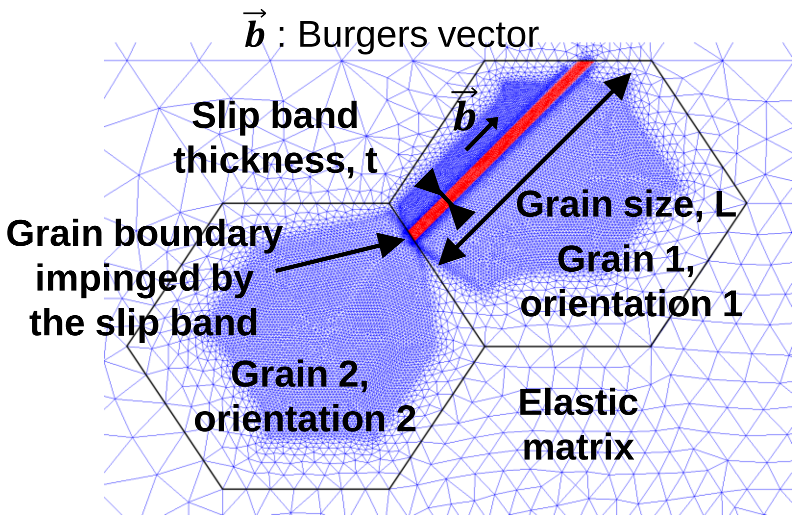
$\Rightarrow$ Resistivity measurements on copper single crystals cycled at 4K [Polák 1987]

$\Rightarrow$ Determination of the vacancy production term [Polák & Sauzay 2009]

p = 3.1 10^{-7} for Copper

$$\varepsilon^{*}_{vacancy} = N_{cycles} * p$$

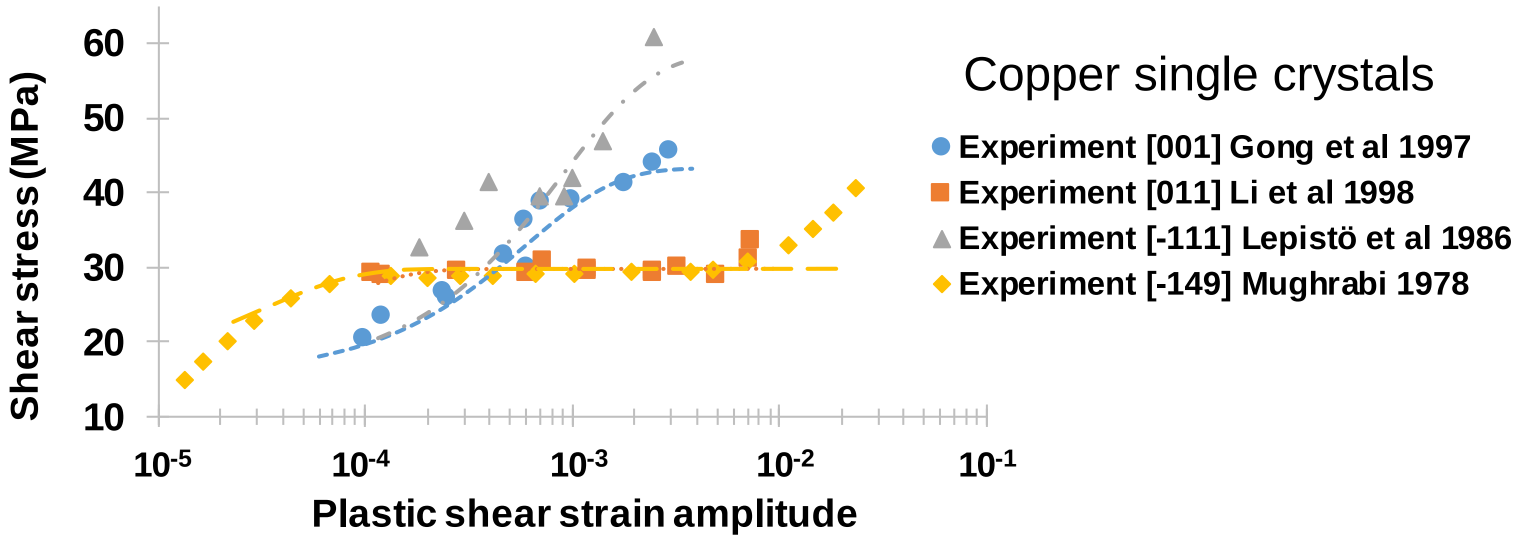




METHOD

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

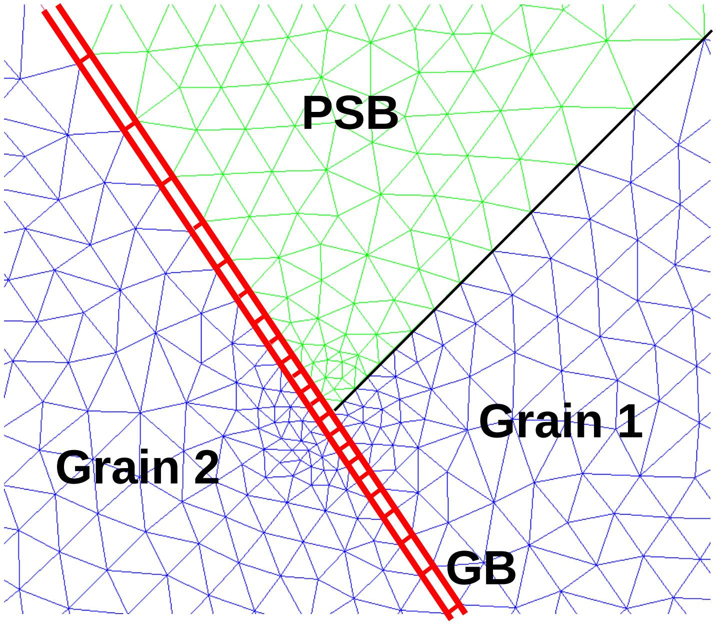
⇒ Elastic-Plastic behavior of neighbor grain

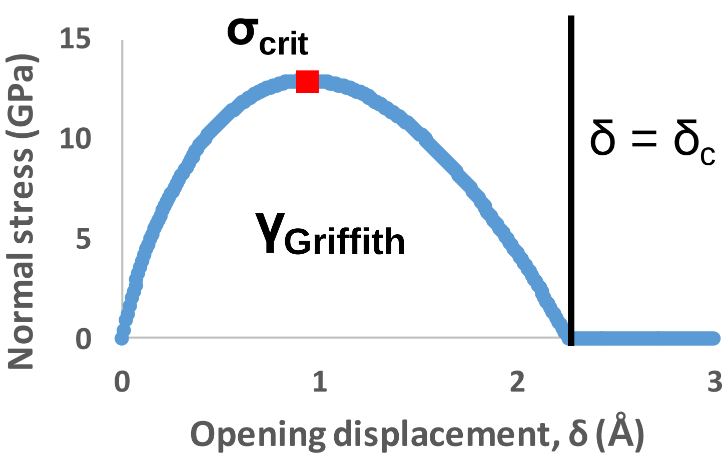
⇒ Elastic matrix

CONTENTS

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

METHOD : COHESIVE ZONE MODELING





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

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

See [Barbé et al 2018]

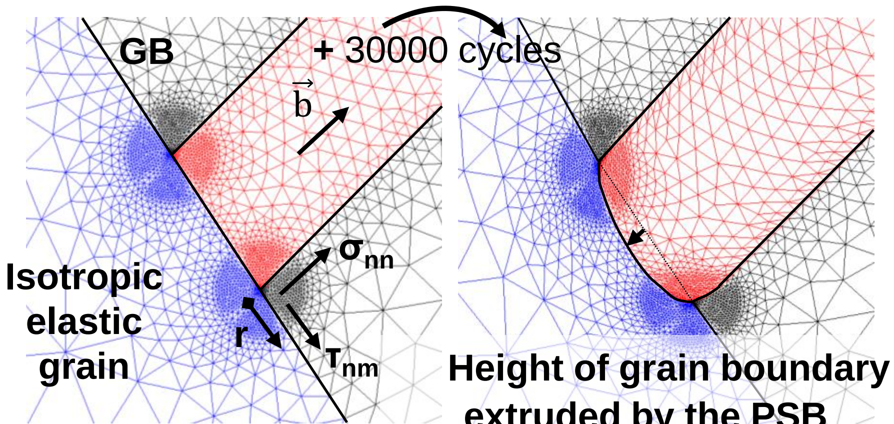
Output: Opening of the interface, δ

=> $\delta/\delta_c = 1$: Complete separation

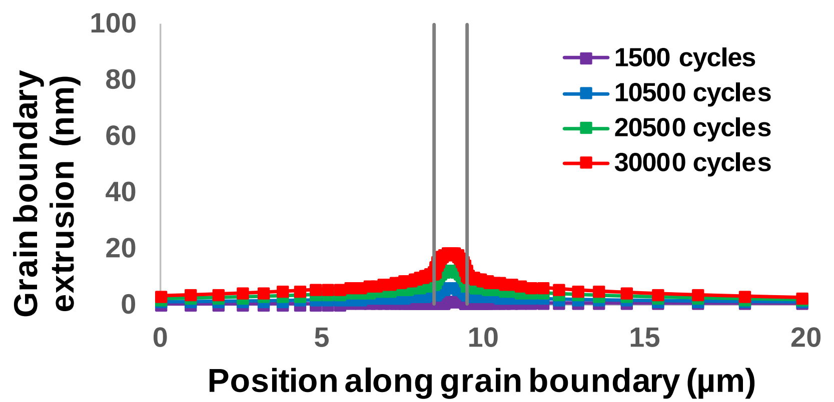
CONTENTS

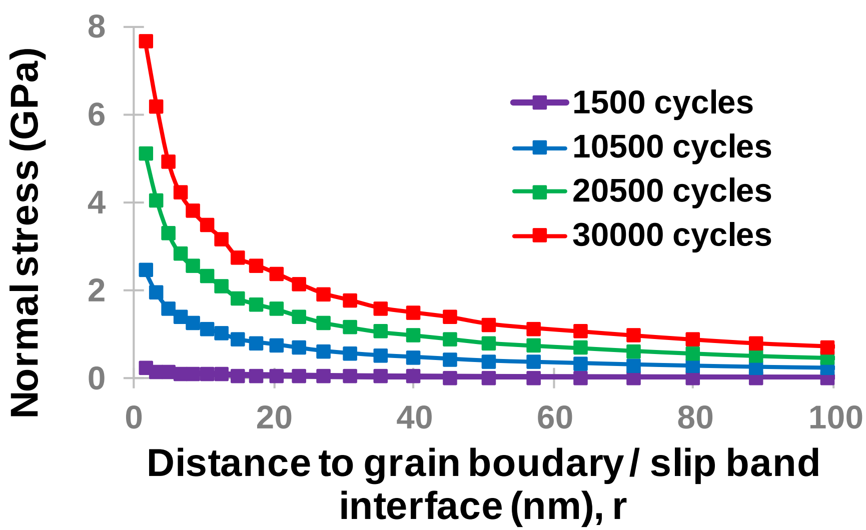
RESULTS : PREDICTION OF MECHANICAL FIELDS

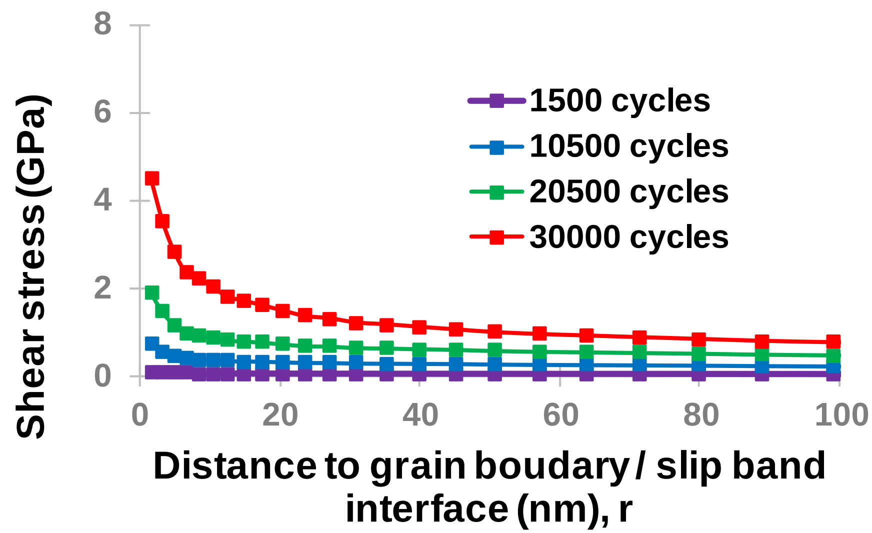
Copper | PSB thickness = 1 µm | Grain size = 50 µm | 30 000 cycles



Height of grain boundary extruded by the PSB impingement





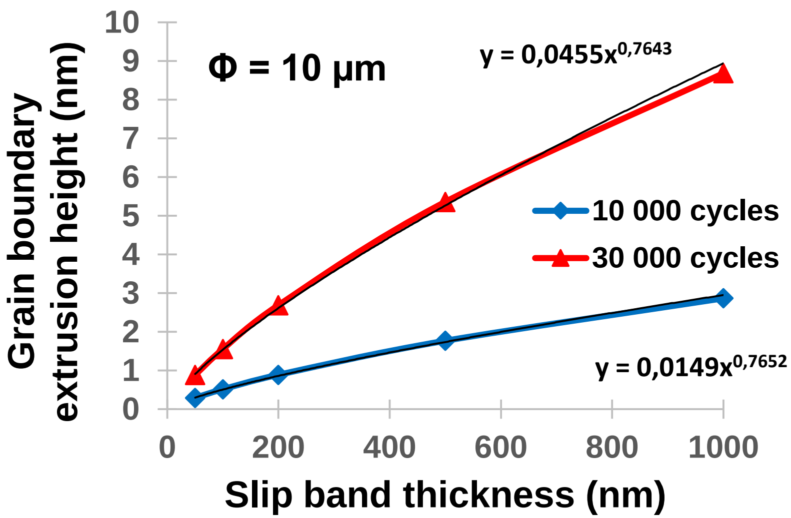


RESULTS: PREDICTION OF MECHANICAL FIELDS

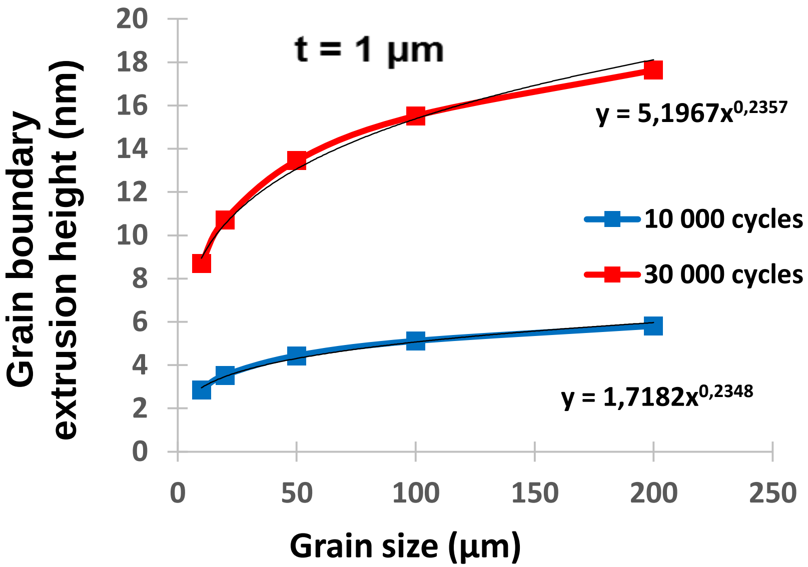
Influence of the persistent slip band characteristic lengths:

=> grain boundary extrusion

Influence of slip band thickness, t



Influence of grain size, L



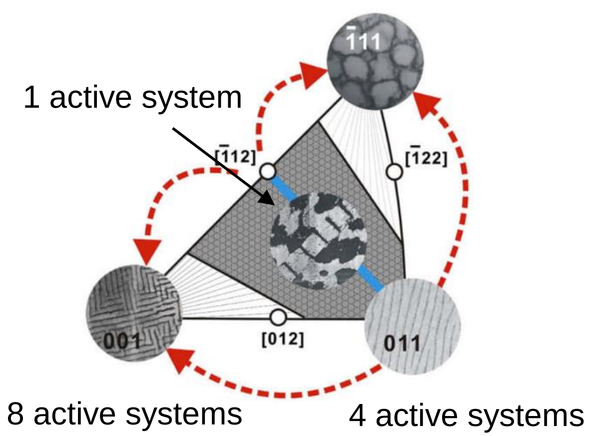
$$\boldsymbol{h\,(N) = 0,56\,.\,p.\,N.\,t^{0,77} * L^{(1-0,77)}}$$

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

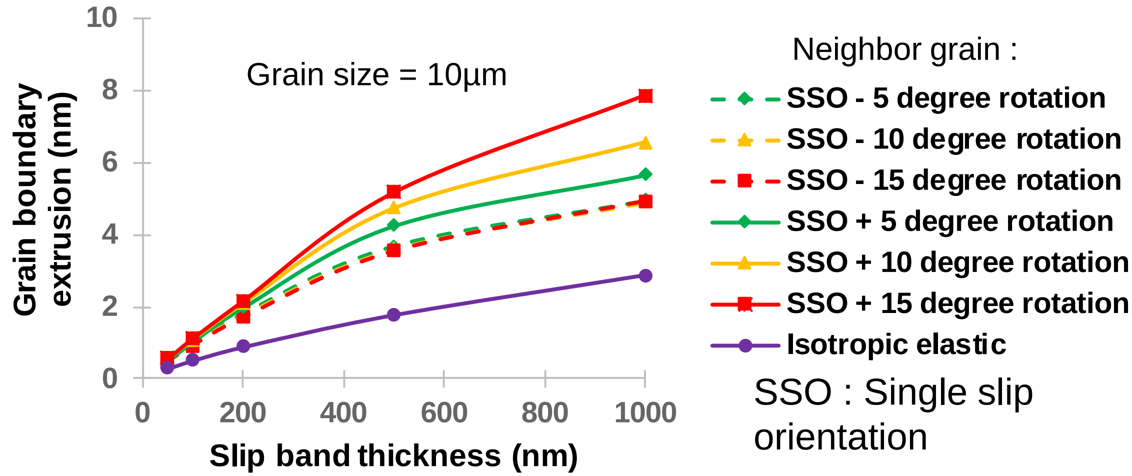
RESULTS: PREDICTION OF MECHANICAL FIELDS

Influence of neighbor grain crystallographic orientation ?

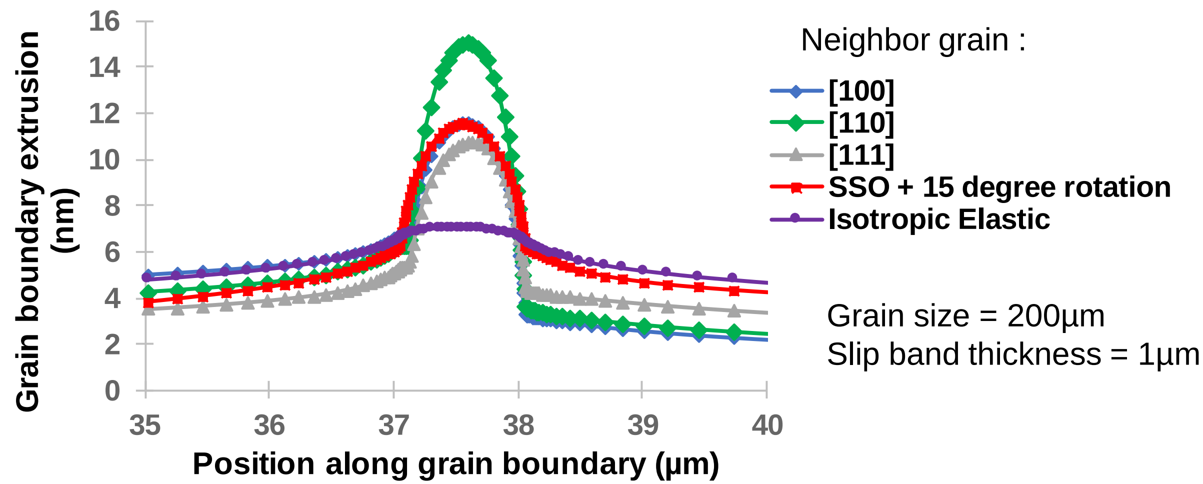
10000 cycles



[Li et al 2010]



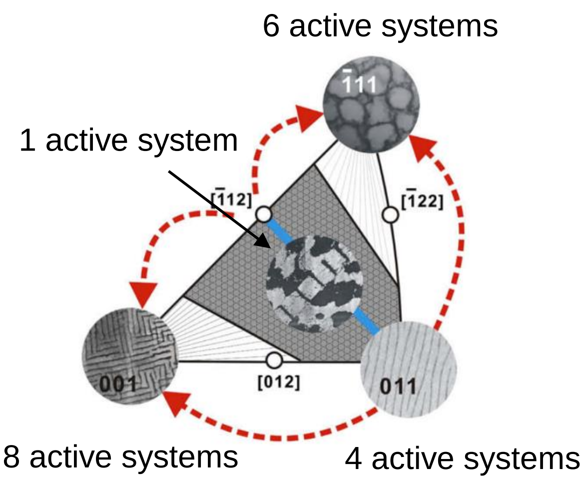
SSO : Single slip orientation



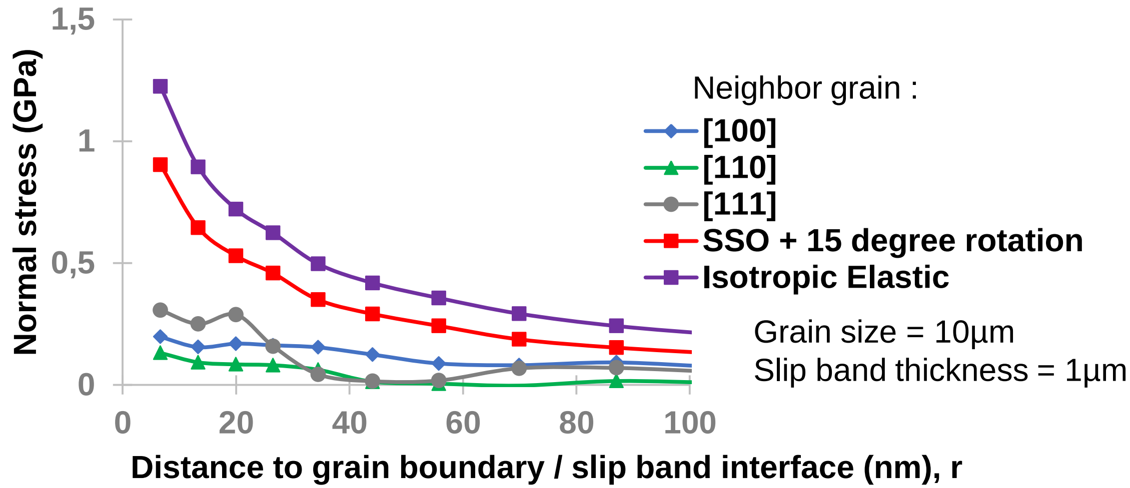
High increase in the grain boundary extrusion due to plasticity in the neighbor grain

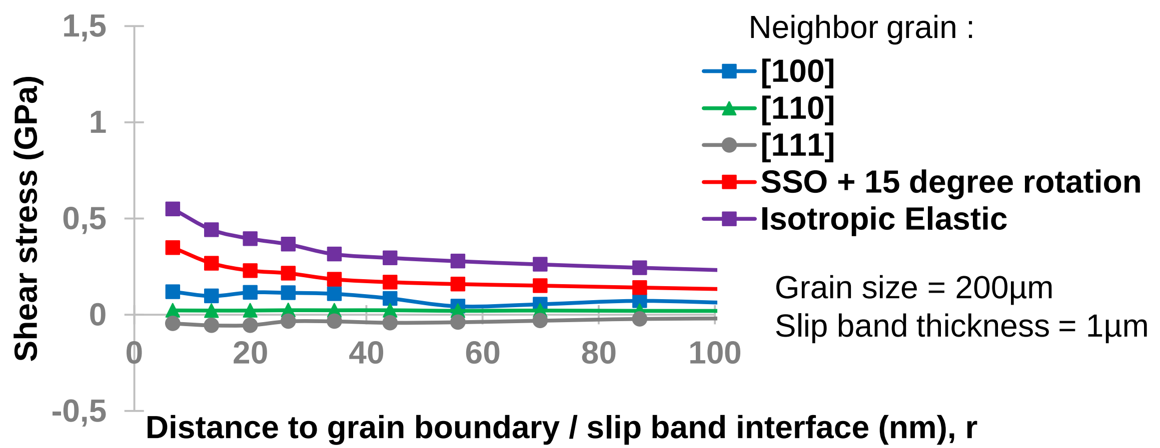
RESULTS: PREDICTION OF MECHANICAL FIELDS

Influence of neighbor grain crystallographic orientation ?



[Li et al 2010]

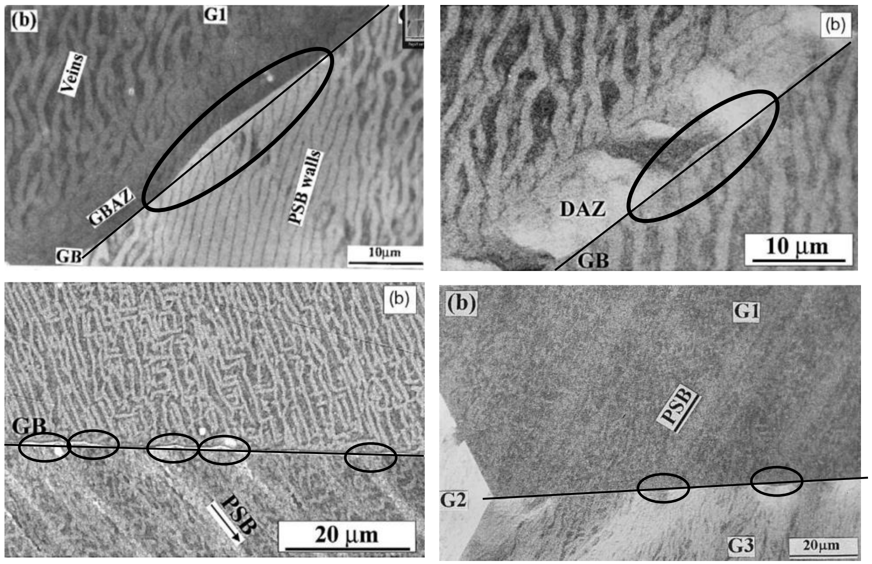




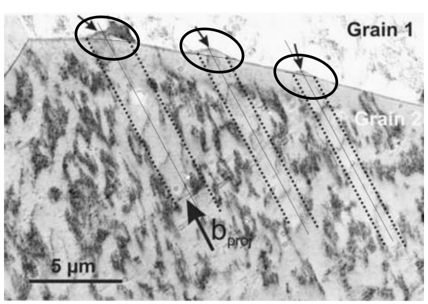
Expected decrease of GB stress fields due to plasticity in the neighbor grain

RESULTS: PREDICTION OF MECHANICAL FIELDS

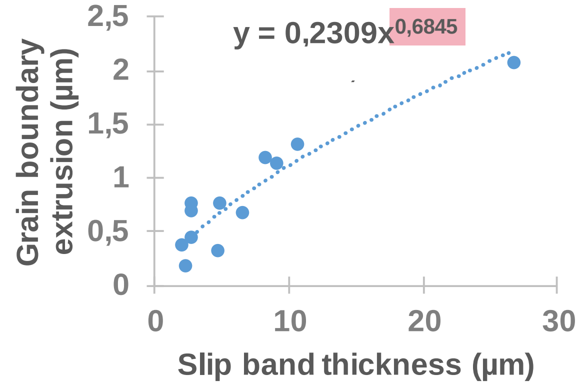
Comparison of the prediction to experimental data from literature :
Impact of PSB thickness on GB extrusion height ?

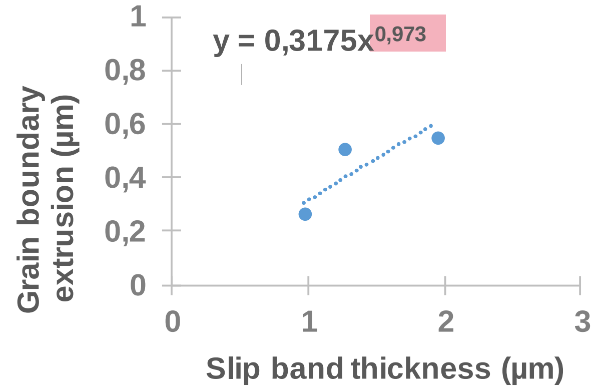


[Zhang & Wang]



[Weidner et al. 2010]





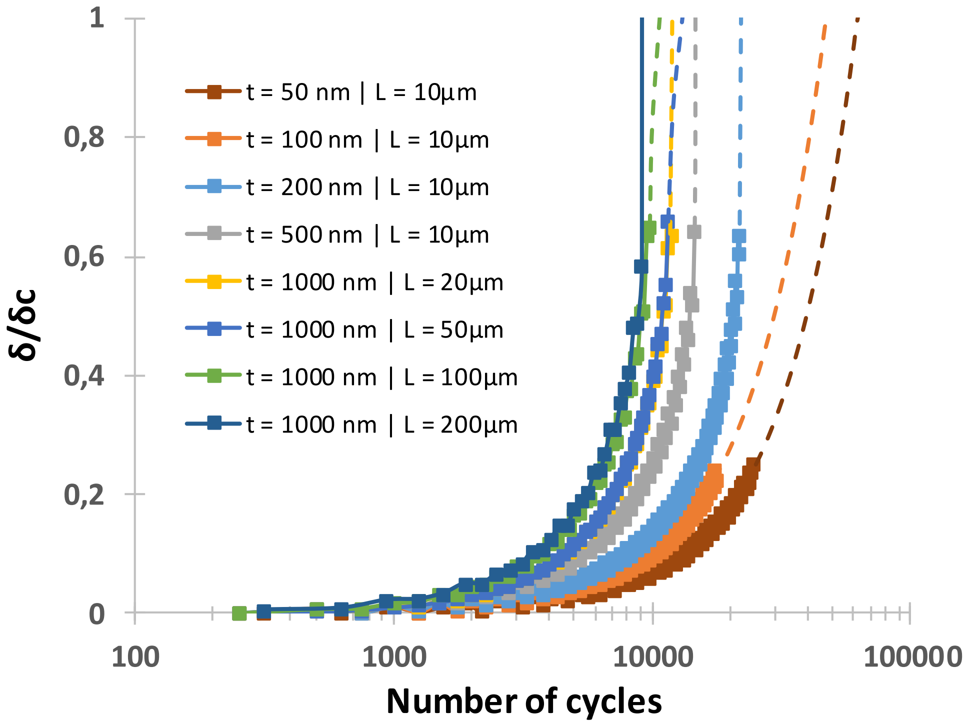
Exponents adjusted using experimental data in reasonable agreement with the exponents provided by the FE computations ~0.7

CONTENTS

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

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

First prediction are in the good order of magnitude
=> Precise microstructure needed for more precise comparison

CONTENTS

CONCLUSIONS & WORK IN PROGRESS

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 :

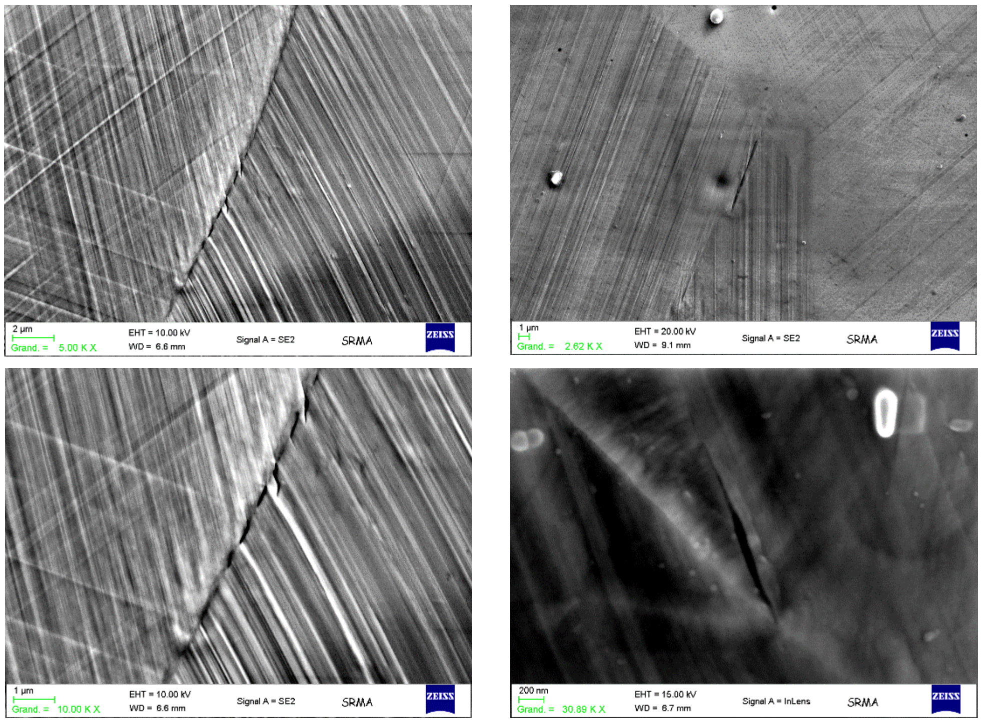
- Prediction of intergranular initiation introducing atomistic considerations in the calculations as M.Sangid did [Sangid et al. 2011]
  - GB type, environment, material, etc.
- Interrupted fatigue test carried out on two 316L SS containing (i) very large grains and (ii) small grains
  - EBSD scan + SEM observations of crack-initiations

  $\Rightarrow$ Comparison of predictions to real cases microstructures
- Analytical model for the prediction of intergranular, transgranular and twin boundaries microcrack initiation

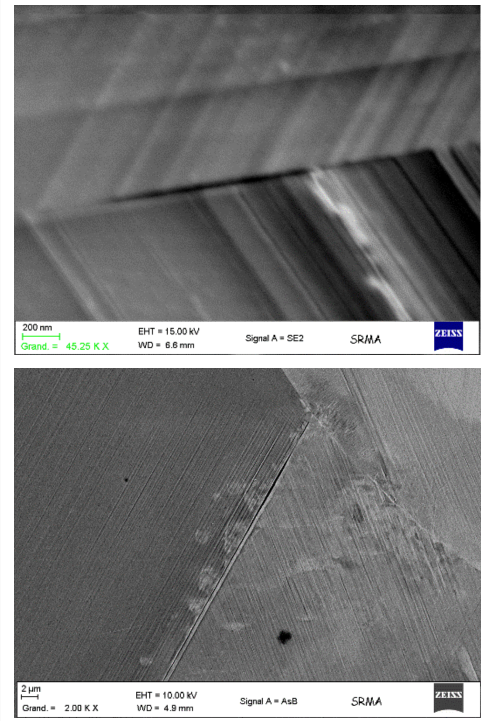
Interrupted fatigue test :

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

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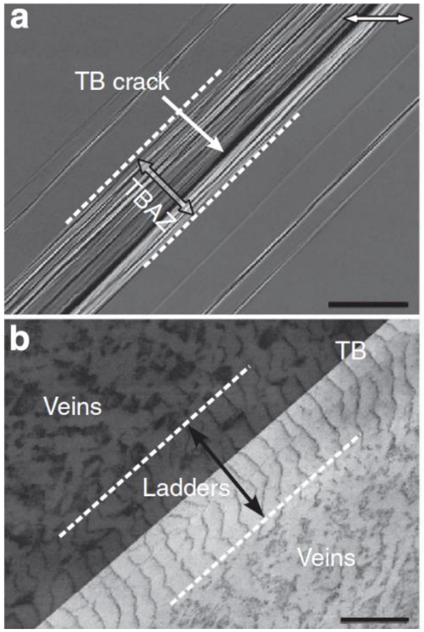
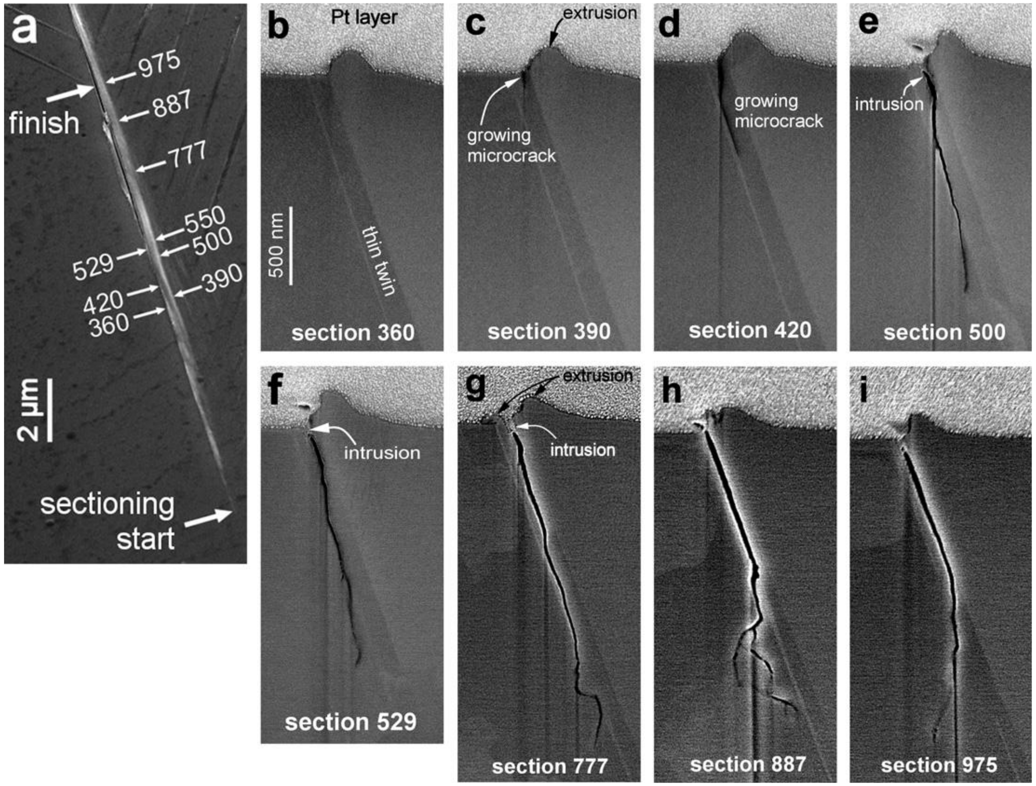
Nuclear Energy Division
Nuclear Material Department
Section for Applied Metallurgy Research
Materials Mechanical Analysis Laboratory

=> Case of HCF & VHCF

Same methodology applicable for twin boundary cracking



[Li et al. 2014]



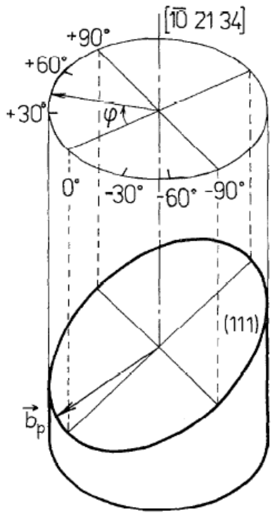
[Man et al. 2012]

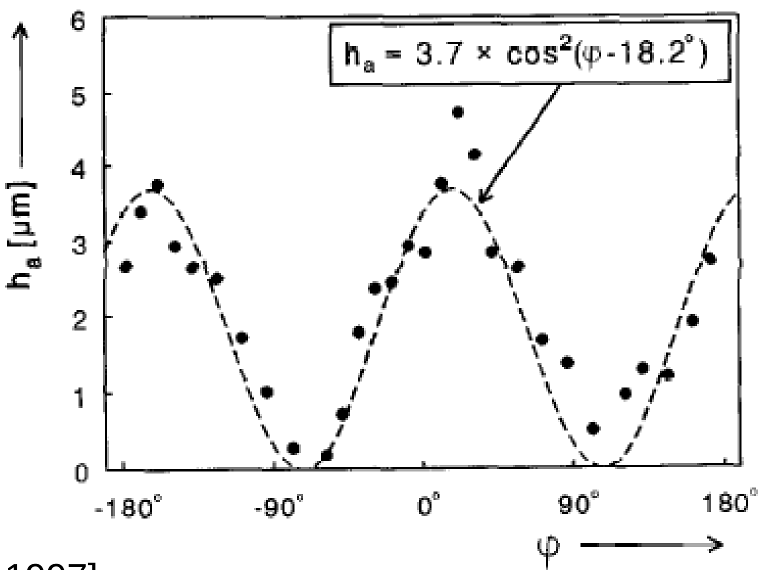
TRANSGRANULAR OR INTERGRANULAR INITIATION ?

Cylindrical Copper single crystal cyclically deformed :

- Each peak is offset by 180°

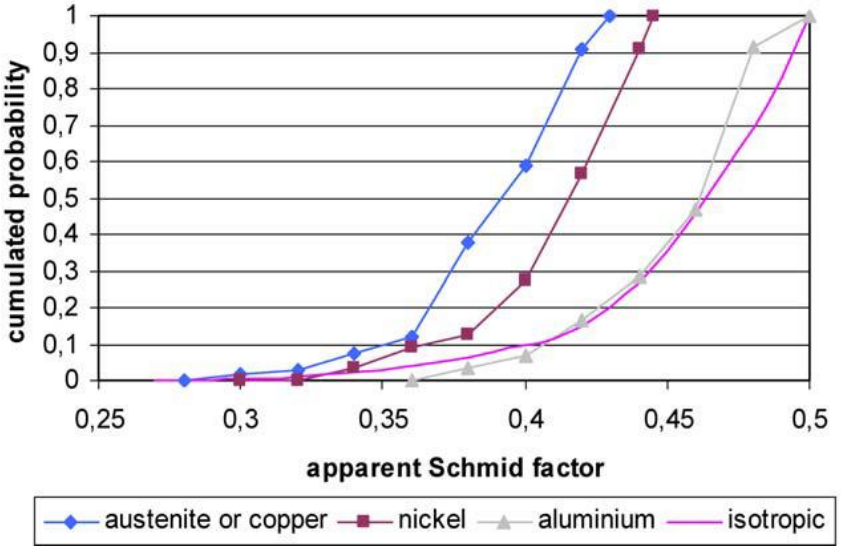
=> Preferential direction of slip

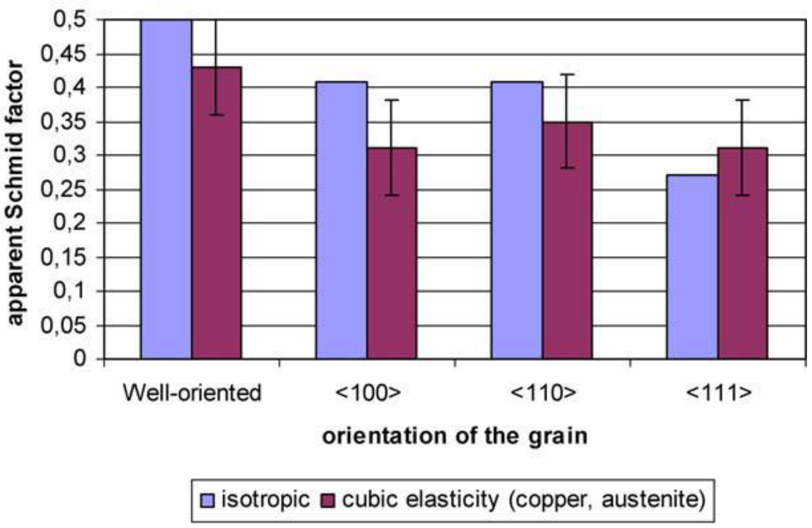




[Obrtlik et al, 1997]

NUMBER OF GRAINS CONTAINING PSBs

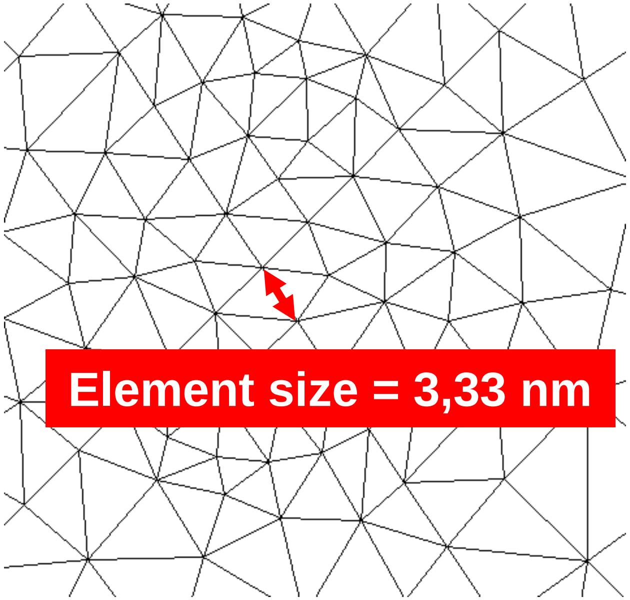




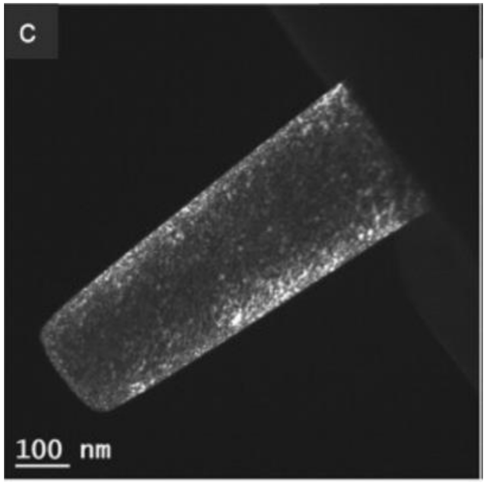
[Sauzay 2006]

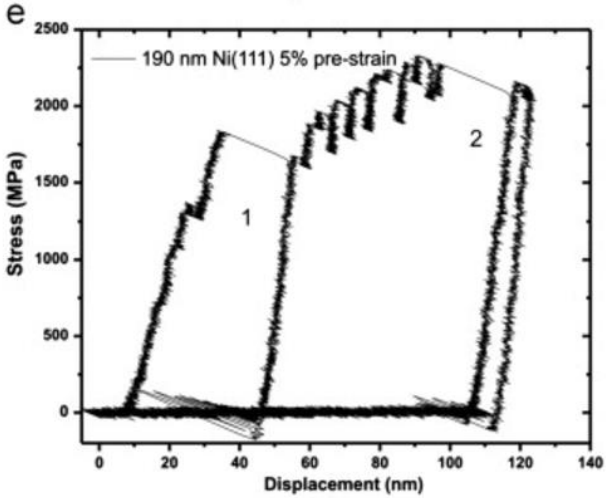
VALIDITY DOMAIN ?

Why matrix is supposed to be elastic ?



Compression test on Ni micropillar [Legros 2014]



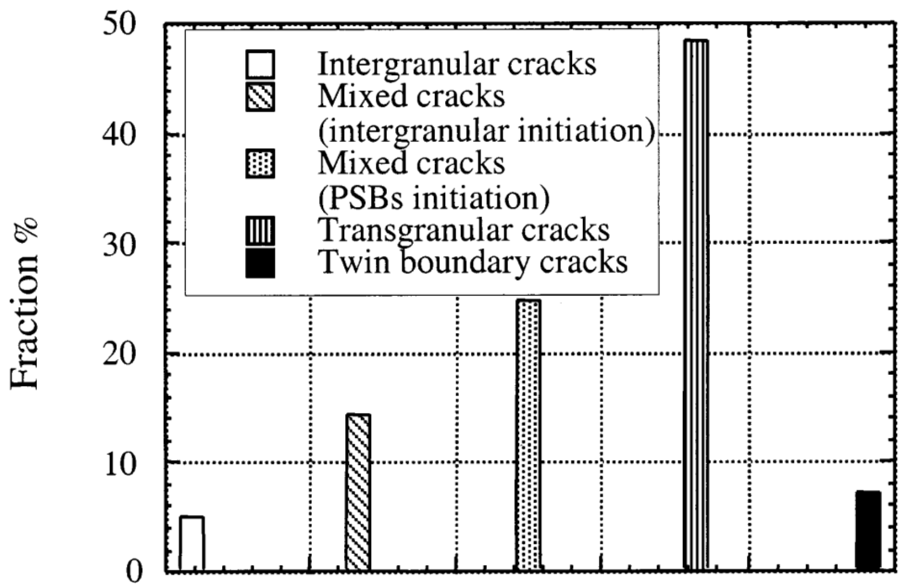


$10^{13}\ m^{-2} < \rho_{Matrix} < 10^{15}\ m^{-2}$

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

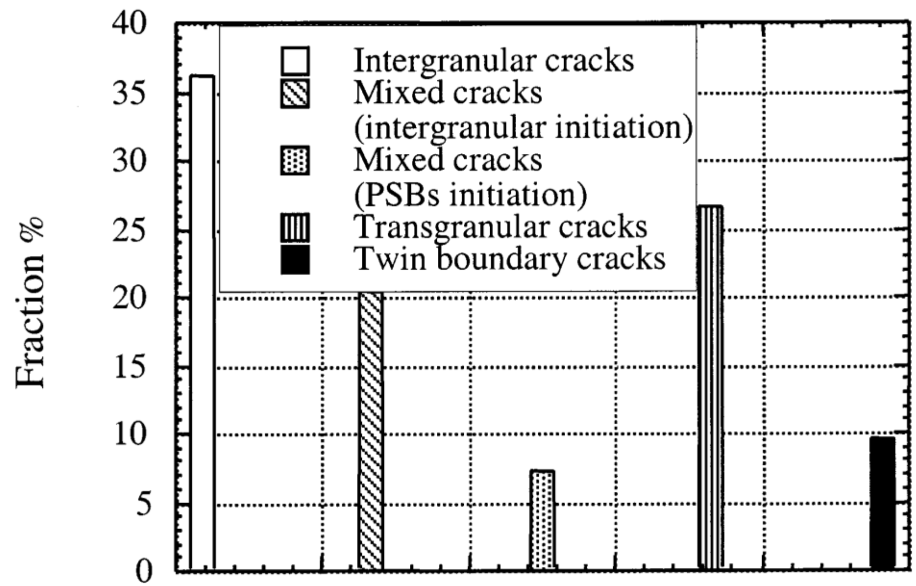
ENVIRONMENT EFFECT ON MICRO-CRACK INITIATION

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



Mostly transgranular initiation

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

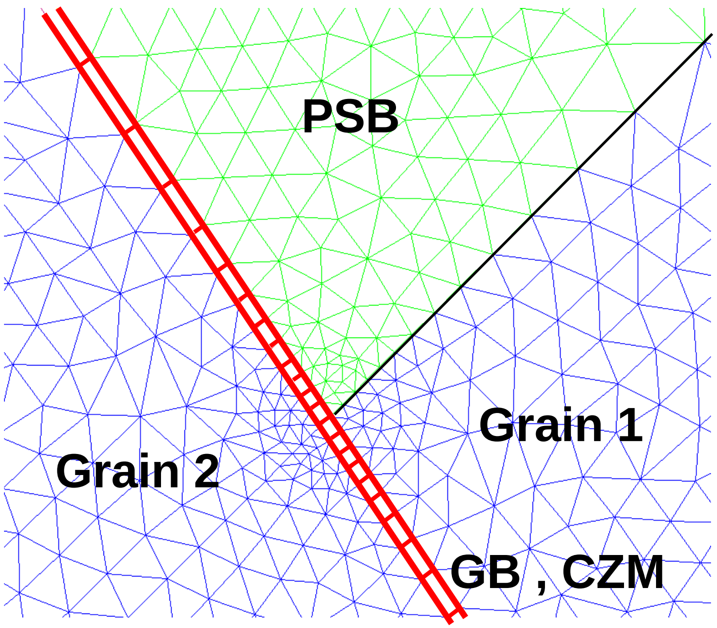


Mostly intergranular initiation

[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/m²)	1.9	2	2
γ_{surf} max (J/m²)	2.2	2.4	3
γ_{GB} min (J/m²)	0.3	0.45	0.48
γ_{GB} max (J/m²)	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]

METHOD : COHESIVE ZONE MODEL

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