SOTERIA FINAL WORKSHOP

DOSE-DEPENDENT NANO-FEATURES AND THEIR EFFECT ON INTER-GRANULAR CRACKING SUSCEPTIBILITY (INTERNALS)

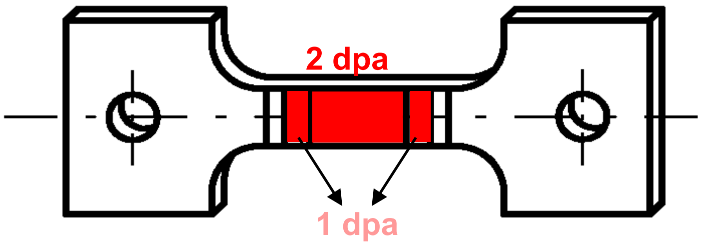
OUTLINE

- Previous findings, up to PERFORM60 (up to 2012)
- Subsequent sub-grain modelling developments (2012-)
- Observations and poly-crystalline model (SOTERIA 2015-2019)

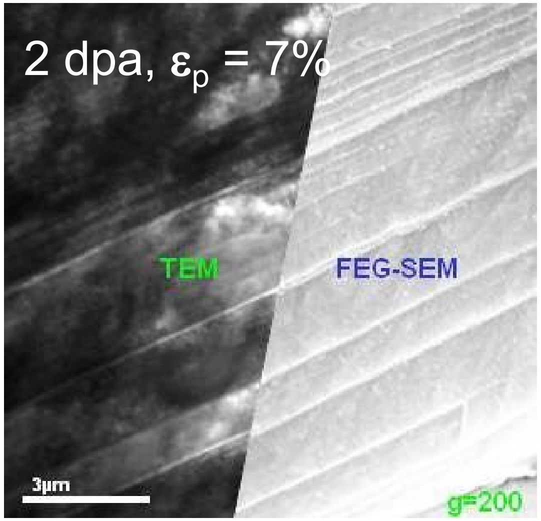
Contribution to SOTERIA WP2
Co-workers: B. Tanguy, J. Hure
Speaker: **Christian Robertson**

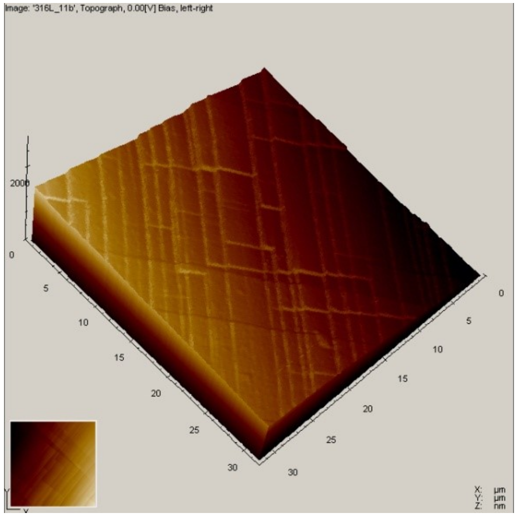
Post-irradiation plasticity mechanisms

Ions irradiations: p+ or Fe^{8+}, 300 °C

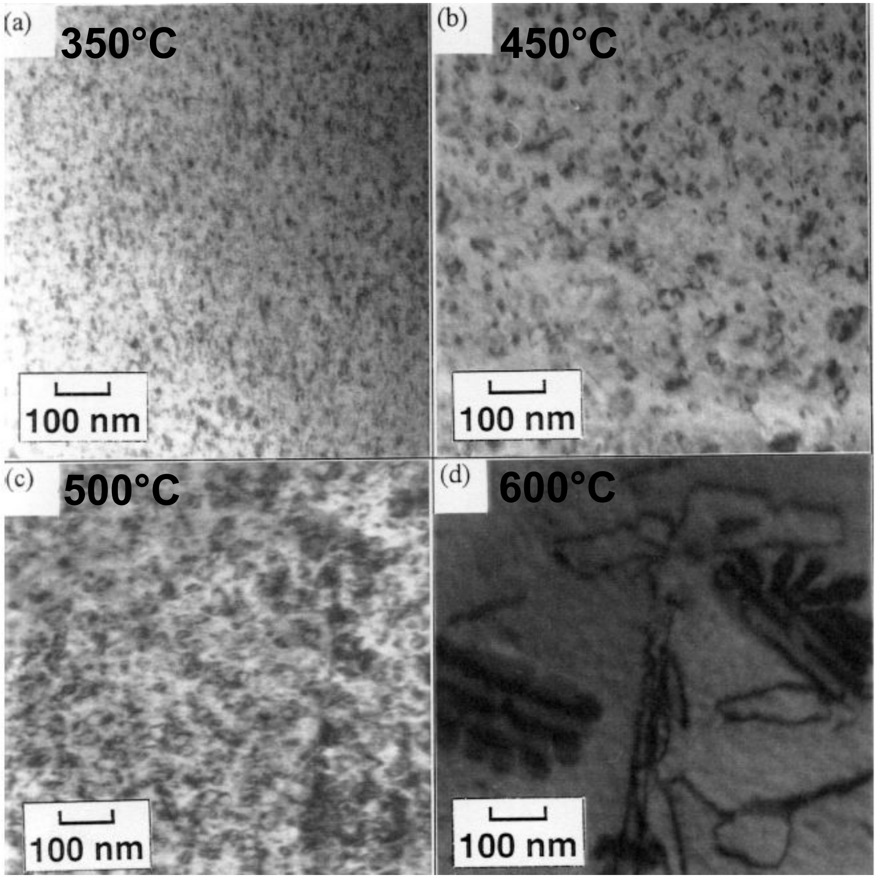


Ion irradiations & observations

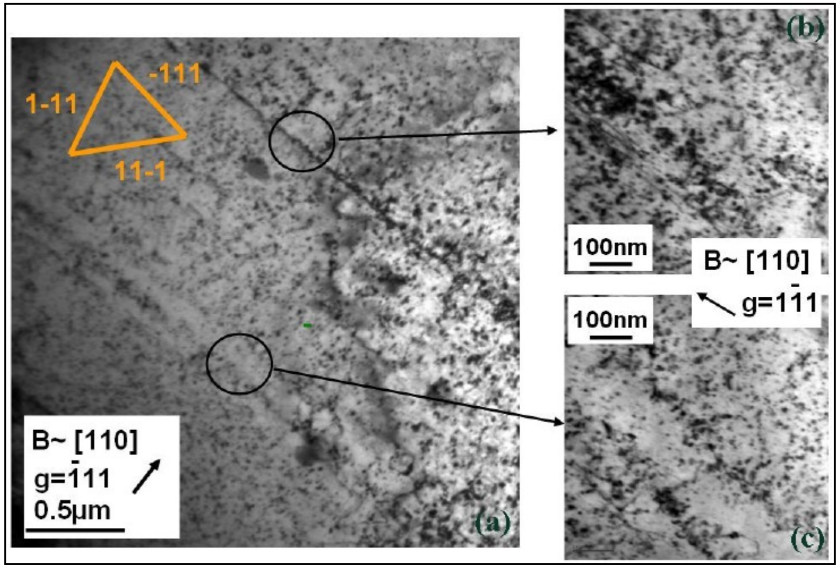




Irradiation defect microstructure



C.Robertson (1998), 3 dpa, Kr ions



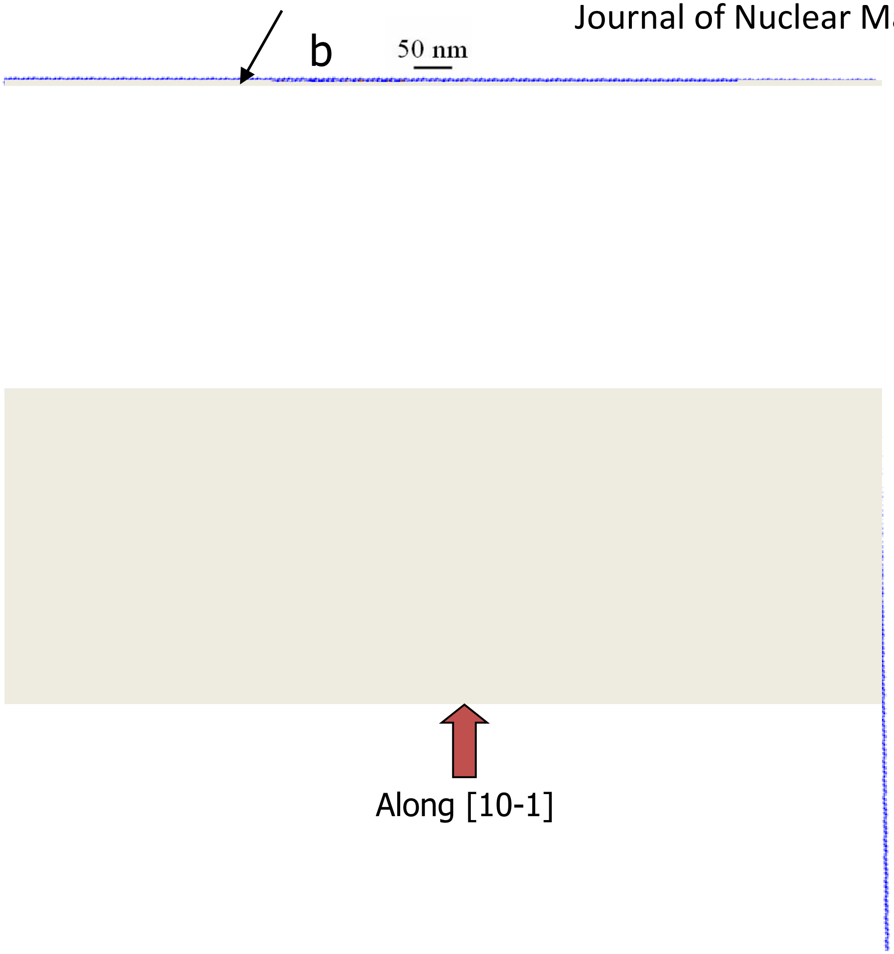
Deformation: in the form of shear bands

i. Dislocation pile-ups: $L_{PU} \propto D_g$

ii. Secondary shear bands and then gradual band broadening

Shear band dislocation substructure

Journal of Nuclear Materials 380 (2008) 22–29



X cleaning **dislocations**

X piled-up **dislocations**

X arrested **dislocations**

Leading dislocations

Dislocations with helix/jogs

Clear and broaden channels

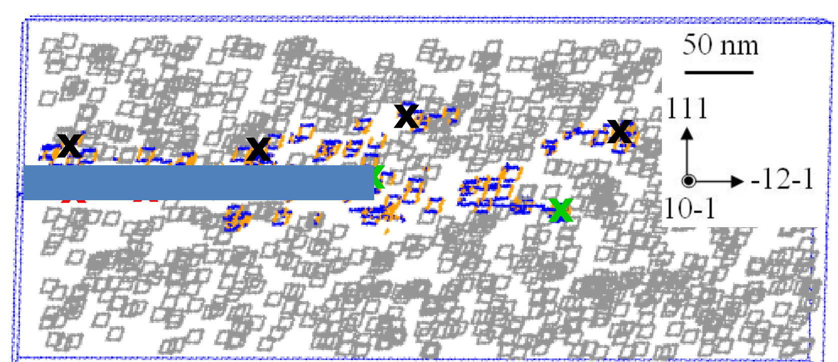
Trailing dislocations

Straight piled-up dislocations

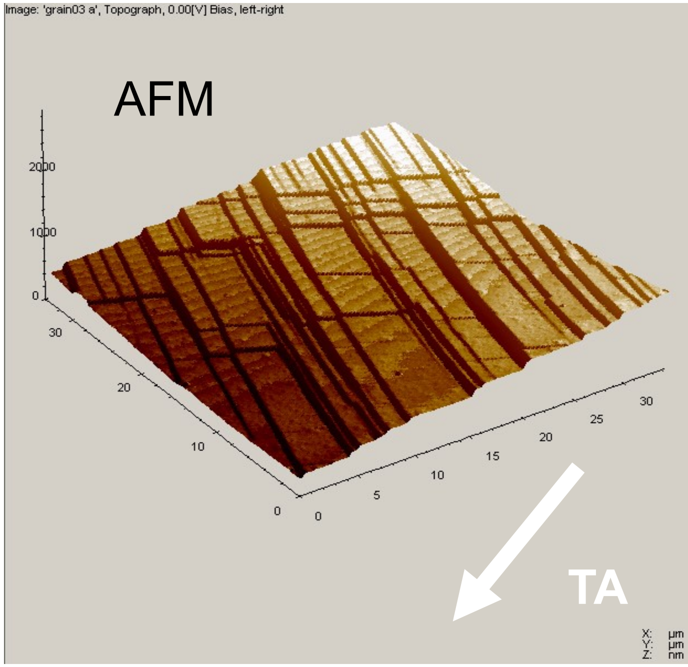
“Push” the leading dislocations

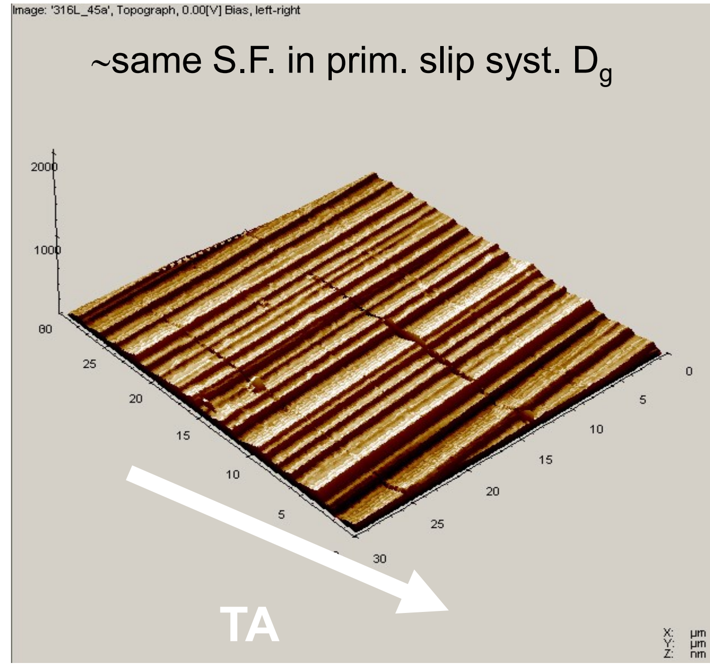
At the channel periphery:

accumulation of coarse loop debris

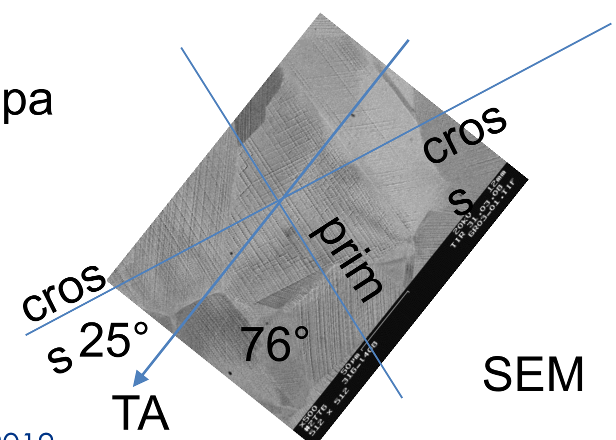


Post-irradiation plasticity mechanisms (P60)

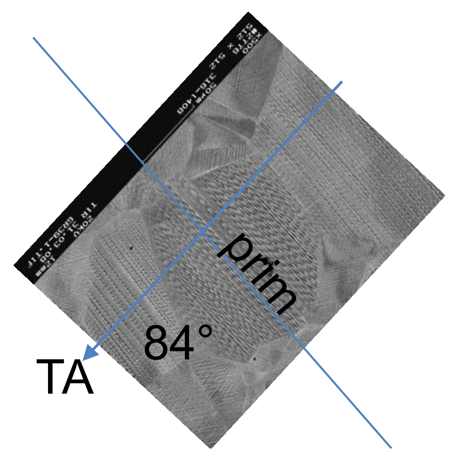




2 dpa



0 dpa



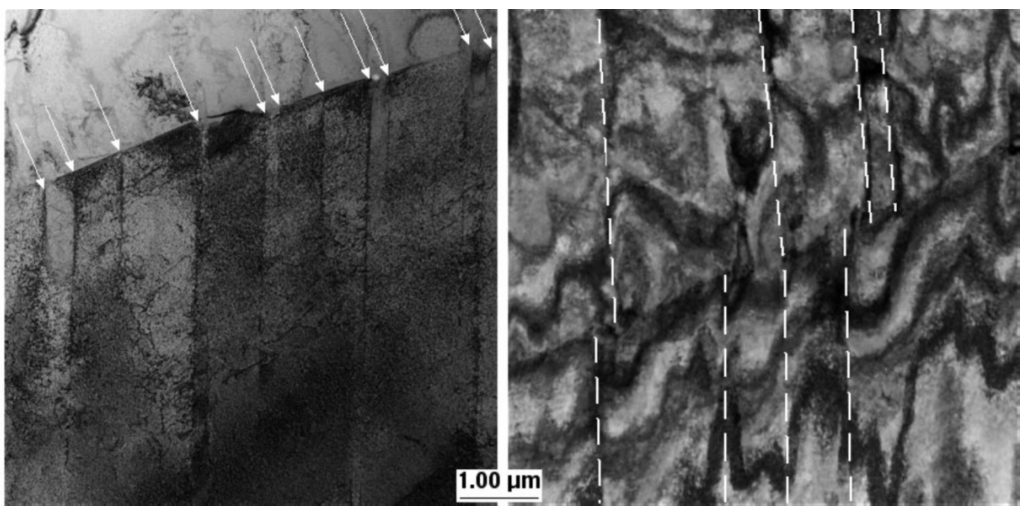
Partial summary… (up to P60)

- Slip steps are fewer and smaller, after irradiation ☞ strain localization
- Loop-depleted channel (or clear band) is merely a particular shear-band type

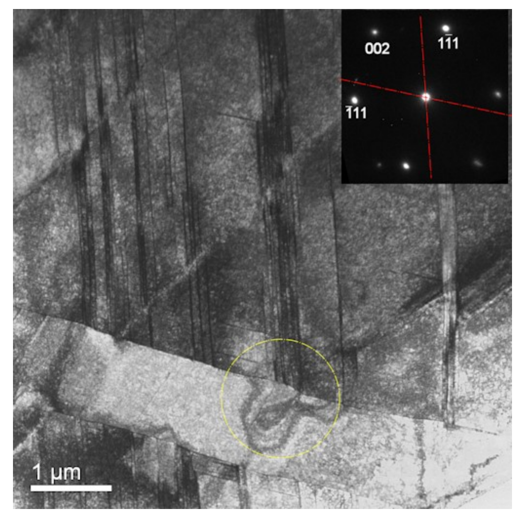
- Channels include dislocation pile-ups (unlike in BCC, where tangles form), generating a long-range, out of plane stress field

- Channel (shear band) thickness and spacing controls the stress concentration magnitude at the GBs and hence, crack initiation susceptibility thereof

W. Karlsen, VTT



0.89 dpa 304L
Tensile test B7, specimen ”nec4”

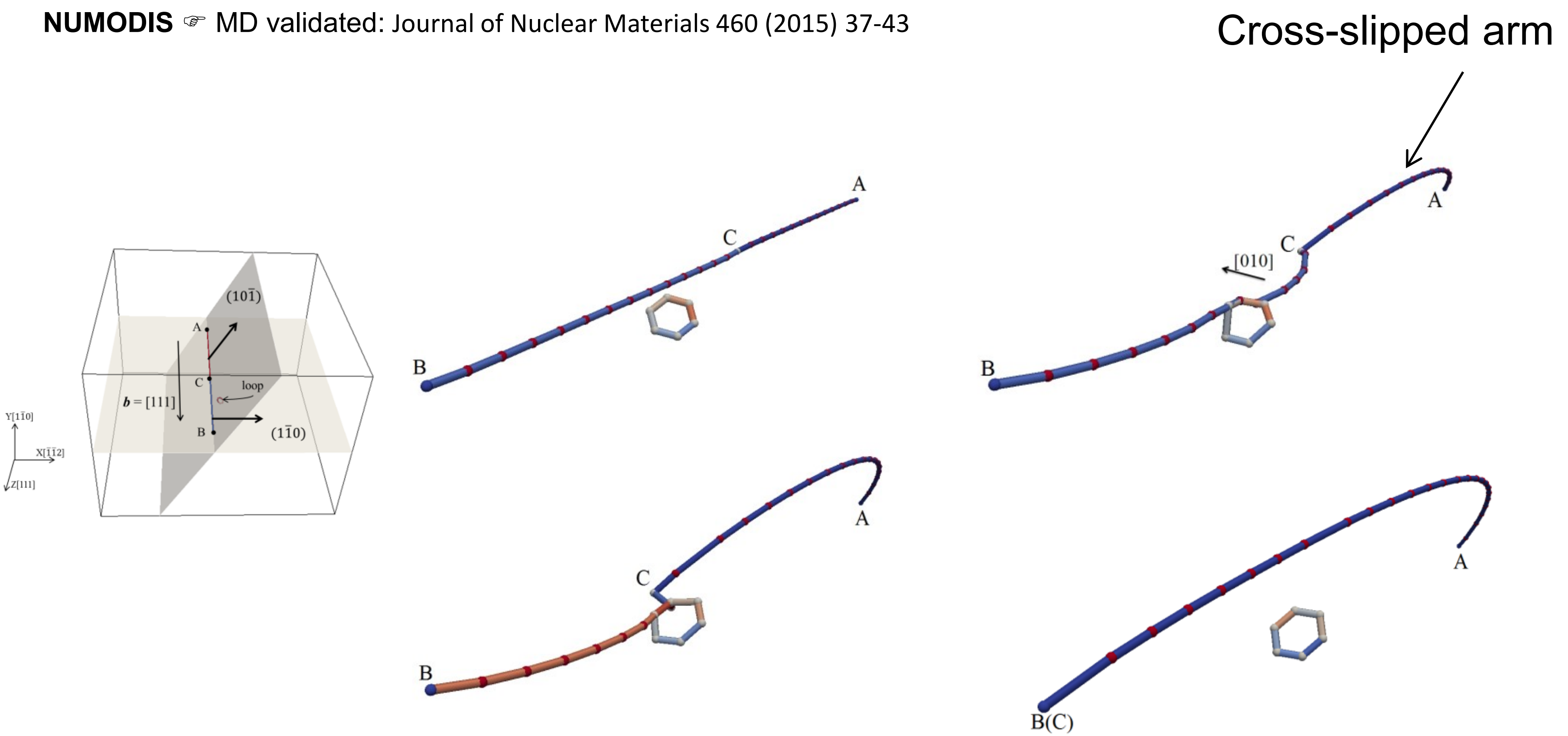


11 dpa CW 316
Tensile test B7, specimen ”nec4”

Cross-slip: interaction with defects

Next step: include the ubiquitous cross-slip mechanism
Interaction with $1\bar{1}1$ & 111 loops

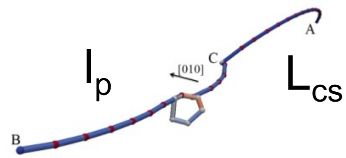
NUMODIS ☞ MD validated: Journal of Nuclear Materials 460 (2015) 37-43

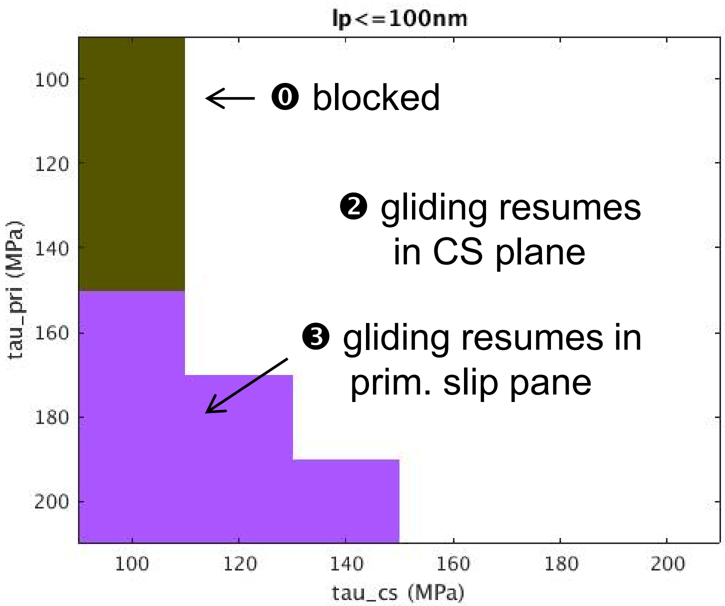


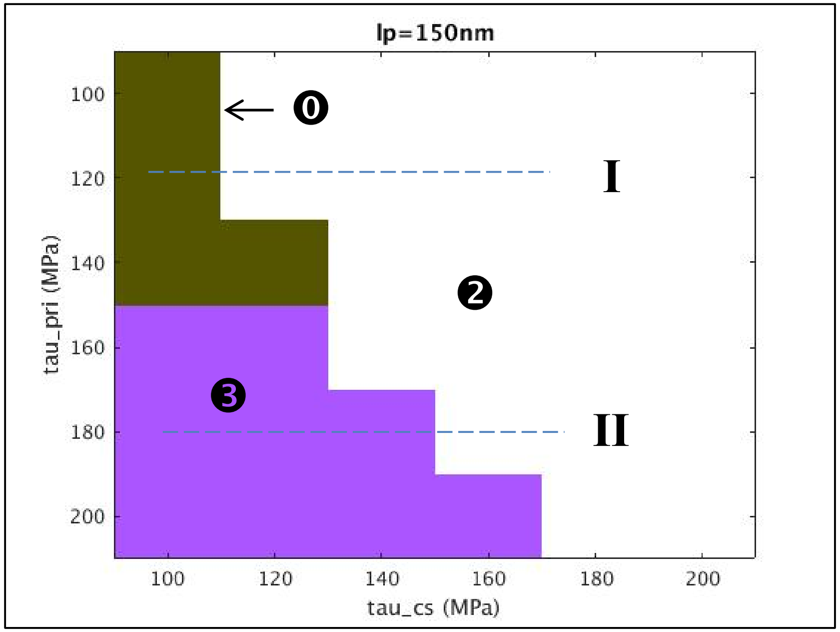
Y. Li, C. Robertson, Model. Simul. Mater. Sci. Eng. 26 (2018) 055009

Cross-slip: interaction with defects

Stress controlled simulations
l_p: segment length in primary SS
$l_p + L_{cs} = 300$ nm

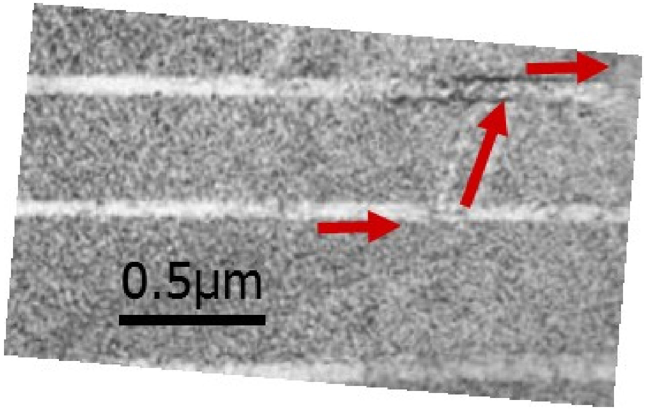






☞ **In presence of cross-slip: interaction strenght < loop strength**
☞ **Cross-slip provides an easy path to overcome the defects**

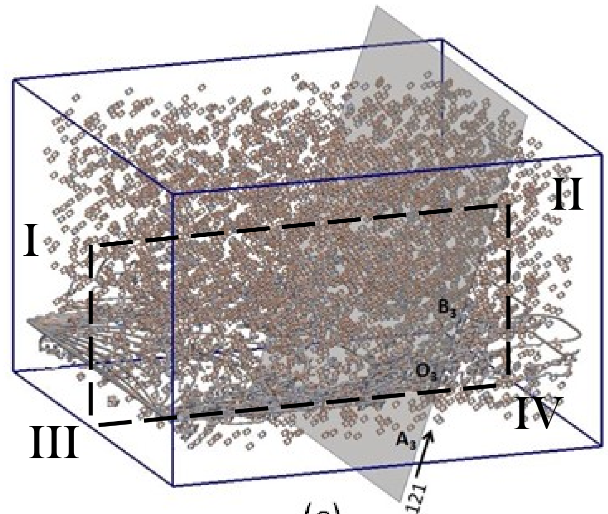
Cross-slip: shear band multiplication



Regular inter-channel spacing ↔ secondary channel in X-slip planes: [Yao 2005]

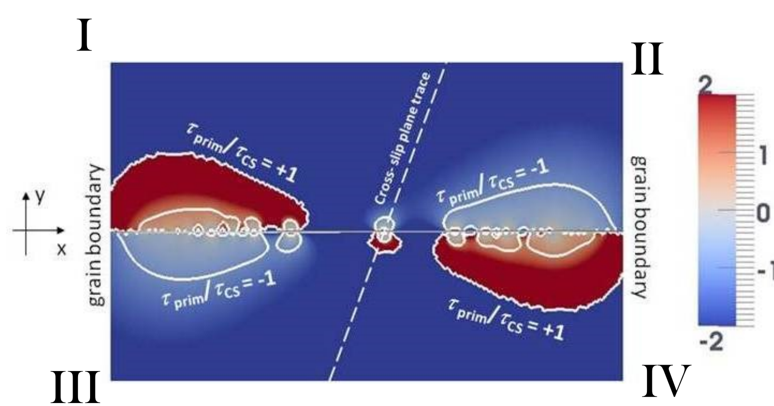
Secondary channels develop wherever CS probability is high, i.e. wherever effective defect interaction strength is minimal (path of least interaction)

In presence of obtacles P(cross-slip) highest: $\tau_{prim}/\tau_{CS} = \pm 1$



(c)

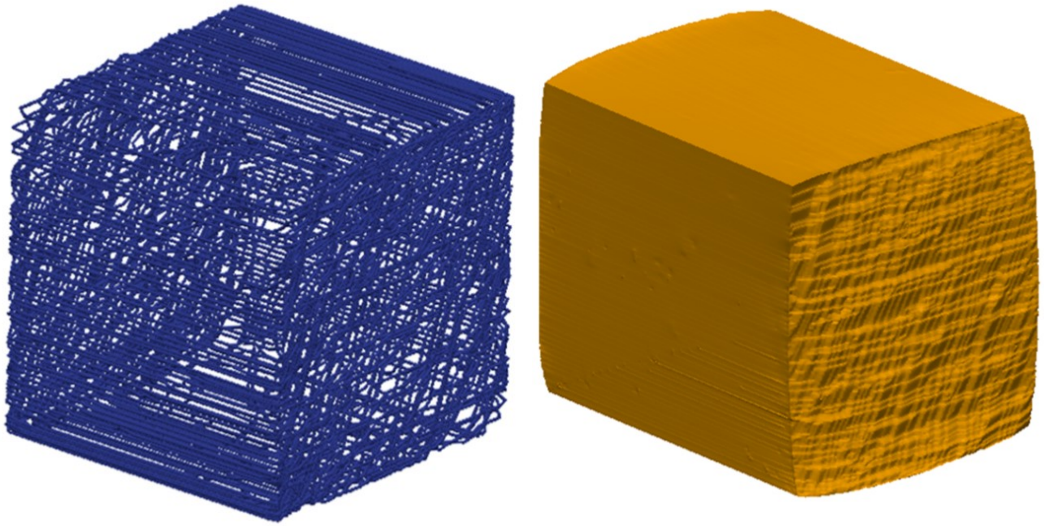
K. Gururaj etal, Phil. Mag. 95 No.12 (2015) 1368-1389

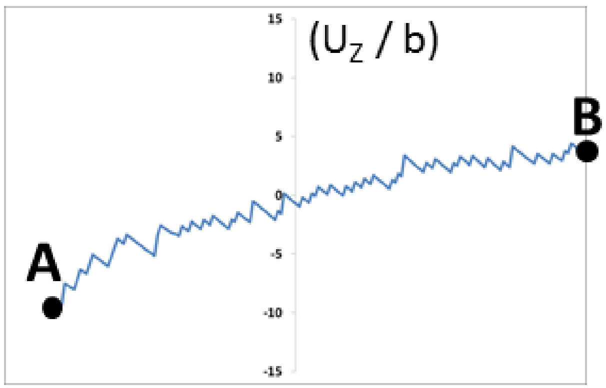


Stress mapping: τ_{prim}/τ_{CS}

Shear band spacing scales with internal stress field characteristic distance

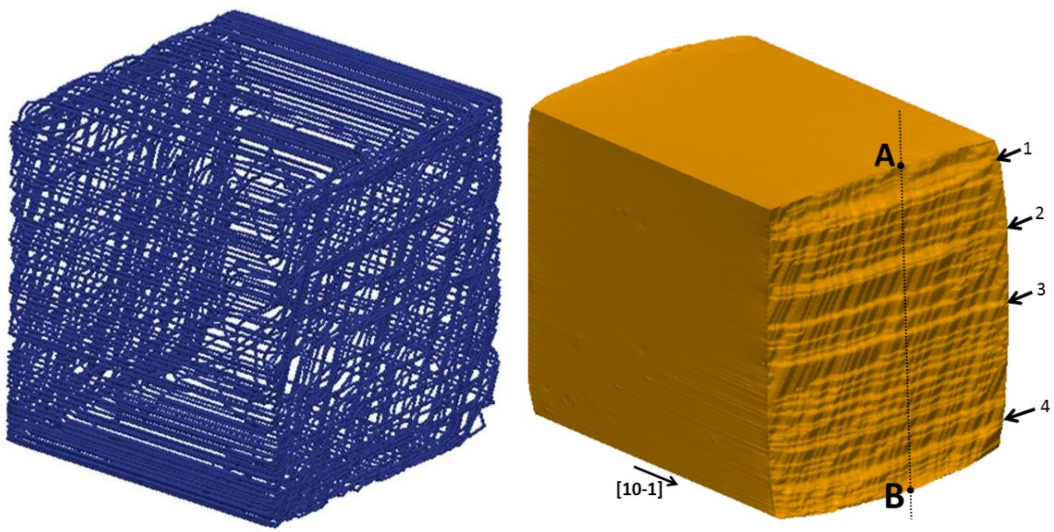
Shear band spacing: simulation…

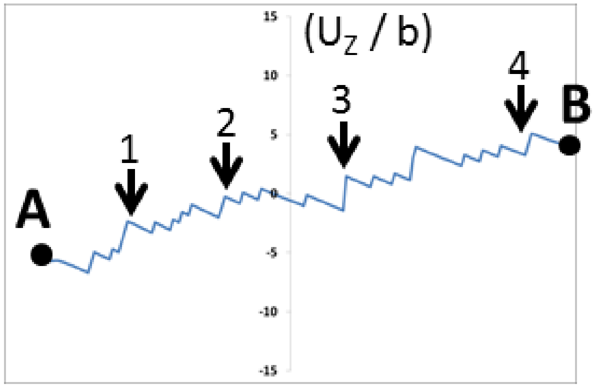




00 loops

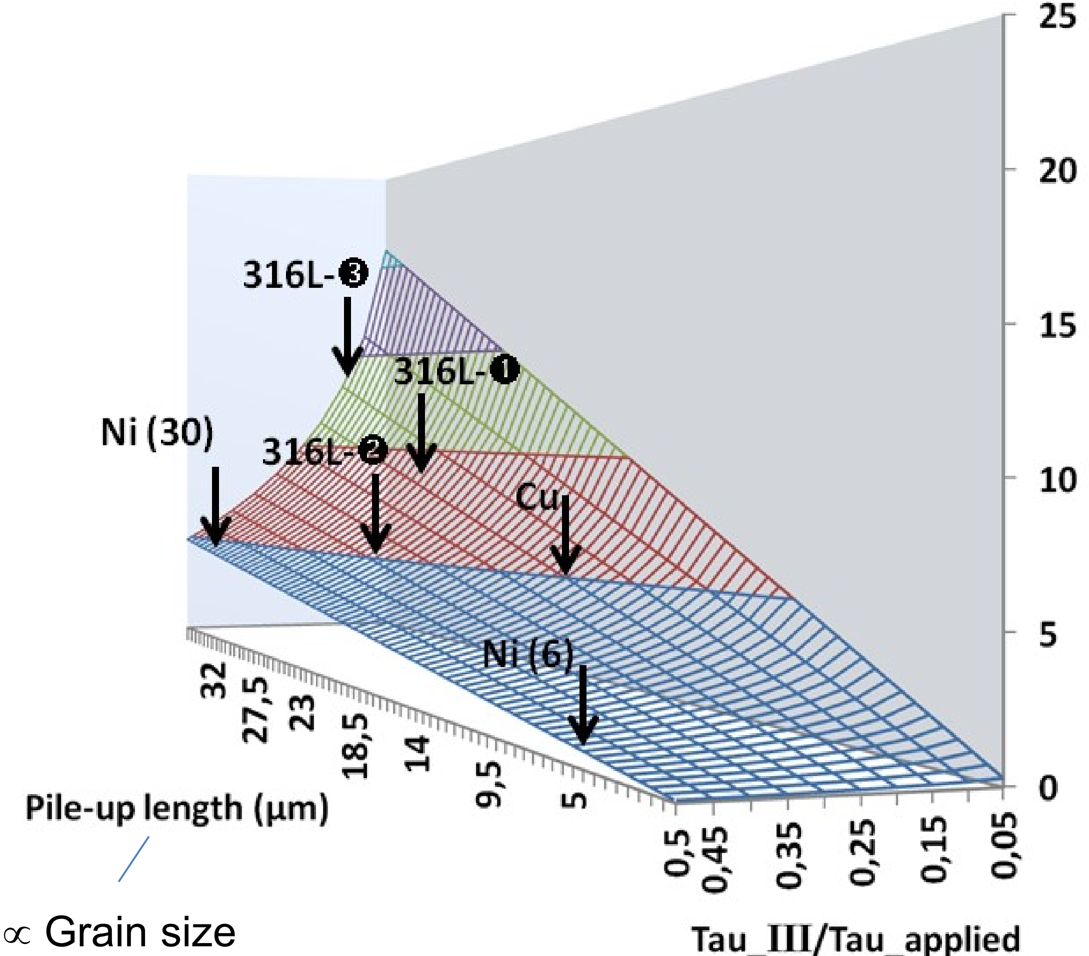
$\varepsilon_p = 1,4\times10^{-3}$





10^{22} loops/m^3 (~ 0.5 dpa)

Shear band spacing prediction?



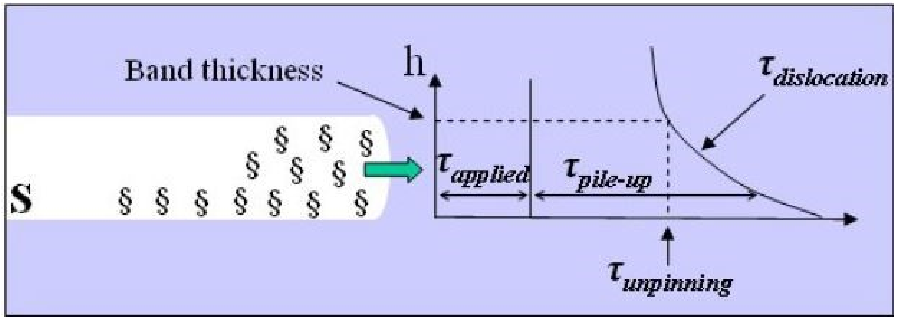
Shear band spacing « d »

$\propto$ Grain size

$f(d_0)$, $f(\mathrm{SFE})$

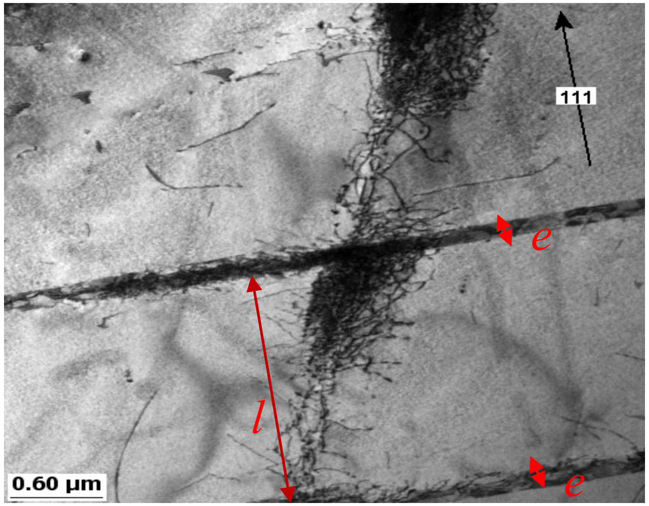
$\approx (\tau_{YS} - \tau_0) + \Delta\tau$ (irradiation-dose, ε_p)

Shear band thickness prediction ?



Dislocation can glide inside shear bands wherever verifies:

$$\tau_{app} + \tau_{pu(band)} > \tau_{defect}$$



[W. Karlsen, VTT, 2006]

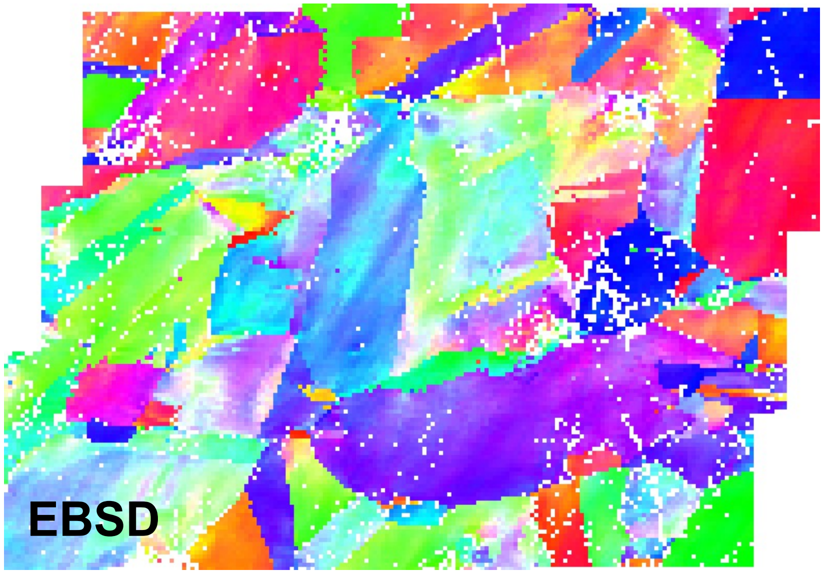
How to chose these different terms?

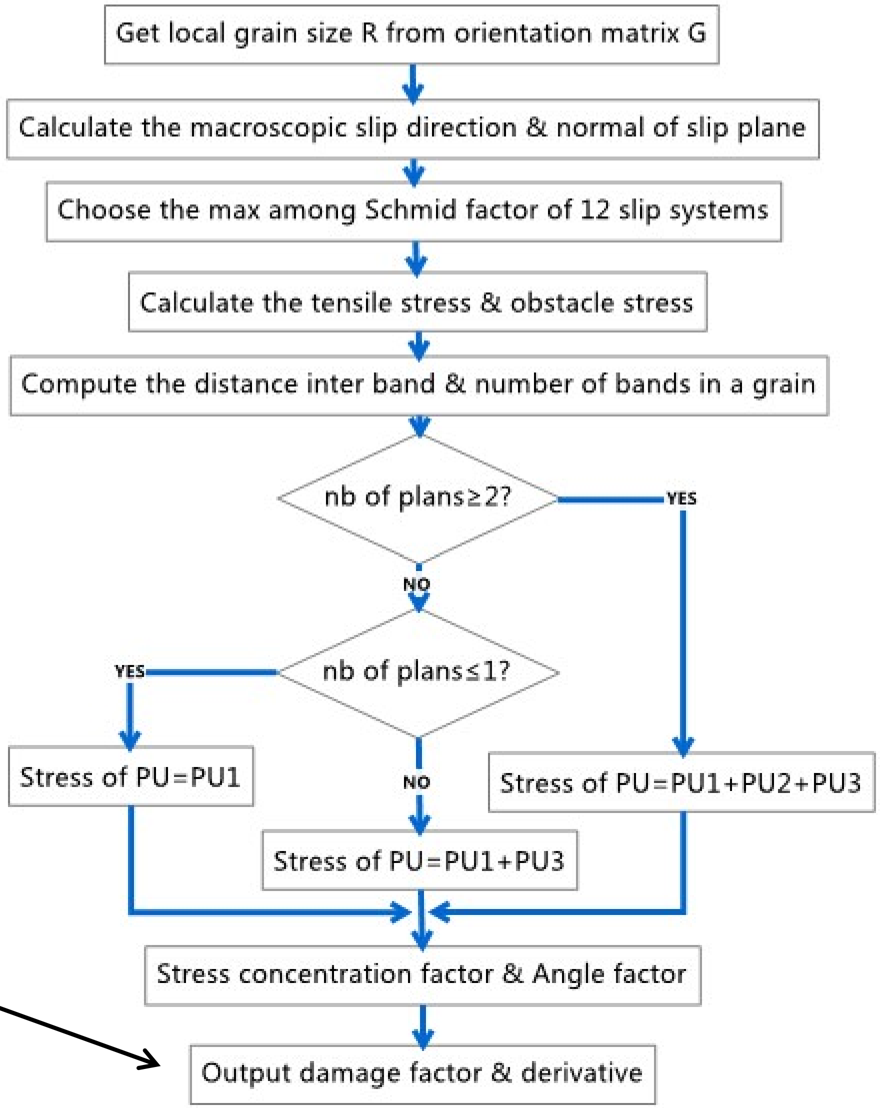
☞ Applied stress level τ_{app} (tensile testing data or hardening theory)
☞ τ_{pu} (inter-band long pile-ups, analytical H&L model)
☞ Obstacle strength τ_{defect} (MD & continuum S&B theory).

☞ Both τ_{app} & τ_{obs} relate to the irradiation conditions

- Defect cluster size
- Defect cluster number density
- Other hardening mechanisms?

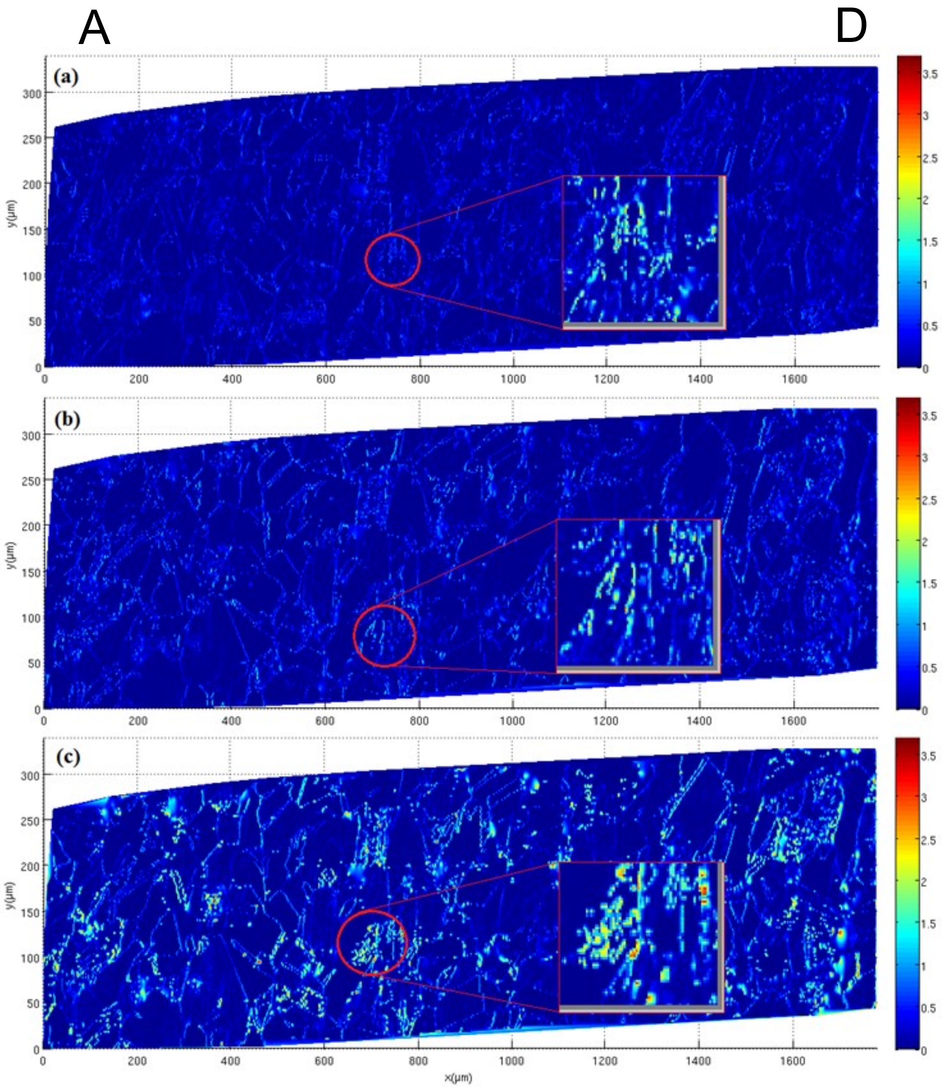
Application to poly-crystals



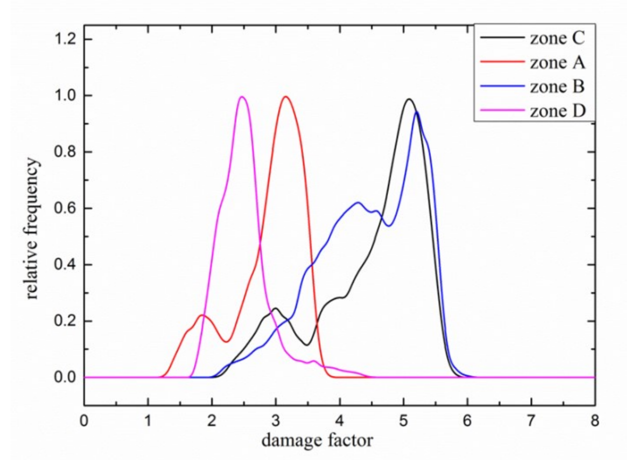


Damage factor include stress concentration and crystallographic orientation contributions.

Application to poly-crystals

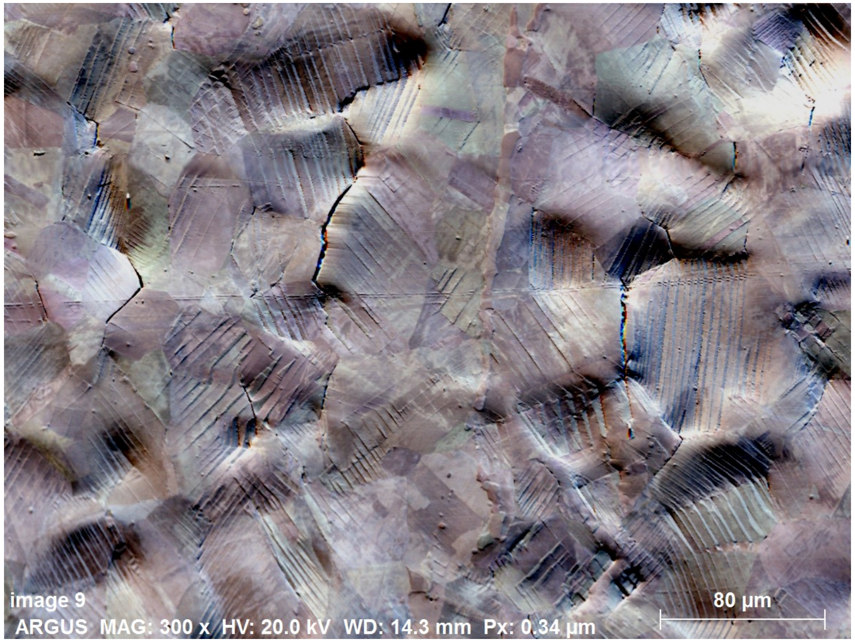


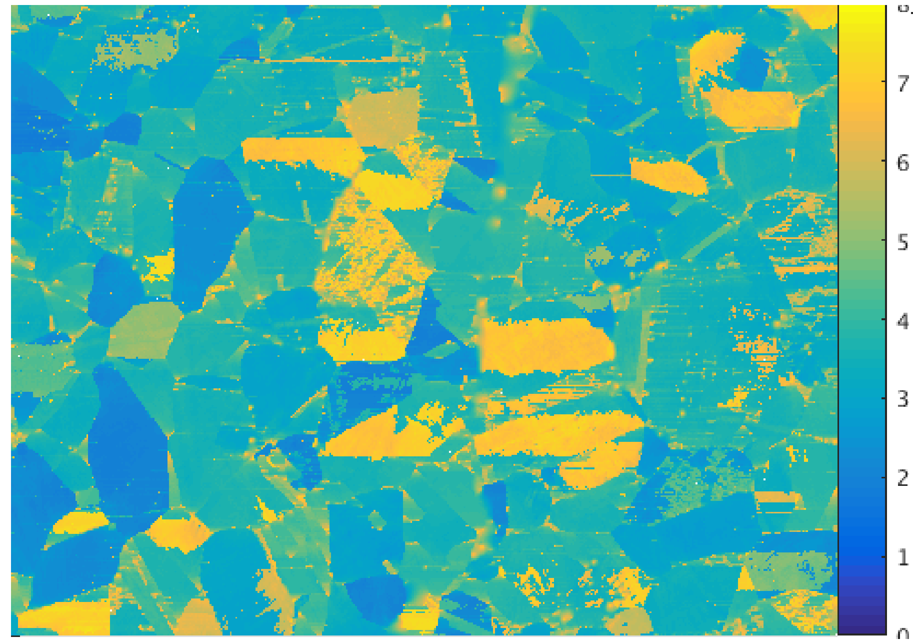
Zone to zone variations of GB loading



Effect of rising dose on GB loading

Comparison with observation (P+ irradiation)

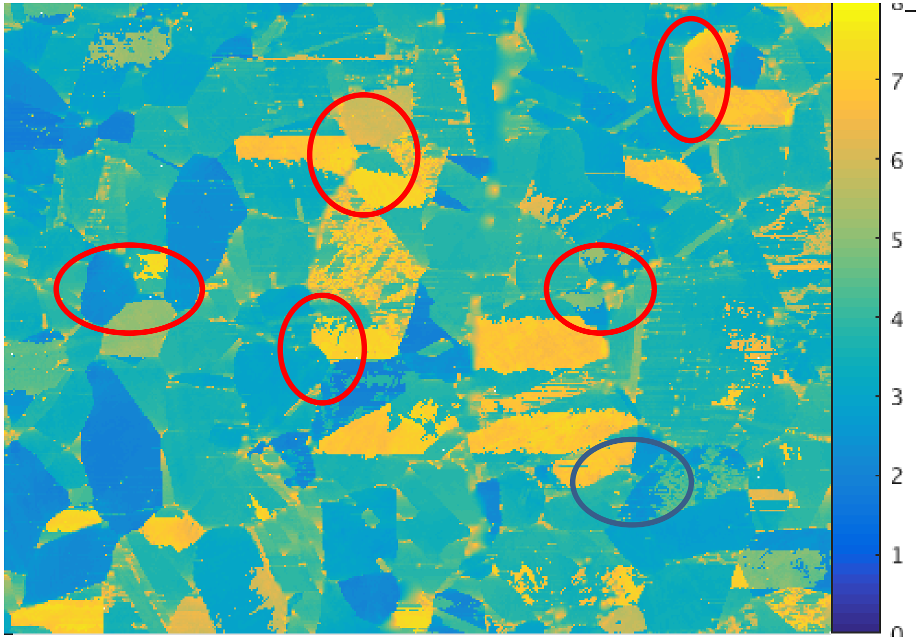




[B. Tanguy, DEN/DMN/SEMI]

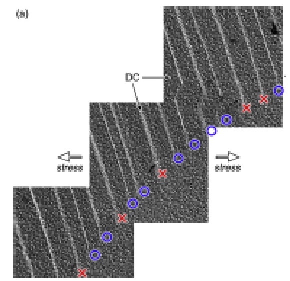
Irradiated 316L steel p+ 2dpa/350℃, 10^{-7} s^{-1} up to $\varepsilon_P = 4\%$ in autoclave (primary water)
Applied stress considering the hardening effect: 684MPa, Area: 411.02 µm X 298.92µm
Mean Defect cluster size: 13.8nm, defect number density 3.6e22 m^{-3}

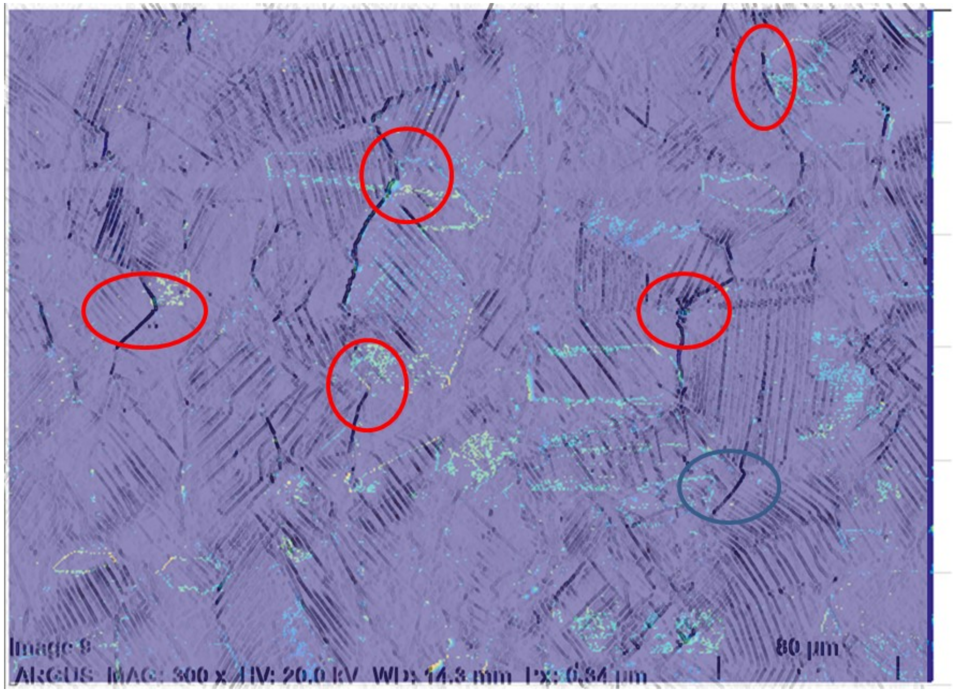
Comparison with observation (P+ irradiation)



Most likely to crack nucleation sites: GB presenting the largest plastic strain contrast.

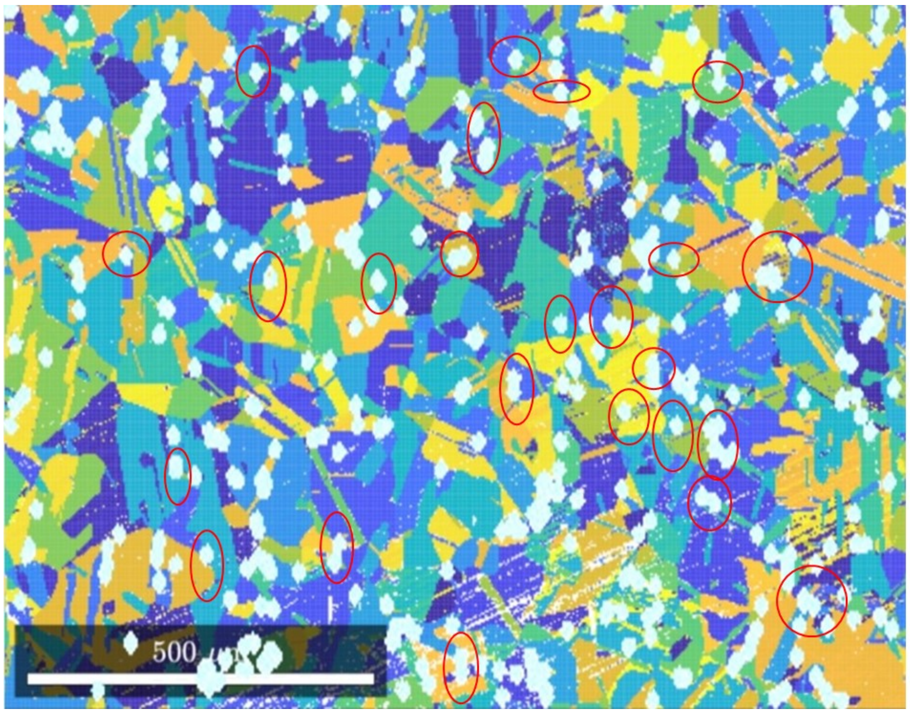
He, Johnson, Was, Robertson
Acta Materialia 138 (2017) 61-71

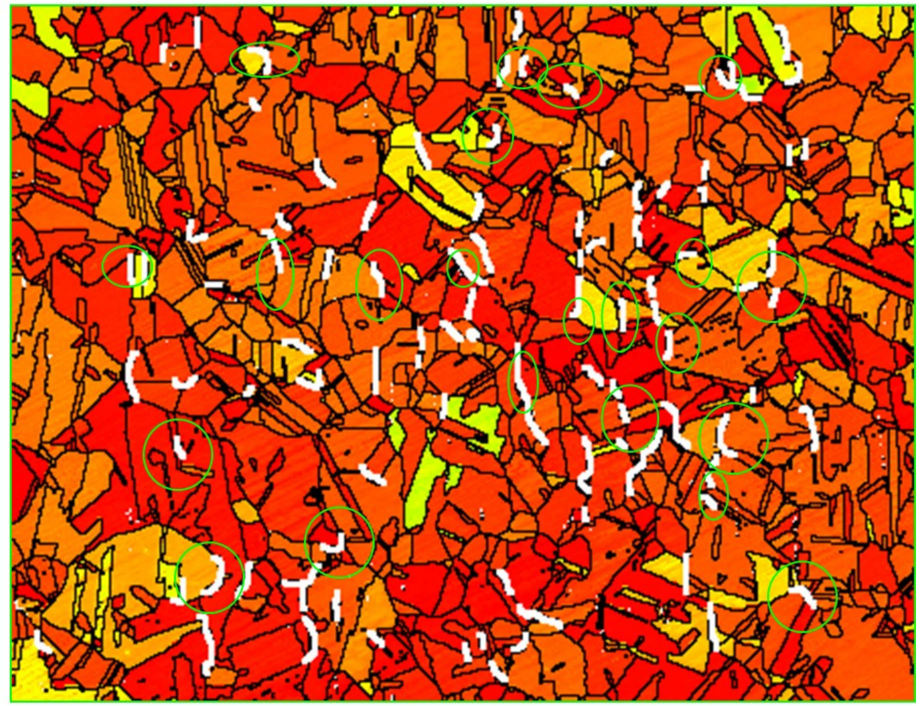




- Damage threshold identification (quantitative evaluation)
- Correct crack nucleation probability in surface grains

Comparison with observation (Fe irradiation)

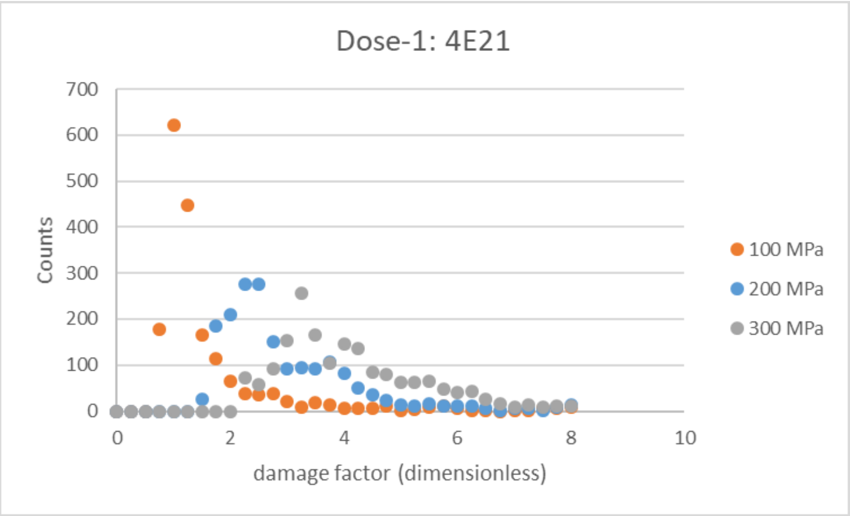


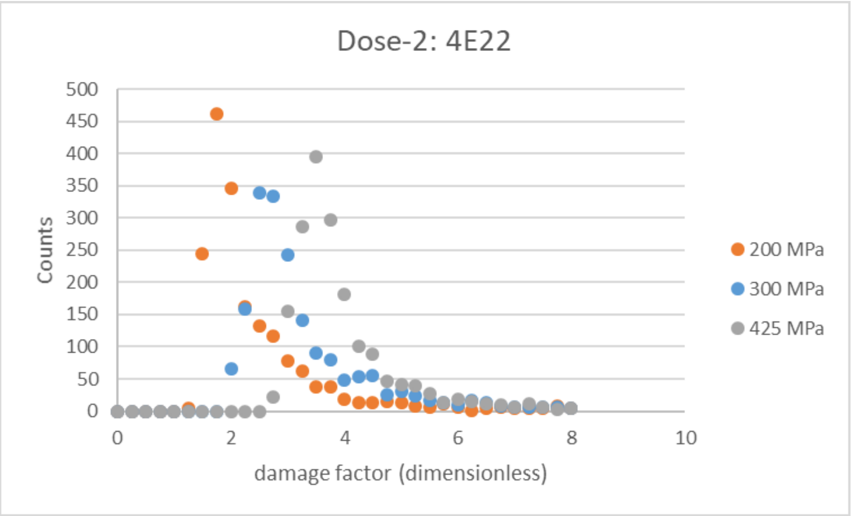


[B. Tanguy, DEN/DMN/SEMI]

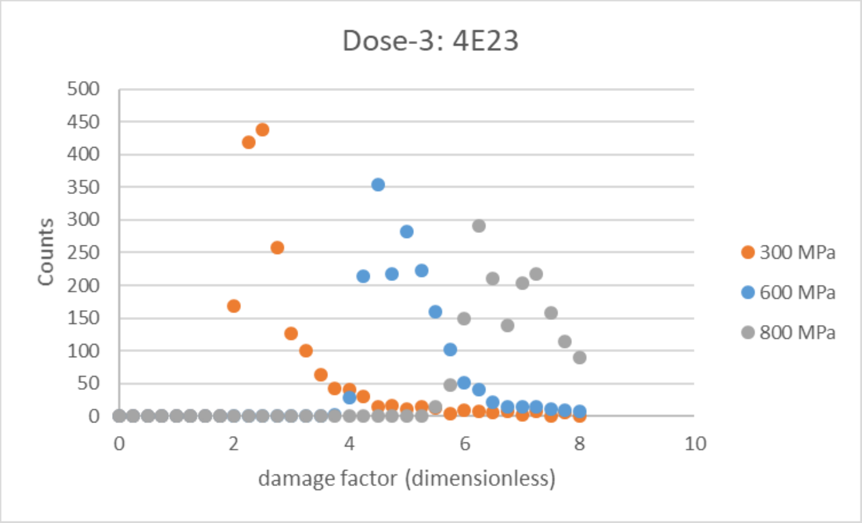
- Predicted crack length comparable to observed crack length
- Crack initiation site correspondance at least 50%
- Damage threshold(s) identification: (mostly) confirmed

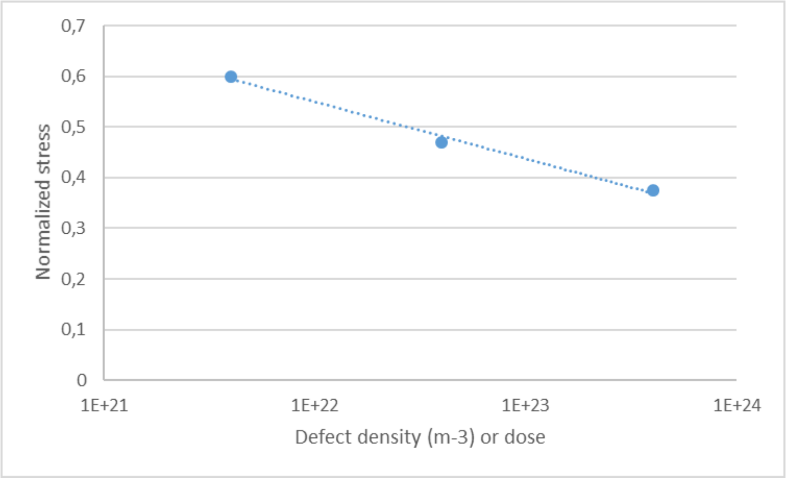
Model predictions

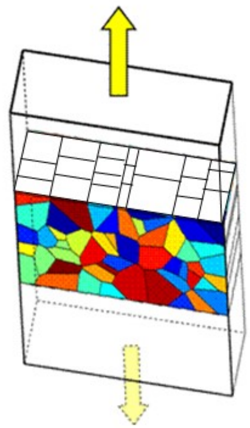


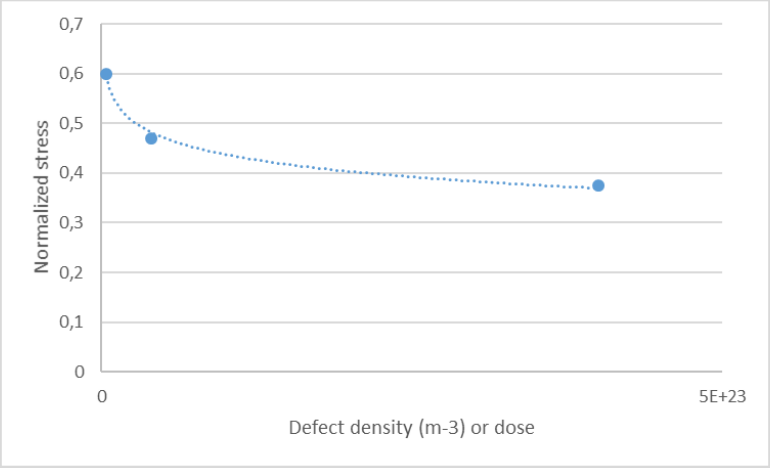


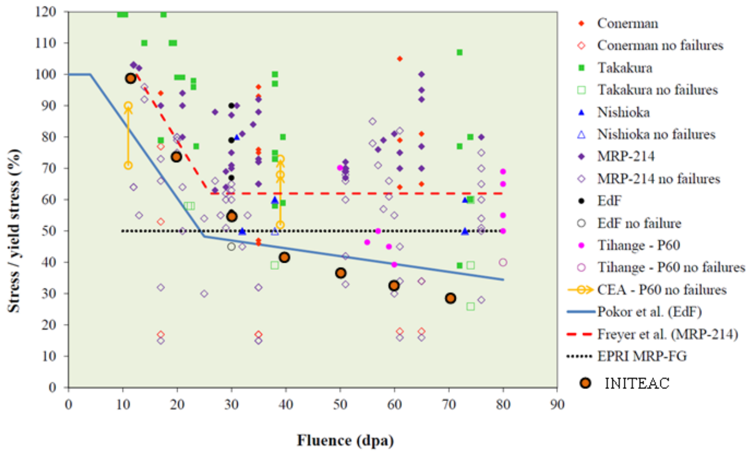
- Including a stress correction according to GB surface energy




0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
Normalized stress
1E+21
1E+22
1E+23
1E+24
Defect density (m-3) or dose




0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
Normalized stress
0
5E+23
Defect density (m-3) or dose


Stress / yield stress (%)
Fluence (dpa)
Conerman
Conerman no failures
Takakura
Takakura no failures
Nishioka
Nishioka no failures
MRP-214
MRP-214 no failures
EdF
EdF no failure
Tihange - P60
Tihange - P60 no failures
CEA - P60 no failures
Pokor et al. (EdF)
Freyer et al. (MRP-214)
EPRI MRP-FG
INITEAC

Conclusion & Perspectives

Analysis of plastic strain spreading in presence of disperse defect populations:

• Dislocation displacement is controlled by cross-slip: i-helps mobile dislocations **overcoming** the disperse defect clusters (enables choosing path of least interaction), ii-helps **spreading** shear bands across the whole grain (secondary channel formation)

• Shear bands dislocation substructures include extended dislocation **pile-ups**
• Shear band spacing controlled by **grain-wide** pile-ups
• Shear band broadening is gradual; controlled by **inter-band wide** pile-ups
• Grain boundary stress → depend on shear bands distribution

• Inter-granular crack initiation susceptibility is higher wherever the **plastic strain contrast** is maximal, between adjacent pairs of grains

Perspectives:

• Improve the estimation of applied stress level, including additional hardening mechanisms (dislocation source decoration)
• Consider 3D effects of grain diameter versus grain depth

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This project received funding under the Euratom research and training programme 2014-2018 under grant agreement N° 661913.

Shear band multiplication: cross-slip

Cross-slip of a bowed-out screw, due to obstacles

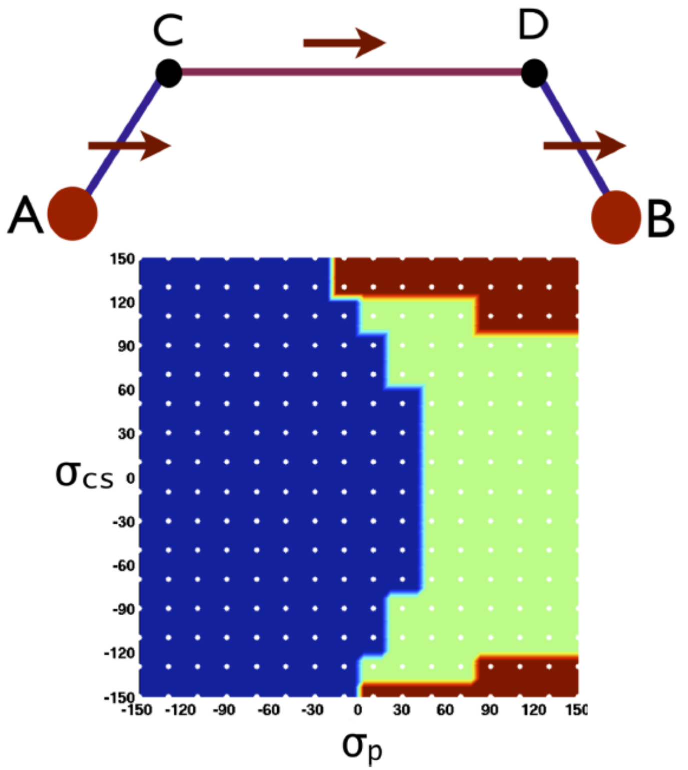


Figure 6.12 – *The set-up and result corresponding to the set 9 of the table 6.3. The image on the left is explained in the text. The image on the right corresponds to the result of primary and cross-slip stress acting on this configuration. The x-axis refers to the stress acting on the primary slip system, $\sigma_p = \overleftrightarrow{\sigma}.n_p.b$ in MPa and y-axis is the stress resolved in the cross-slip plane, $\sigma_{cs} = \overleftrightarrow{\sigma}.n_{cs}.b$ in MPa The regions in red indicate the (σ_p, σ_{cs}) combination that makes the length CD equal to AB, and region in blue indicates the (σ_p, σ_{cs}) combination that makes the length CD tend to zero. The regions in green indicate the (σ_p, σ_{cs}) values where the length of cross-slip segment CD neither goes to 0 nor equals distance between pinning points AB.*

- In presence of obstacles (radiation defects, GB, etc), cross-slip probability is maximal for **τ_{prim}/τ_{CS} = ±1**
- This validates our model for predicting inter-band distance in irradiated metals (see 06/13)

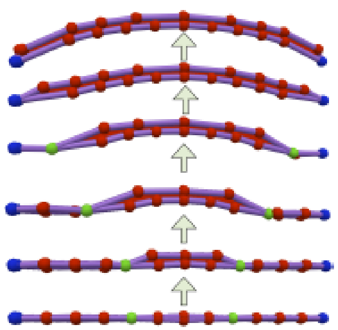
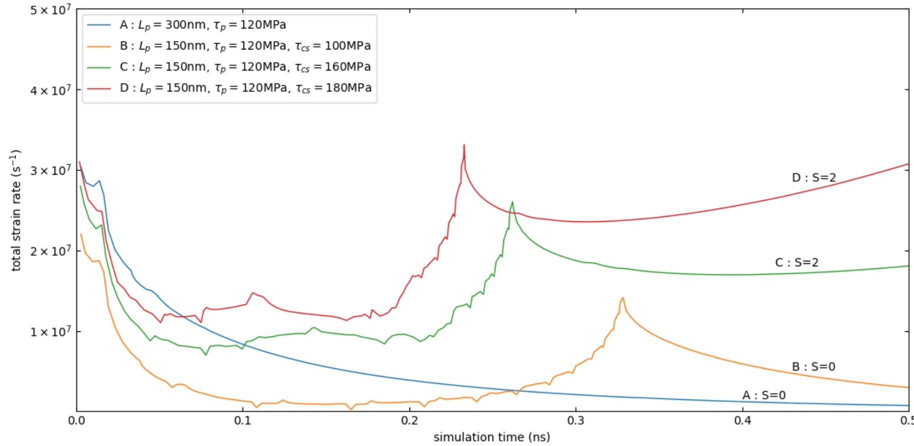


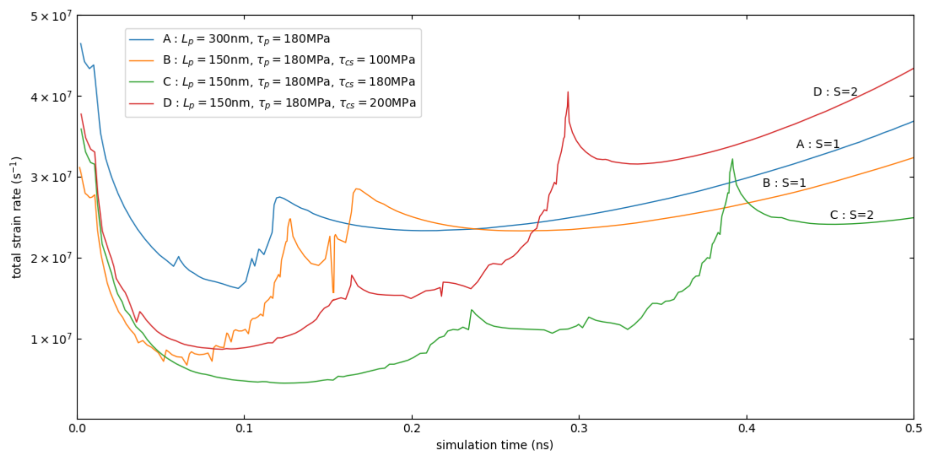
Figure 6.8 – *The evolution of a three segment split composite FR source of the form shown in the figure 6.5b. The figures from top to bottom illustrate the cross-slip segment spreading over the whole dislocation length.*

Cross-slip: interaction with defects

I: tau_prim_I



II: tau_prim_II



☞ **Rising tau_CS facilitates dislocation unpinning regarless of tau_prim!**