SOTERIA training school

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

OUTLINE

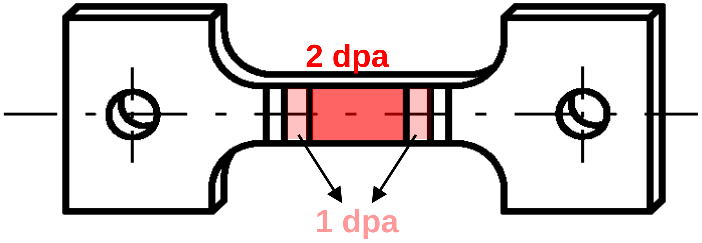
- Previous findings, up to PERFORM60 (up to 2012)
- Subsequent sub-grain modelling developments (2012-)
- Observations and poly-crystalline model (SOTERIA 2015-)

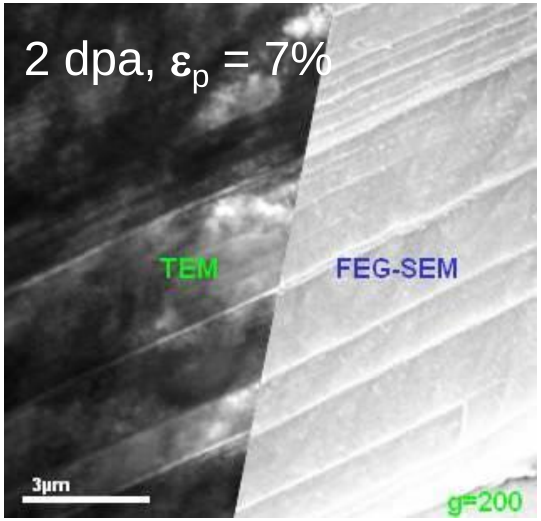
Contribution to SOTERIA WP2
Co-workers: B. Tanguy, J. Hure
Speaker: **Christian Robertson**

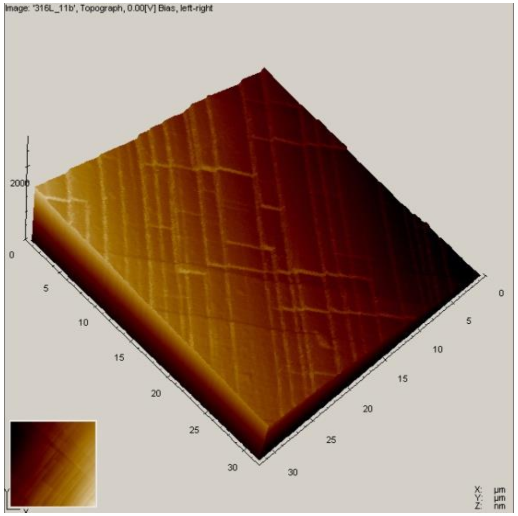
Post-irradiation plasticity mechanisms

Ion irradiations & observations

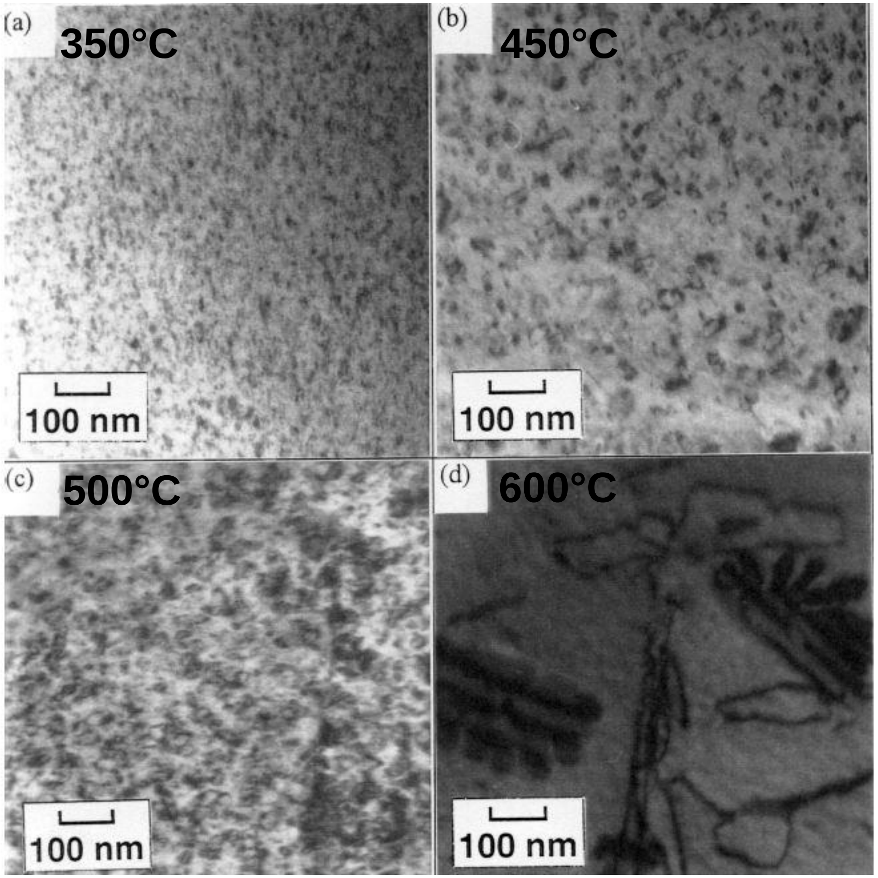
Ions irradiations: p+ or Fe^{8+}, 300 °C



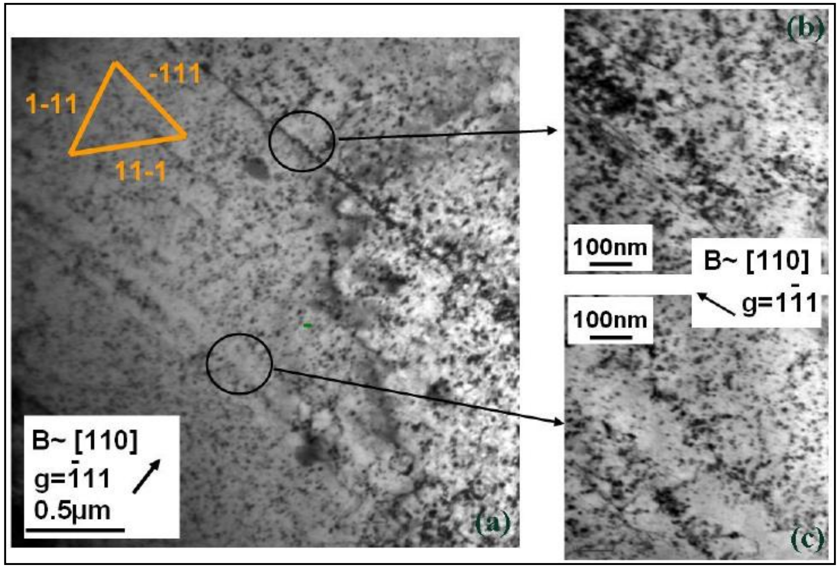




Irradiation defect microstructure



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



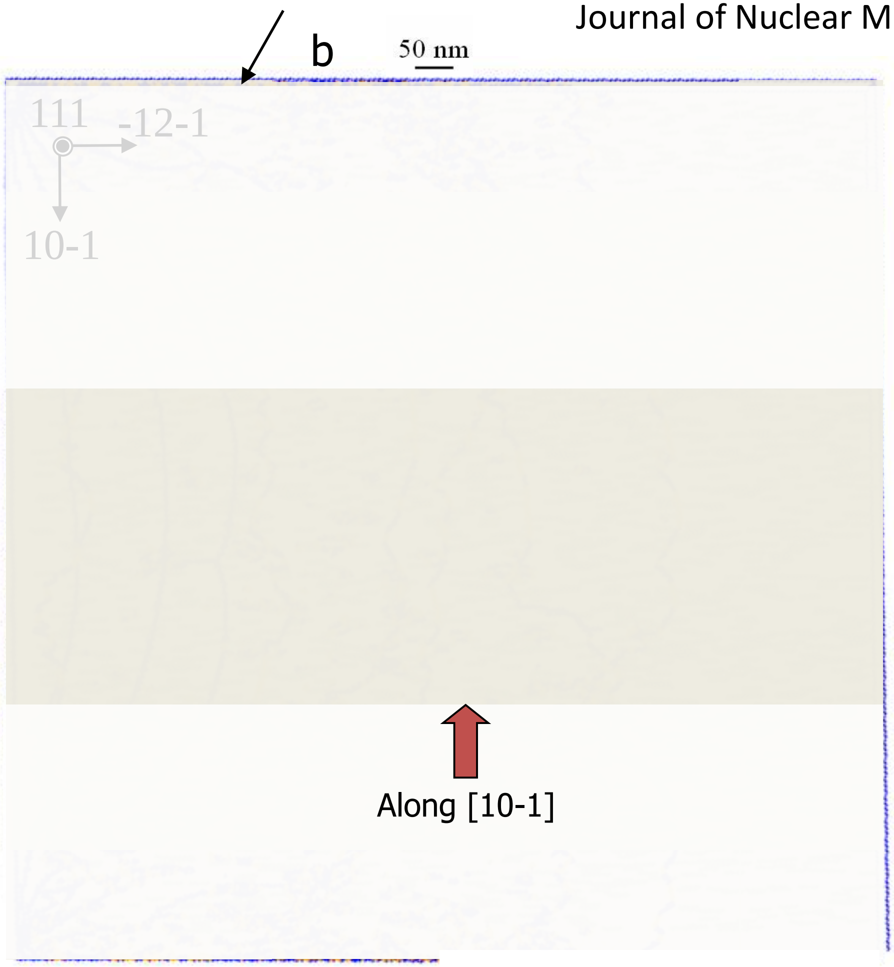
Deformation: in the form of shear bands

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



Leading dislocations

Dislocations with helix/jogs

Clear and broaden channels

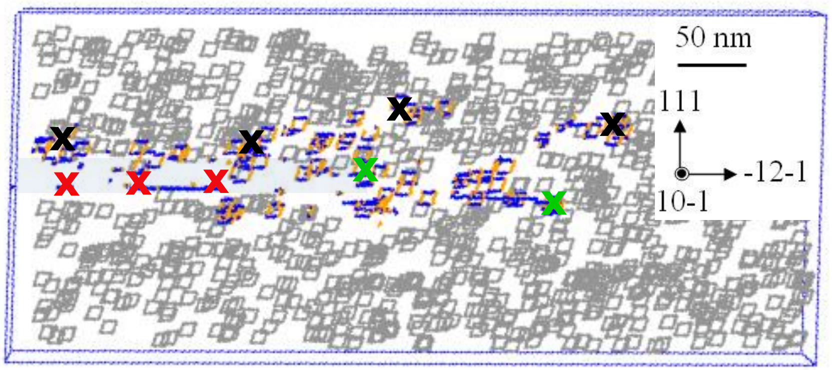
Trailing dislocations

Straight piled-up dislocations

“Push” the leading dislocations

At the channel periphery:

accumulation of coarse loop debris

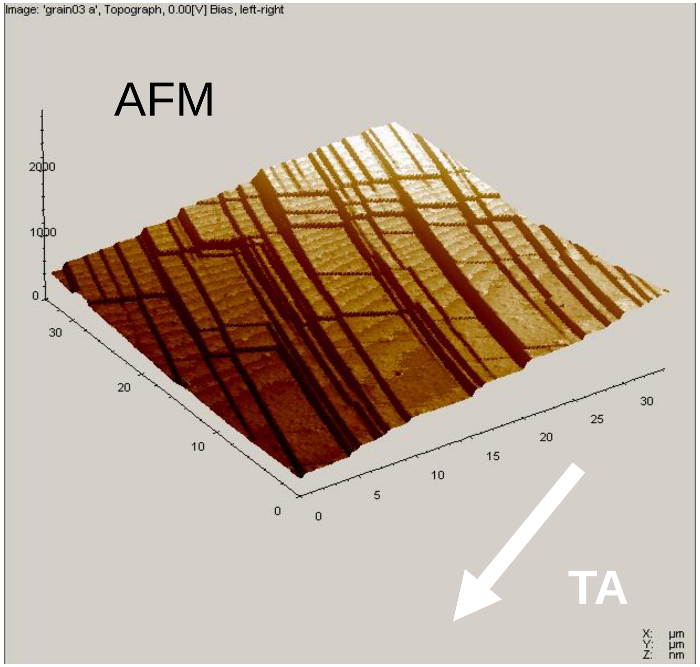


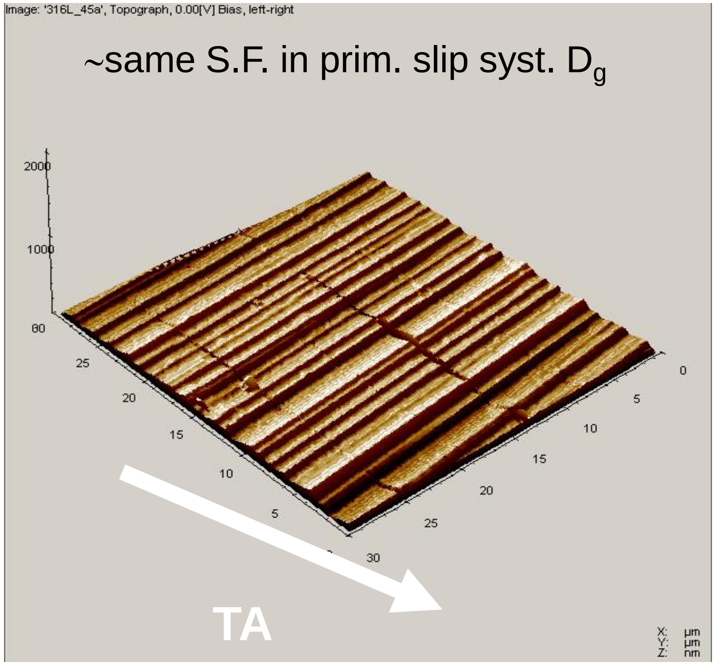
X cleaning **dislocations**

X piled-up **dislocations**

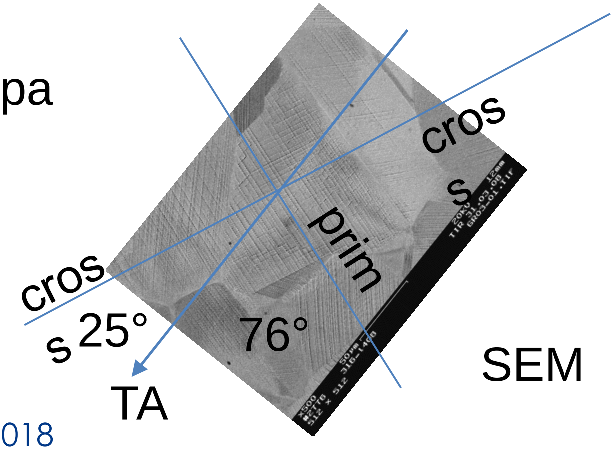
X arrested **dislocations**

Post-irradiation plasticity mechanisms (P60)



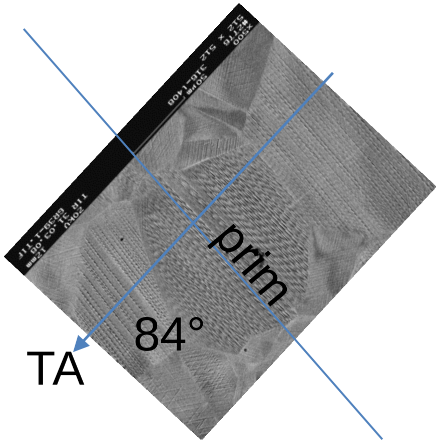


2 dpa



SEM

0 dpa



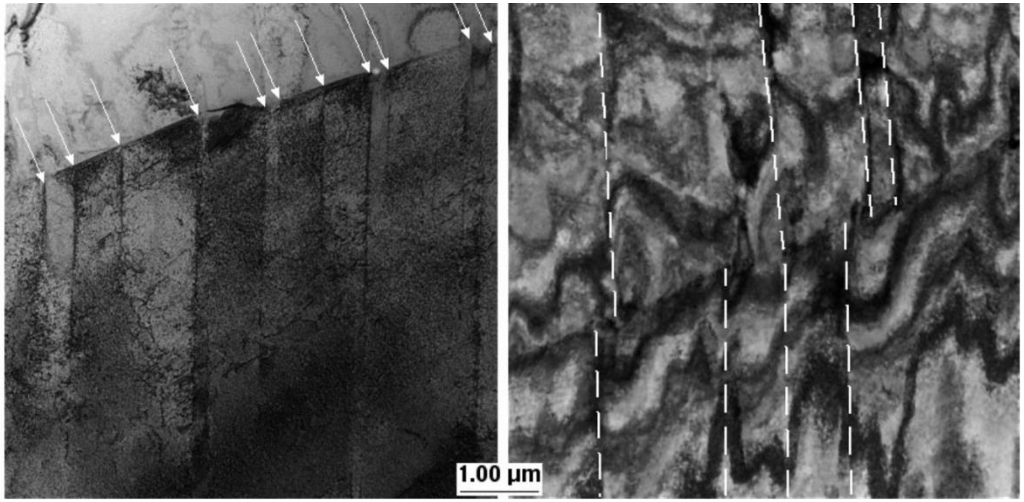
Partial summary… (up to P60)

- Slip steps are fewer and smaller, after irradiation ☞ strain localization

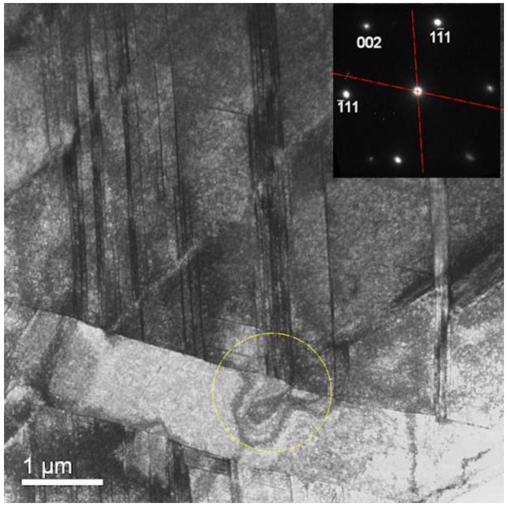
- Channel (shear band) thickness and spacing controls the stress concentration magnitude at the GBs and hence, crack initiation susceptibility thereof

- Loop-depleted channel (or clear band) is merely a particular shear-band type

W. Karlsen, VTT



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



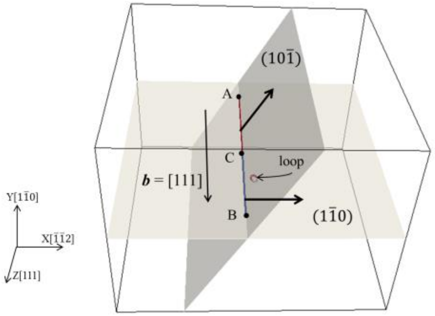
11 dpa CW 316
Tensile test B7, specimen ”nec4”

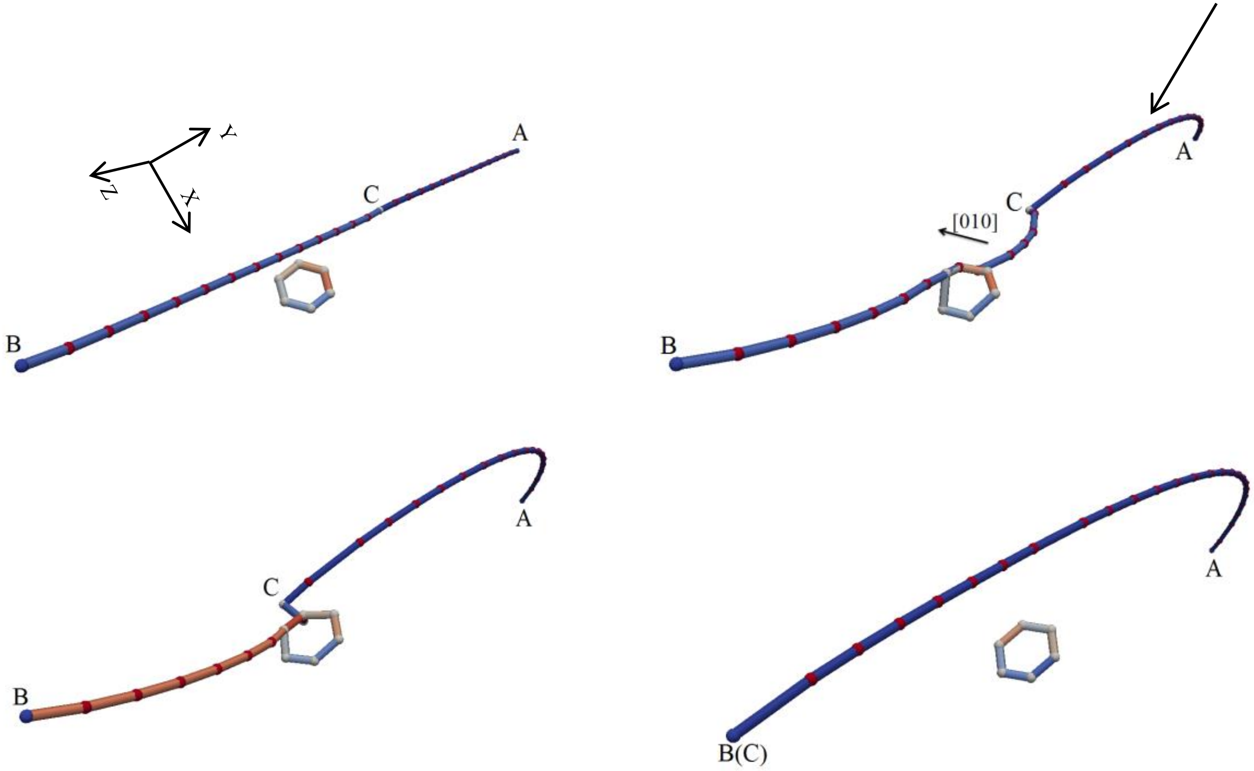
Cross-slip: interaction with defects

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

Cross-slipped arm





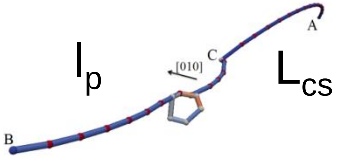
Y. Li, C. Robertson, Model. Simul. Mater. Sci. Eng. 26 (2018) 055009

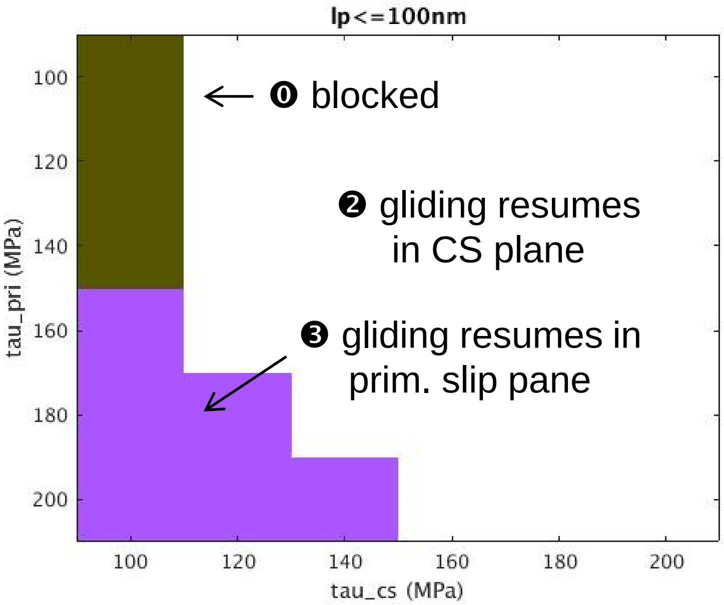
Cross-slip: interaction with defects

Stress controlled simulations

l_p: segment length in primary SS

$l_p + L_{cs} = 300$ nm

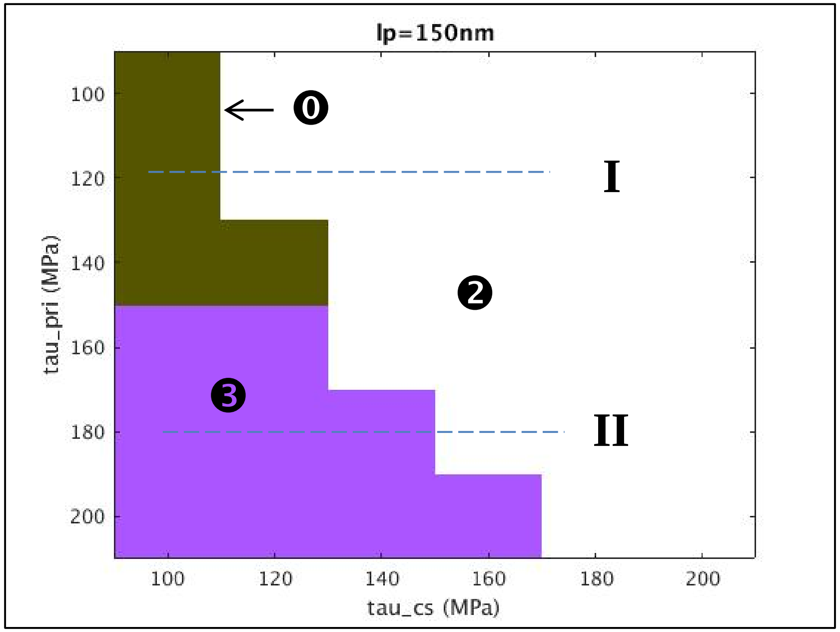




⓿ blocked

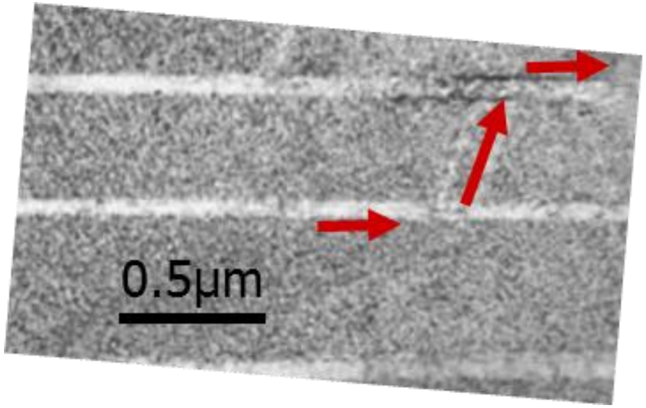
❷ gliding resumes in CS plane

❸ gliding resumes in prim. slip pane



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

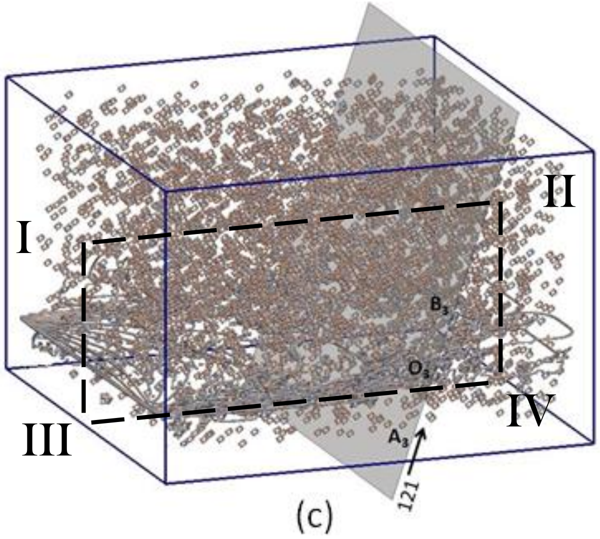
Cross-slip: shear band multiplication



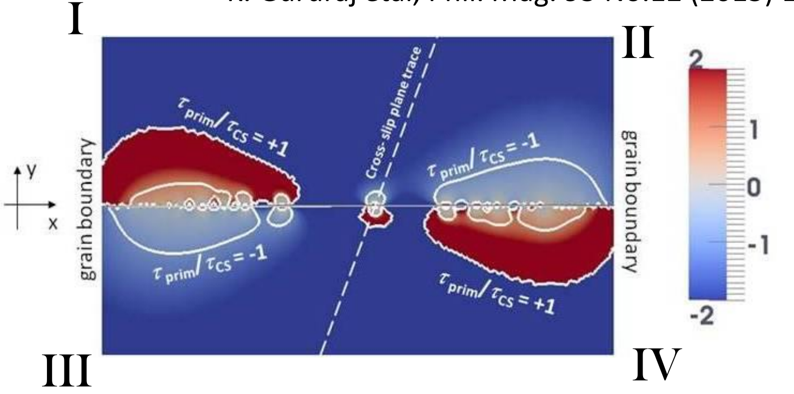
Regular inter-channel spacing ↔ secondary channel in X-slip planes: [Yao 2005]

Secondary channels develop wherever CS probability is high, i.e. wherever defect interaction strength is minimal

In presence of obtacles P(cross-slip) highest: τ_{prim}/τ_{CS} = ±1



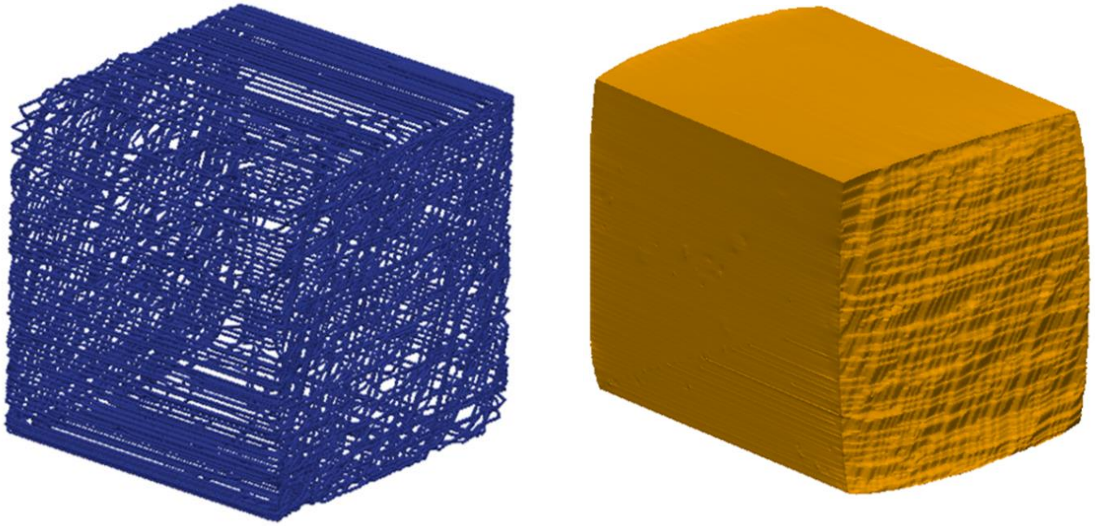
K. Gururaj etal, Phil. Mag. 95 No.12 (2015) 1368-1389

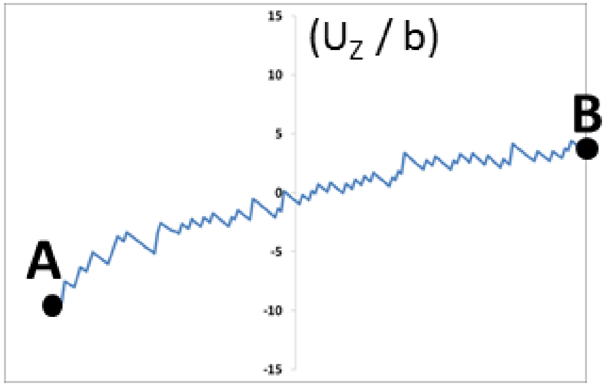


Stress mapping: τ_{prim}/τ_{CS}

Shear band spacing scales with internal stress field characteristic distance

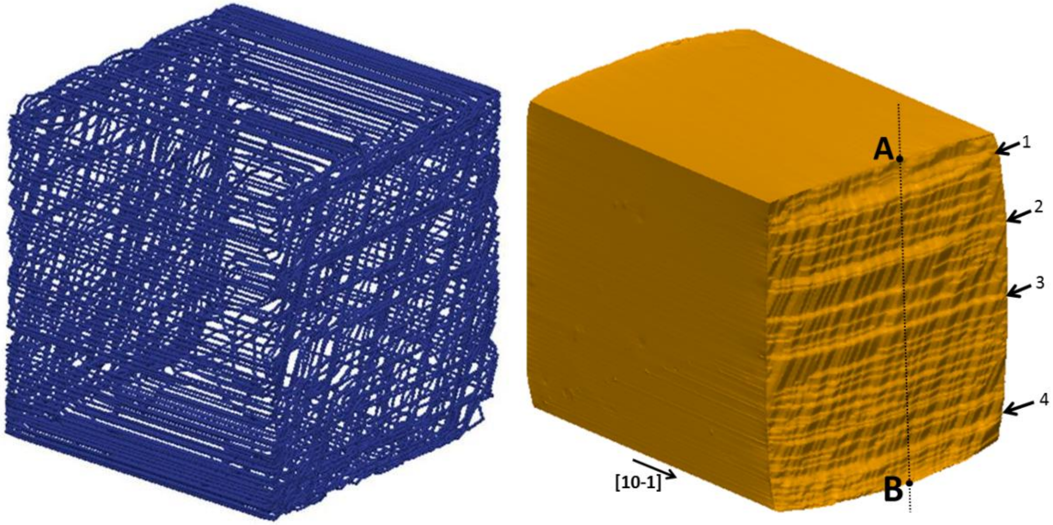
Shear band spacing: simulation…

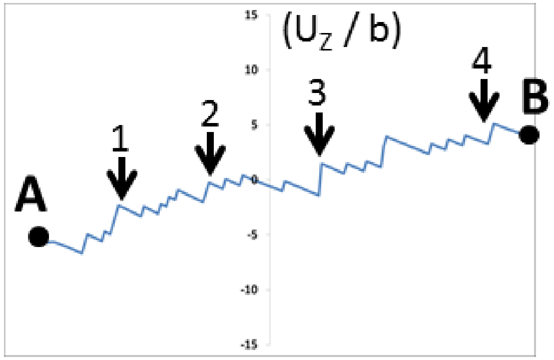




00 loops

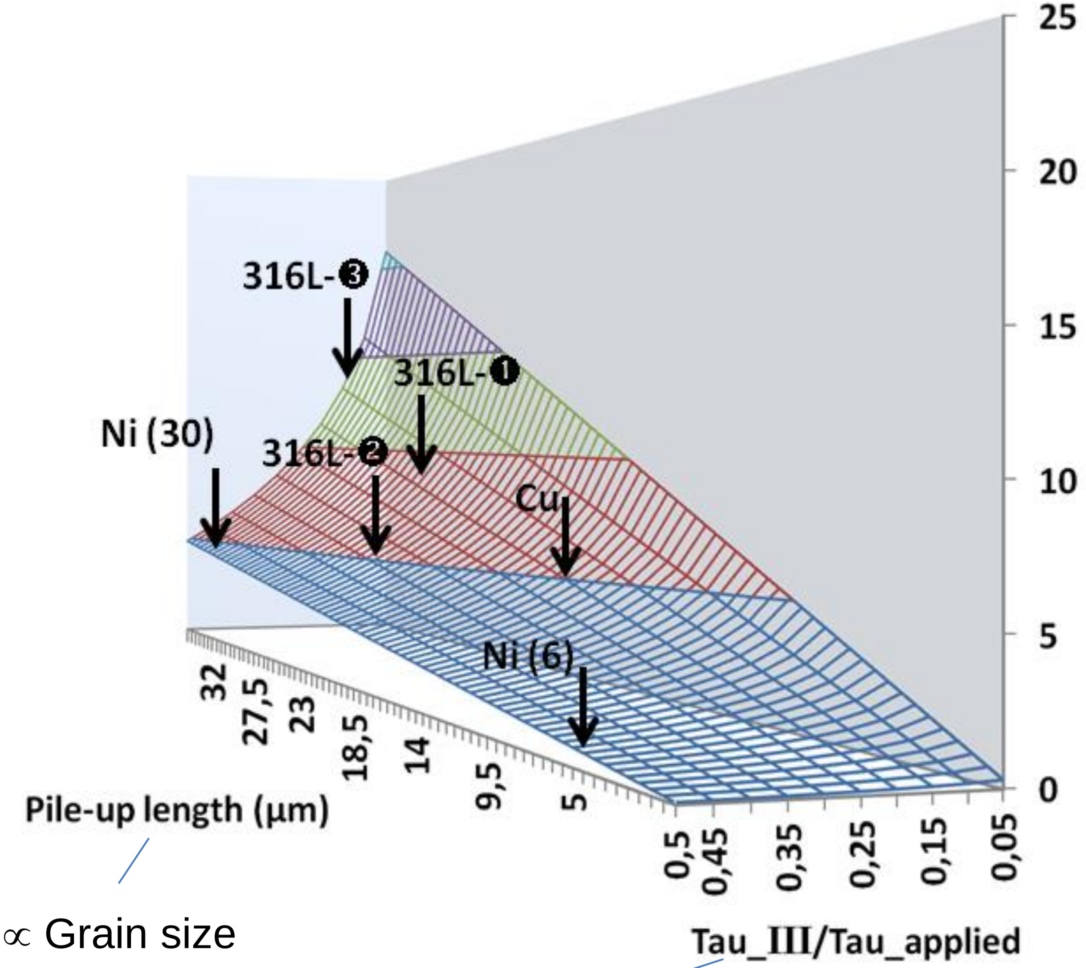
$\varepsilon_p = 1{,}4\times10^{-3}$





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

Shear band spacing prediction?



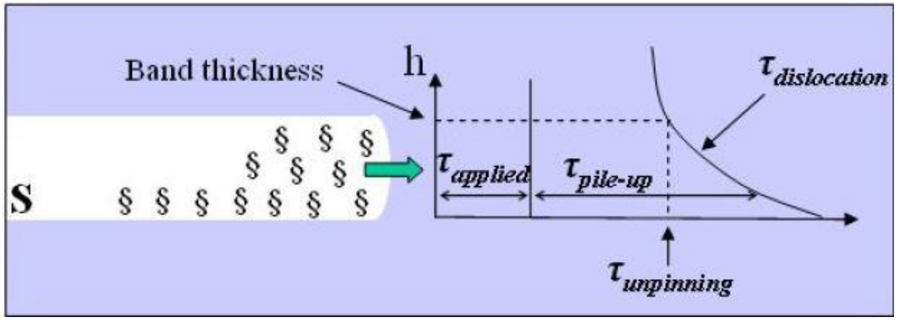
Shear band spacing « d »

$\propto$ Grain size

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

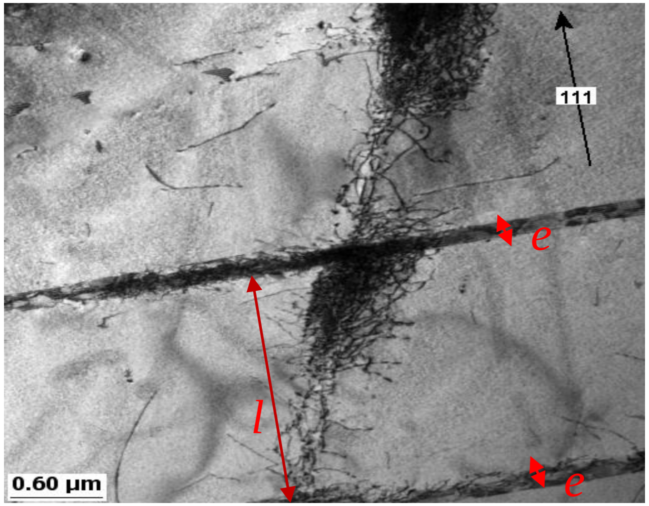
$\approx (\tau_{YS} - \tau_0) + \Delta\tau$ (irradiation-dose, ε_p)

Shear band thickness prediction ?



Dislocation can glide inside shear bands wherever the stress verifies:

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



[W. Karlsen, VTT, 2006]

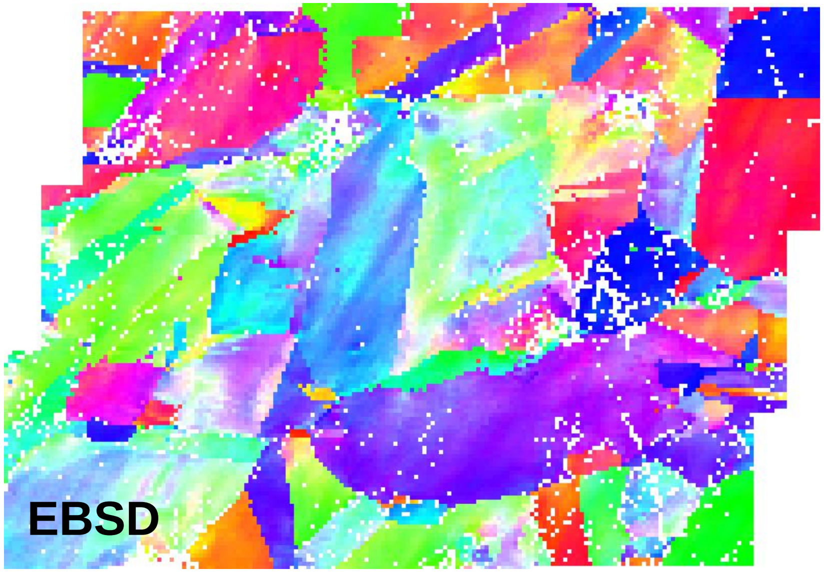
How to chose these different terms?

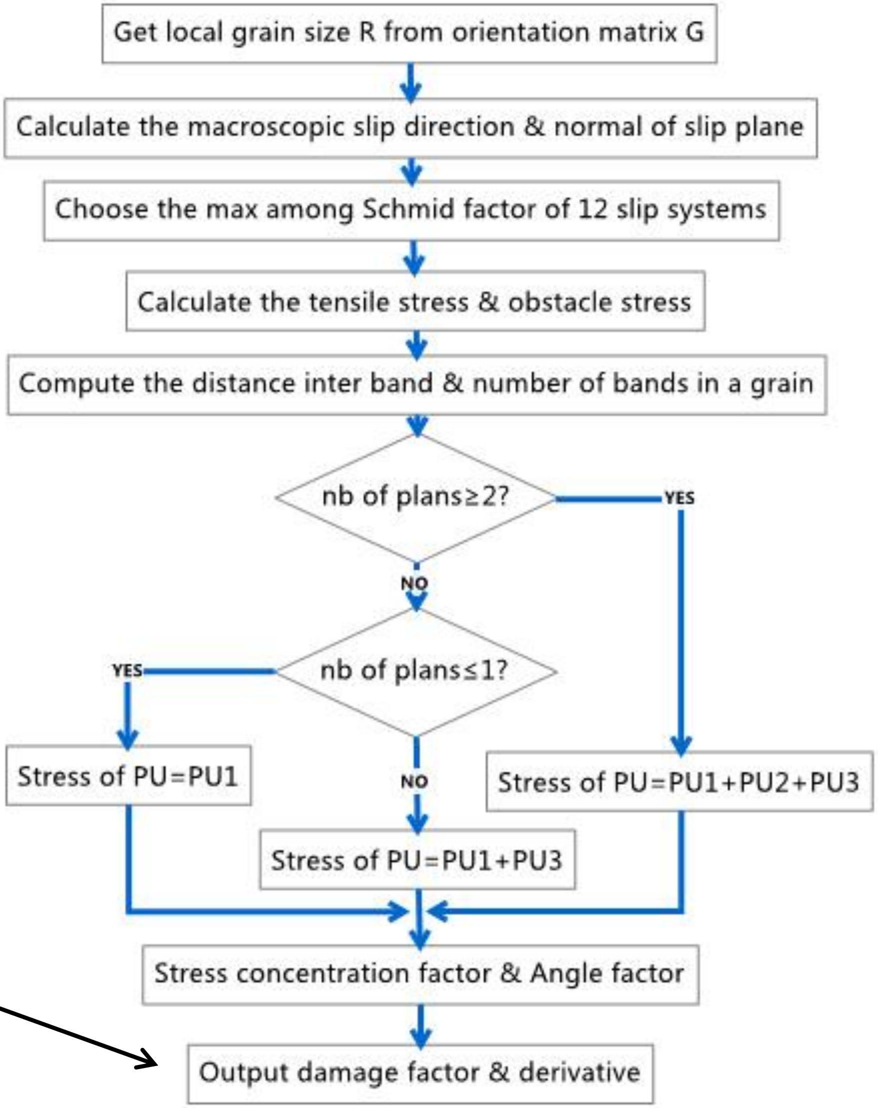
☞ Applied stress level τ_{app} (tensile testing data or hardening theory)
☞ τ_{pu} (inter-band pile-ups, analytical H&L model)
☞ Obstacle strength τ_{defect} (MD & continuum S&B theory).

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

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

Application to poly-crystals




Get local grain size R from orientation matrix G

Calculate the macroscopic slip direction & normal of slip plane

Choose the max among Schmid factor of 12 slip systems

Calculate the tensile stress & obstacle stress

Compute the distance inter band & number of bands in a grain

nb of plans≥2?

nb of plans≤1?

Stress of PU=PU1

Stress of PU=PU1+PU2+PU3

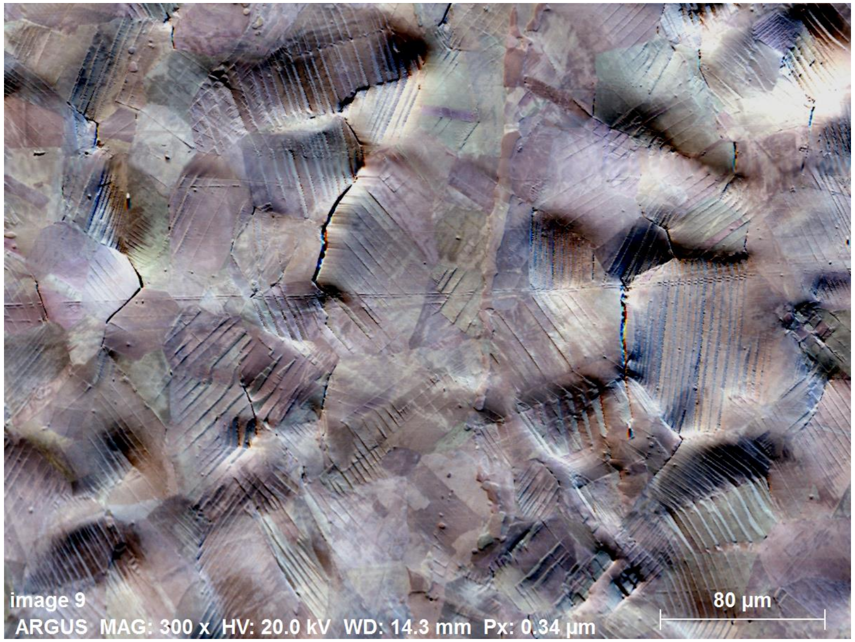
Stress of PU=PU1+PU3

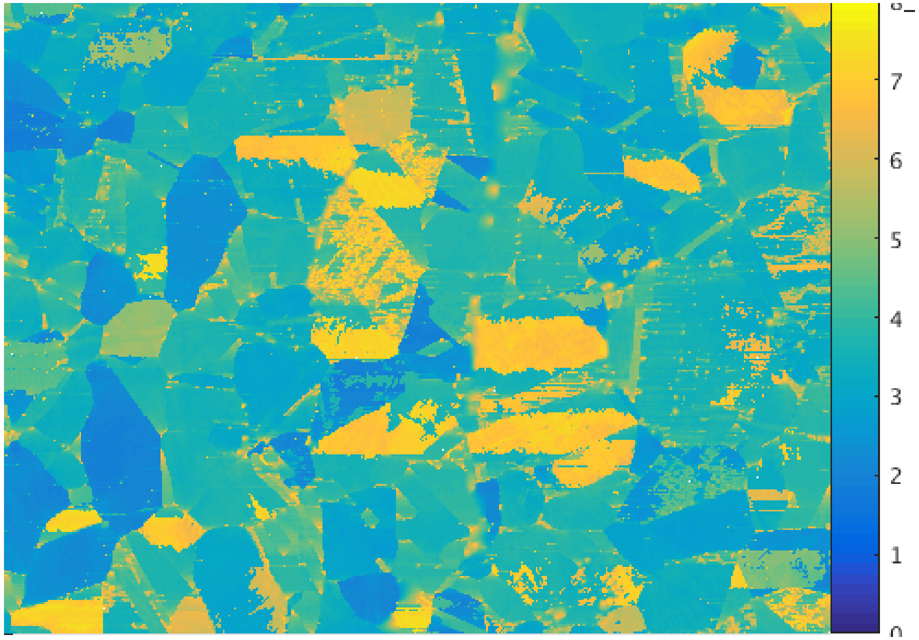
Stress concentration factor & Angle factor

Output damage factor & derivative

Damage factor include stress concentration and crystallographic orientation contributions.

Comparison with observation (P+ irradiation)

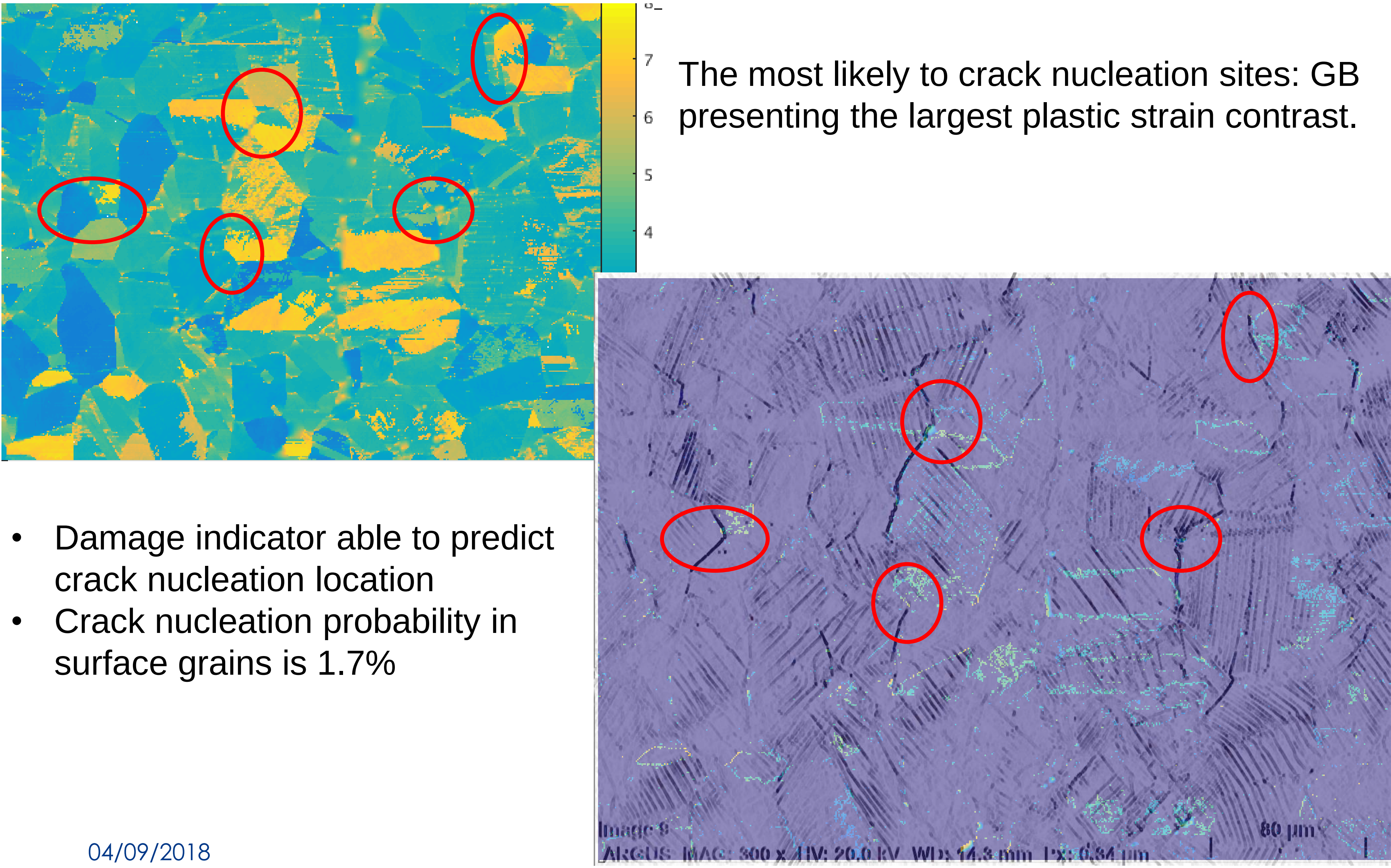




[B. Tanguy, 2014, DEN/DMN/SEMI]

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)



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

- Damage indicator able to predict crack nucleation location
- Crack nucleation probability in surface grains is 1.7%

Conclusion & Perspectives

<u>Plastic strain in presence of disperse defect populations:</u>

- Dislocation spreading is controlled by <u>cross-slip</u>: i-helps mobile dislocations **overcoming** the disperse defect clusters, ii-helps **spreading** shear bands across the whole grain

- Shear bands dislocation substructures include extended dislocation **pile-ups**
- Shear band spacing controlled by **grain-wide** pile-ups
- Shear band thickening 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

<u>Perspectives:</u>

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