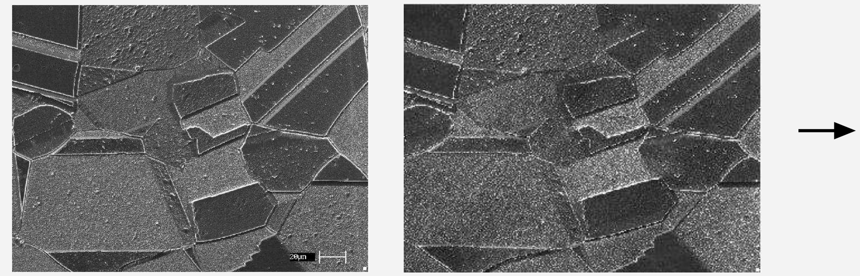
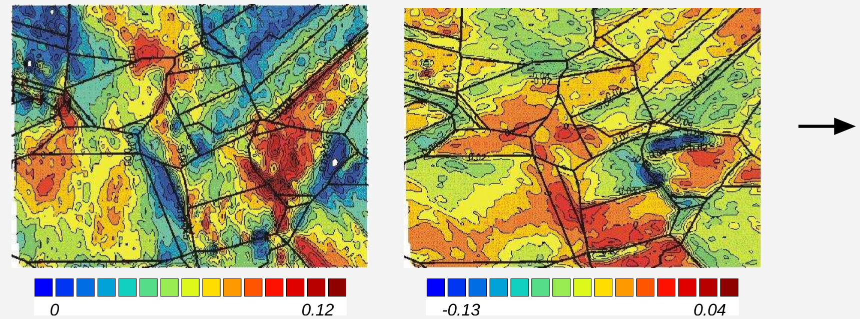
Contents

SEM images and measured strain fields



Initial view — *After 10% average strain*



Axial strain ε_{11} — *Lateral strain ε_{22}*

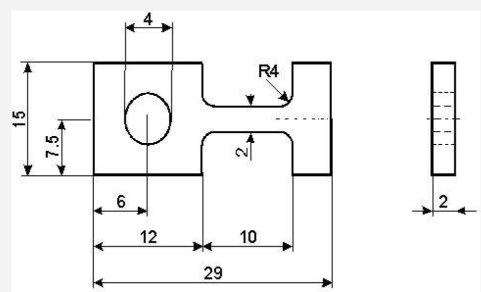
Average strain 5%

FE calculations of crystalline microstructures (ctd)

Georges Cailletaud

Centre des Matériaux
Ecole des Mines de Paris/CNRS

A summary of the experimental data



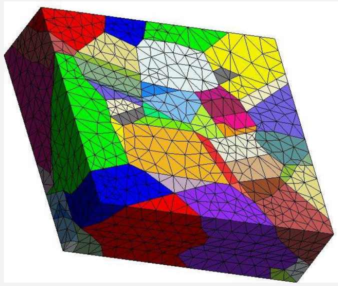
Tension tests on a small flat specimen made of OFHC copper

Data available:
- *Macro stress-strain curve*
- *SEM images*
- *OIM scans*
- *Local strain field*

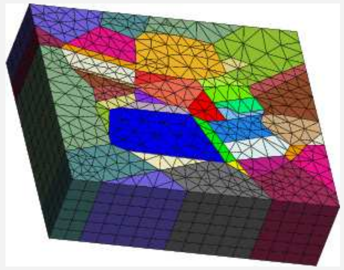
[Tatschl and Kolednik, 2003, Tatschl and Kolednik, 2004]
Erich Schmid Institute of Material Science, Leoben, Austria

Simulations in Musienko's PhD

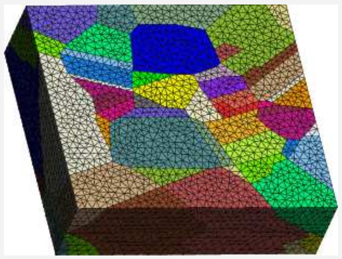
Finite element meshes



3D, 31780 nodes



extended 2D, 14076 nodes



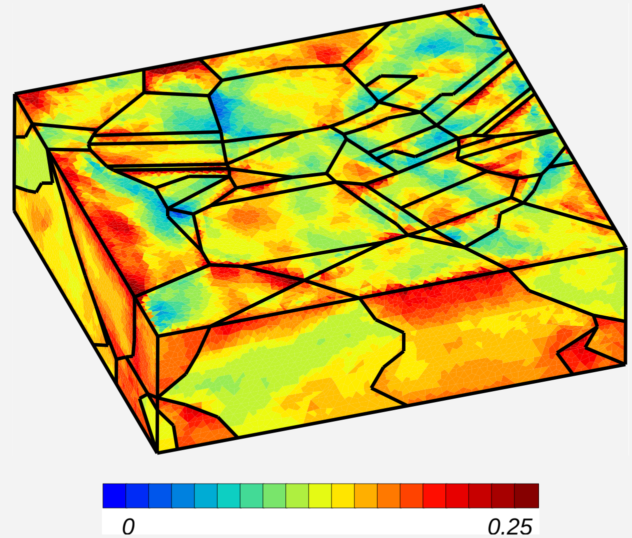
3D-fine, 130818 nodes

Purpose of the computation

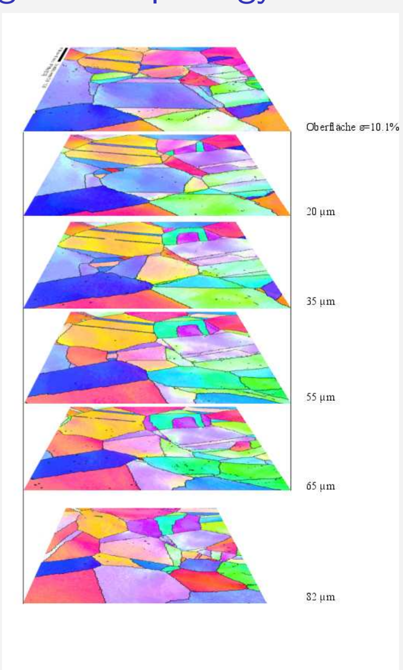
- *Check the local strain fields*
- *Compare 2D and 3D FE computations*

Schmidegg's master thesis

FE result: sum of the plastic slips

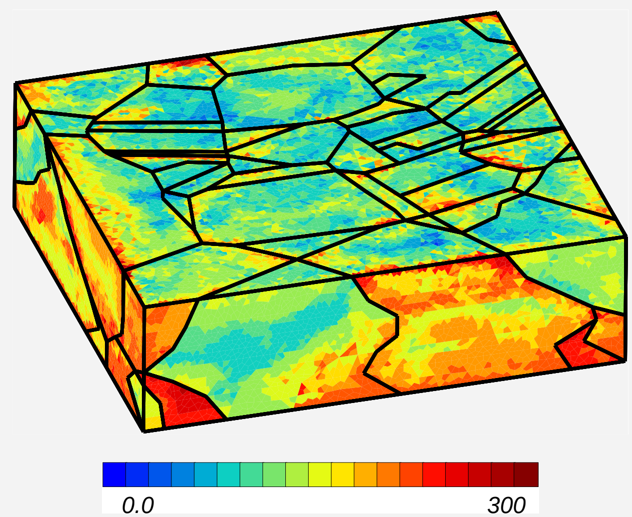


3D grain morphology information

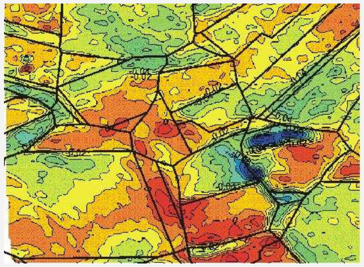


- *After the test, 6 layers of material were successively removed*
- *Final depth – 100 μm*
- *OIM-analysis was made after each removal*
- *3D grain structure can be reconstructed*

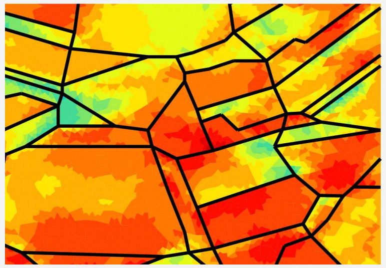
FE result: von Mises stress



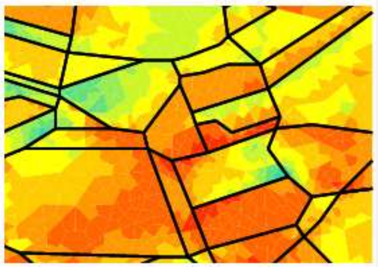
Comparison of sim and exp lateral strain fields



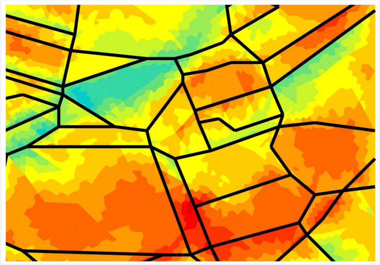
Experiment



3D fine *FE computation*



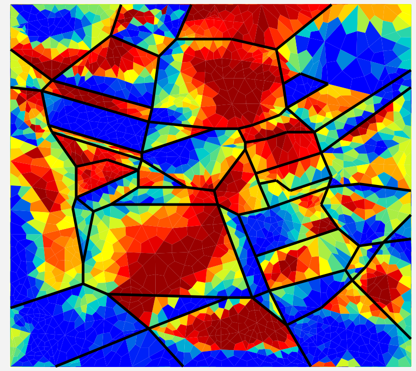
3D *FE computation*



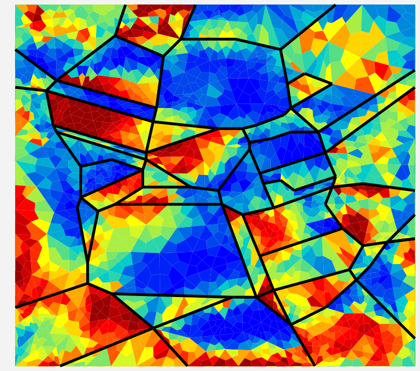
2Dext *FE computation*

Looking for primary slip ($\varepsilon = 0.05$)

Primary slip

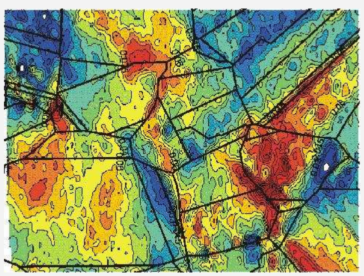


Maximum slip

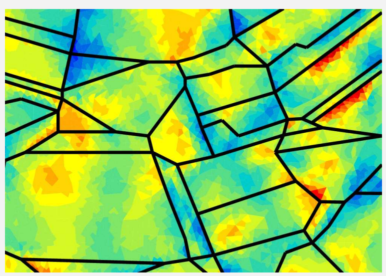


- *Primary slip is predominant in large grains, far from the limit of the aggregate*
- Special effect of twins ?

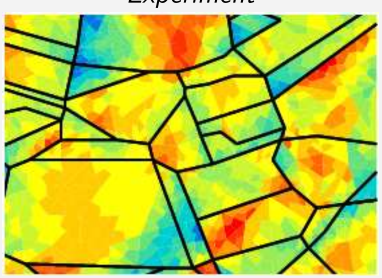
Comparison of sim and exp axial strain fields



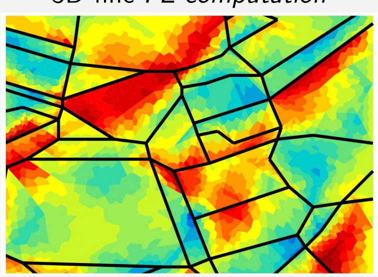
Experiment



3D fine *FE computation*



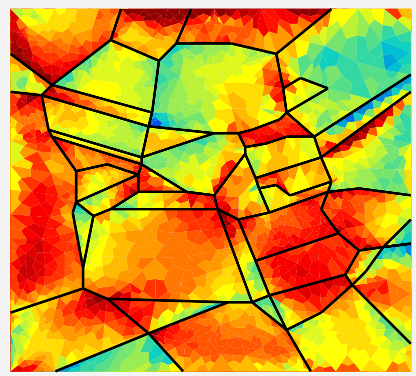
3D *FE computation*



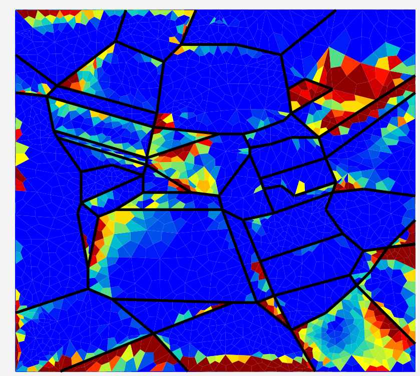
2Dext *FE computation*

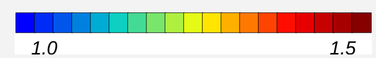
Resolved shear stress

τ^{B4}, *resolved shear stress on syst B4*



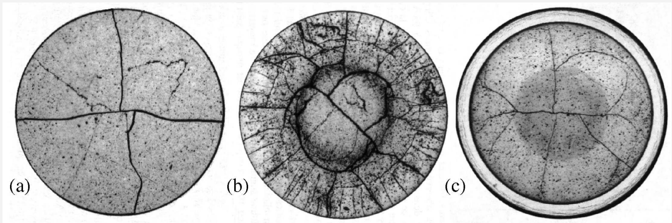
Ratio τ^{max}/τ^{B4}





- *B4 is such as it has the highest Schmid factor as a single crystal*
- τ^{max}/τ^{B4} is greater than 1 in perturbated zones

Pellet Crack Patterns

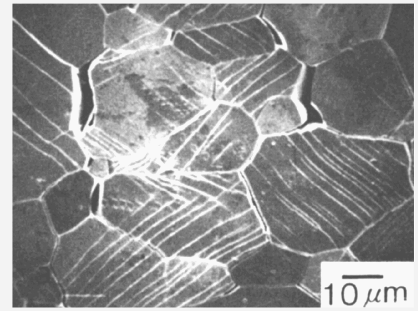


After one irradiation cycle	Two cycles then a ramp	Five cycles

- *Expansion of the uranium oxide, then indentation of the tube by the fragments*
- *Dimension of the tube : diameter 8 mm, thickness 0.7 mm*

PhD O. Diard, A. Musienko with EDF

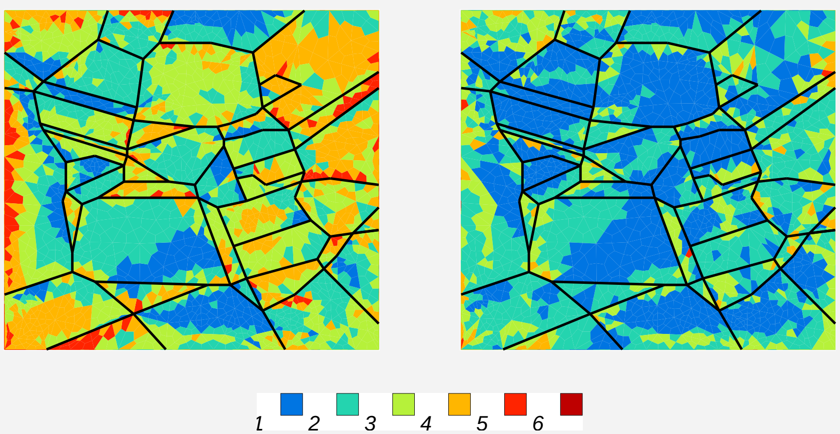
Damage mechanisms



- *Intergranular failure of grain boundaries normal to tension axis*
- *Iodin interaction with grain boundaries (adsorption)*
- *Grain boundaries become prone to damage due to iodin action*
- *Iodin diffusion faster in damaged grain boundaries*
- *After interganular propagation along a few grains, cleavage along basal plan appears*

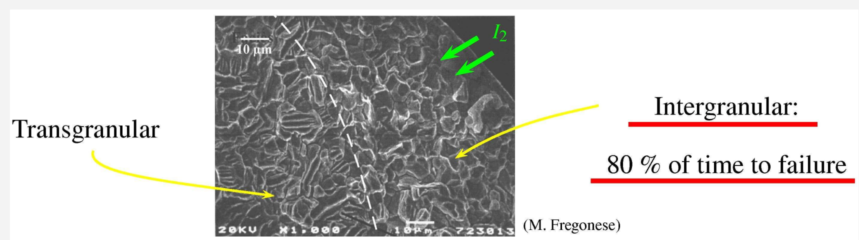
Number of active slip systems

$\varepsilon = 0.002$ $\varepsilon = 0.05$



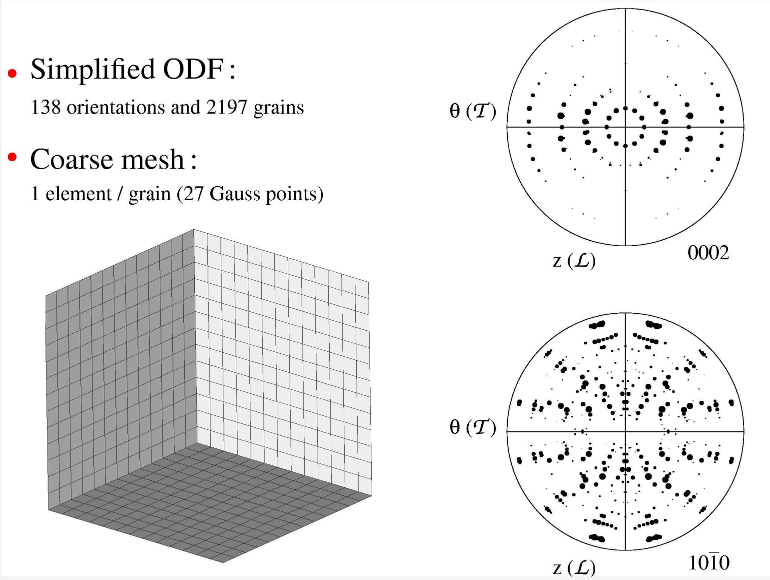
- *Many slip systems at the onset of plastic flow*
- Localization of the deformation process on a small number of slip systems

Cladding failure type

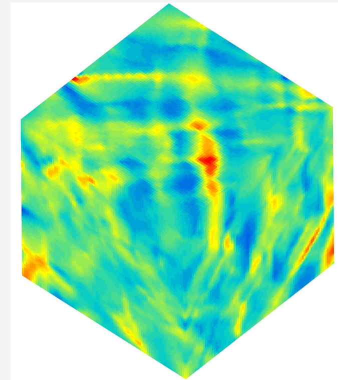


- *Intergranular nucleation and propagation*
- *Inter to trans transition, with quasi-cleavage mechanisms and fluting*
- *Brittle surface of failure*
- *Presence of* Stress Corrosion Cracking

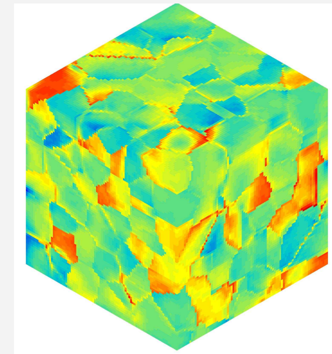
Identification procedure



Results on a 28x28x28 mesh

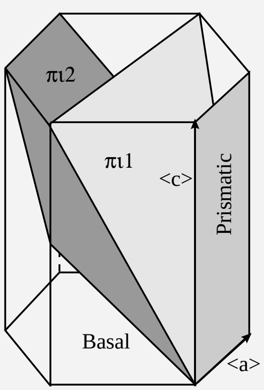


Total axial strain



von Mises equivalent

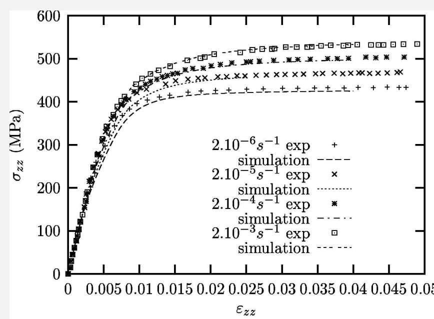
Crystallographic data



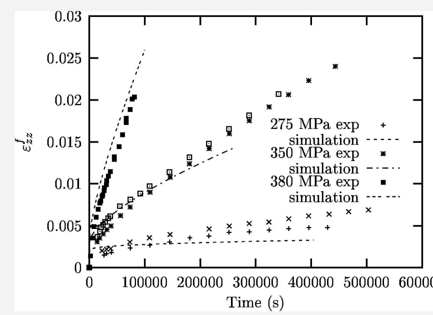
- *Hexagonal lattice until 863° C*
- *Deformation by slip on prismatic, then basal and pyramidal families*

System	Plane	Direction
Prismatic	$\{10\bar{1}0\}$	$<11\bar{2}0>$
Basal	$\{0001\}$	$<11\bar{2}0>$
$\pi 1 <a>$	$\{10\bar{1}1\}$	$<11\bar{2}0>$
$\pi 1 <c+a>$	$\{10\bar{1}1\}$	$<11\bar{2}3>$
$\pi 2 <c+a>$	$\{11\bar{2}2\}$	$<11\bar{2}3>$

Simulation of hardening and creep tests

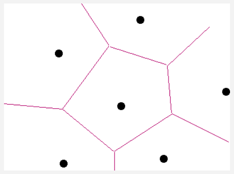


Hardening at various strain rates

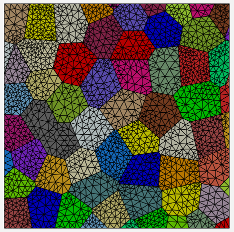


Creep tests

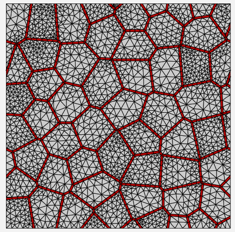
Aggregate fabrication scheme



Voronoi cells



polycrystalline aggregate



grain boundaries added

- *2D and 3D cases are treated*
- *Polycrystalline aggregate generation – then grain boundaries added*
- *Grain boundary is made of 2 elements. We no longer consider "grain boundary modeling", but "behaviour of each grain near the grain boundary"*

Slip system families

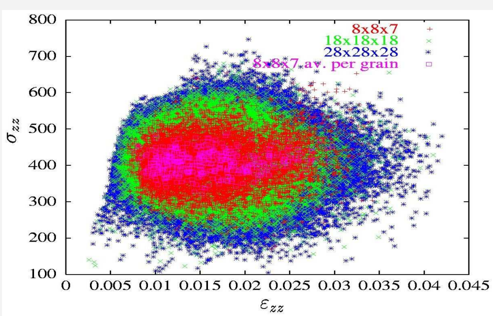
- *Plastic strain is a sum of elementary slips*

$$\dot{\underset{\sim}{\varepsilon}}^p = \sum_s \underset{\sim}{\mathbf{m}}^s \dot{\gamma}^s \qquad \dot{\gamma}^s = \left\langle \frac{|\tau^s| - r^s}{K} \right\rangle^n sign(\tau^s)$$

- *Prismatic slip* — $r_0 = 20$ *MPa*
  Basal slip — $r_0 = 132$ *MPa*
  Pyramidal $< a >$ *slip* — $r_0 = 107$ *MPa*
  Pyramidal $< c + a >$ *slip* — $r_0 = 195$ *MPa*
- *Predominant prismatic slip, possible basal and pyramidal slip*
- *Alternative solution – cleavage at basal plane*

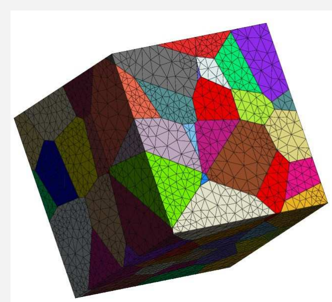
Local intragranular strain–stress state

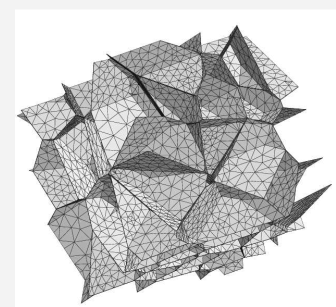
Local state in each grain after a tension at 1.5%



- *The larger meshes are "softer", they allow the material to deform more easily*
- *Coarse meshes underestimate the local scatter*

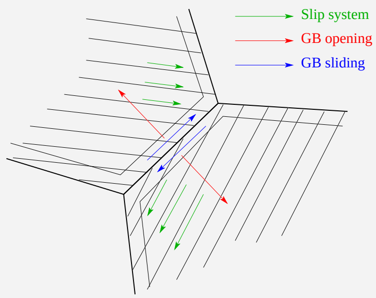
3D - a 100 grain aggregate





- *2 element boundaries, hexahedra, prisms, tetrahedra, quadratic and quadratic/linear elements*
- *Local orientation to determine normal to the grain boundary*

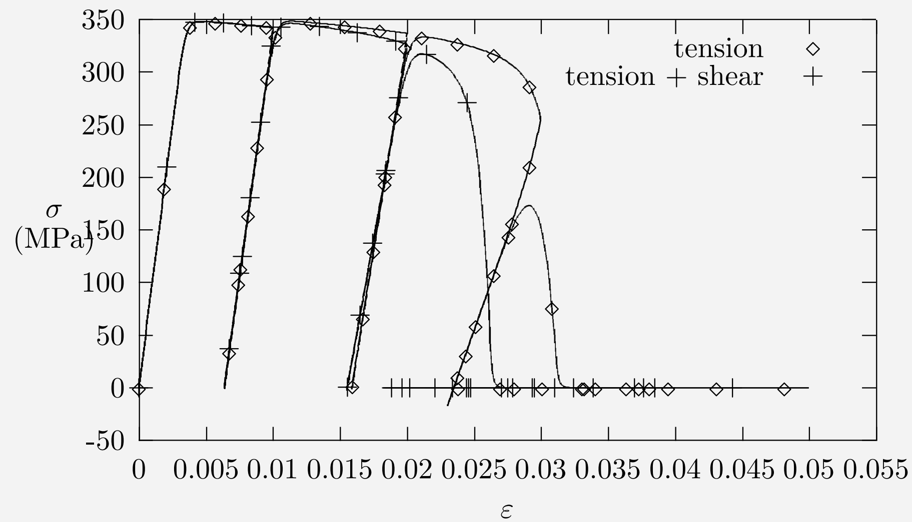
What is a grain boundary material ?



Grain boundary is the result of the behaviour of

- *the normal material*
- plus *additional "slip" capabilities (opening and sliding)*
- Two *half-GB's having each the properties of the host grain*

Illustration of grain boundary behavior



Opening for a loading normal to GB plane and constant superimposed shear ($\beta = 0.1$)

Cleavage representation

- *Additional deformation of "cleavage opening"* $\dot{\underset{\sim}{\epsilon}}^p = \dot{\delta}_c \underline{\mathbf{n}} \otimes \underline{\mathbf{n}}$
- $\underline{\mathbf{n}}$ – *normal to basal plane*
- *Flow rule for "cleavage"* $\dot{\delta}_c = \left\langle \frac{\sigma_c - R_c}{K_c} \right\rangle^{n_c}$, *viscous regularization*
- *Opening* δ *for positive* $(\sigma_c - R_c)$, *with* $\sigma_c = \underset{\sim}{\sigma} : (\underline{\mathbf{n}} \otimes \underline{\mathbf{n}})$
- *Nothing happens if* $(\sigma_c - R_c) < 0$
- $R_c = R_c^0 + Q_c \cdot (1 - exp(-b_c \delta_c))$, *with* $Q_c < 0$

DOS model

- *Elasticity and plastic flow*

Strain decomposition: $\dot{\underset{\sim}{\epsilon}} = \dot{\underset{\sim}{\epsilon}}^e + \dot{\underset{\sim}{\epsilon}}^p$

Elastic law with isotropic damage: $\underset{\sim}{\sigma} = (1 - D)\underset{\approx}{\mathbf{L}} : \underset{\sim}{\epsilon}^e$

Opening and sliding: $\dot{\underset{\sim}{\epsilon}}^p = \dot{\delta}\underline{\mathbf{n}} \otimes \underline{\mathbf{n}} + \dot{\gamma}^{\{}\underline{\mathbf{n}} \otimes \underline{\mathbf{t}}^{\}}$

- *Flow rules for opening and sliding*

Opening:
$$\dot{\delta} = \left\langle \frac{< \sigma_{11} > /(1 - D) - R_n}{K_n} \right\rangle^{n_n}$$

Sliding:
$$\dot{\gamma} = \left\langle \frac{|\tau|/(1 - D) - R_t}{K_t} \right\rangle^{n_t} sign(\tau)$$

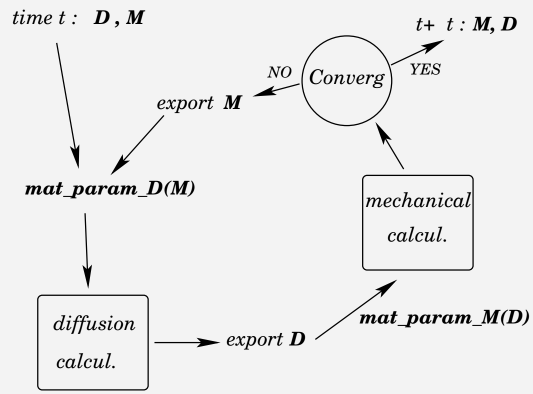
- *Damage evolution*

Critical variable:
$$\sigma_D = \sqrt{\sigma^2 + \beta\tau^2}$$

Damage evolution:
$$\dot{D} = \left\langle \frac{\sigma_D - R_D}{A} \right\rangle^{r} (1 - D)^{-k}$$

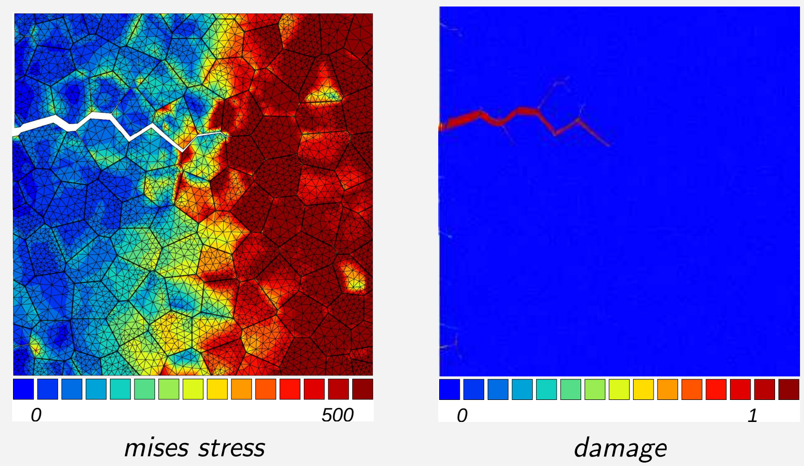
Damage is coupled with elasticity, opening and sliding

Weak coupling procedure in the FE code

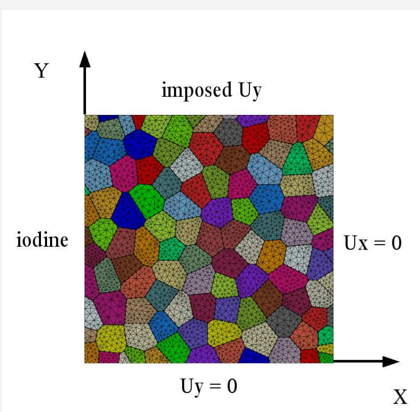


- M *and* D *are resp. the sets of mechanical and diffusion variables*
- mat_param_M *and* mat_param_D *the sets of material parameters*
- *Diffusion variables are seen as external variables for mechanics*
- *Mechanical variables are seen as external variables for diffusion*

2D iodine-influenced intergranular fracture (DOS+iodine)



Zircaloy. Boundary conditions

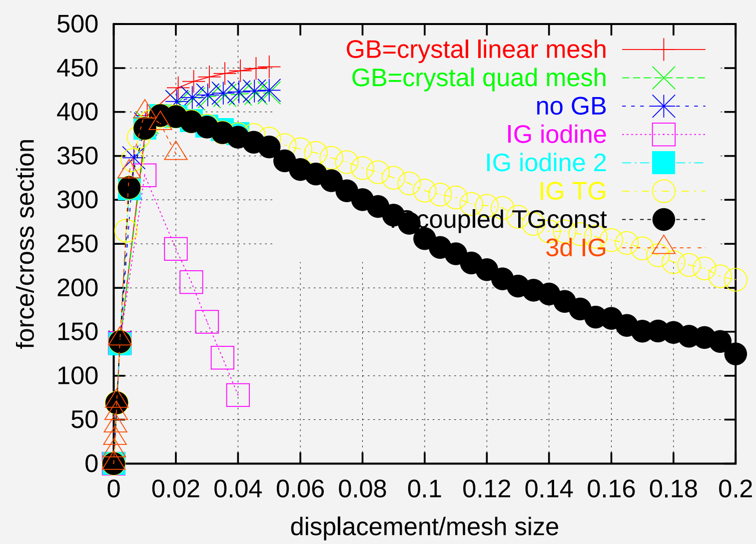


Computation list:

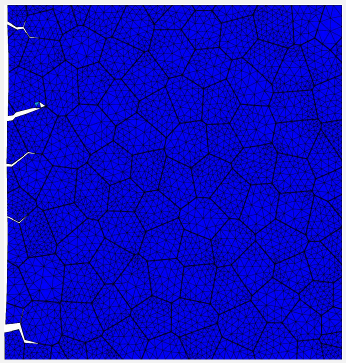
- *2D, DOS only*
- *2D, DOS+iodine*
- *3D, DOS+iodine*
- *2D, DOS+iodine+TG*

With iodine, the computations are made using the weak coupling procedure of the code Z-Set/ZeBuLoN

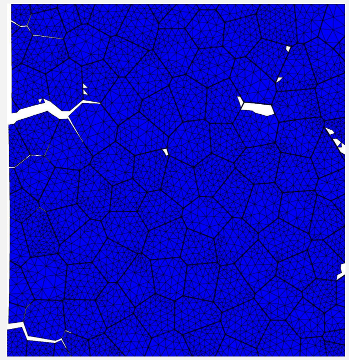
All computations. Macro level



Disconnected inter and transgranular failure



Crack initiation at the surface

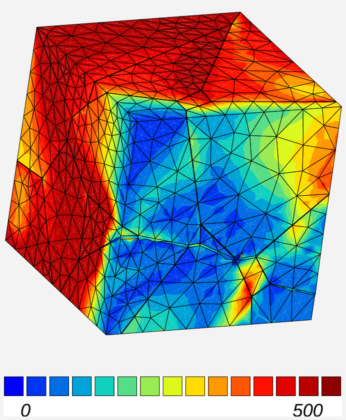


Cleavage far from the crack tip

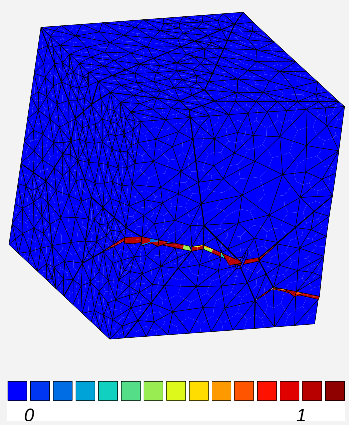
Conclusions and perspectives

- *Crystal plasticity is the proper scale for modeling damage behaviour of Zy4*
- *Grain boundaries are critical, due to mechanics–environment interaction*
- *Intergranular crack propagation was simulated in 2D and 3D using a new concept of grain boundary (grain boundary as a bicrystal with Damage, Opening and Sliding).*
- *It was possible to reproduce the transition form intergranular to transgranular failure.*
- *more in [Cailletaud et al., 2002]*

3D iodine-influenced intergranular fracture (DOS + iodine)



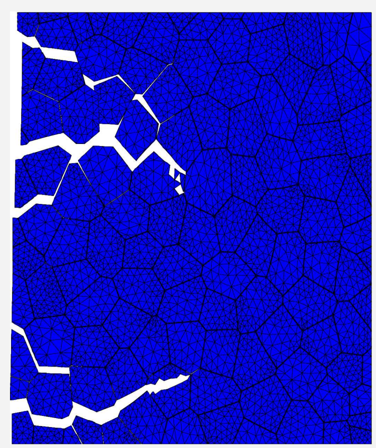
von Mises stress

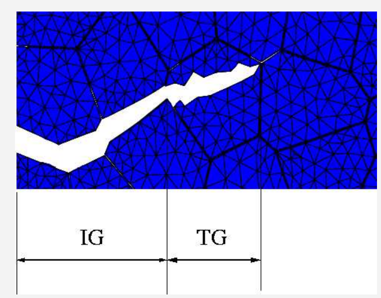


damage

σ = *385 MPa* ε = *1.6%*

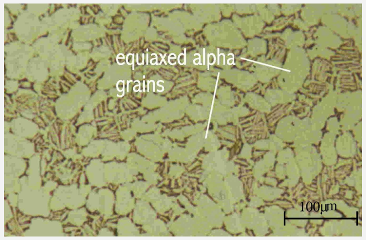
Inter-transgranular passage





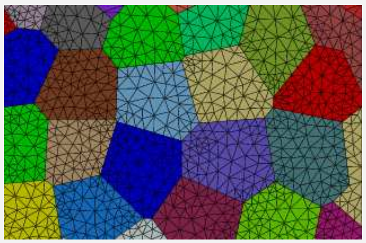
Cleavage at the crack tip

Microstructural model of TA6V



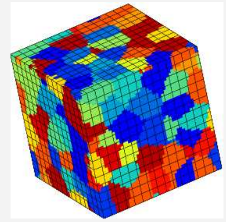
TA6V: *equiaxed α, layered $\alpha+\beta$ zones*

$\Downarrow$



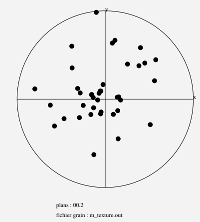
Model: *equiaxed α titanium*

Crystal plasticity: model identification



Representative elementary volume

- *Grain geometry by random Voronoï polyhedra generation*
- *Boundary conditions: periodicity*

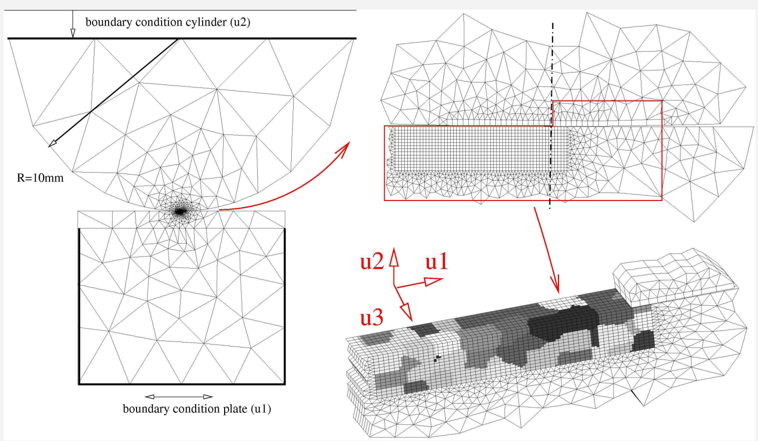


00.2 pole figure

Texture generation

1. *A texture component = vector + tolerance of 20 degrees*
2. *Intensity in Multiple Random Units (MRU)*
3. *Orientation generation by random process*

3D FE model of a fretting wear test (PhD T. Dick/Snecma)



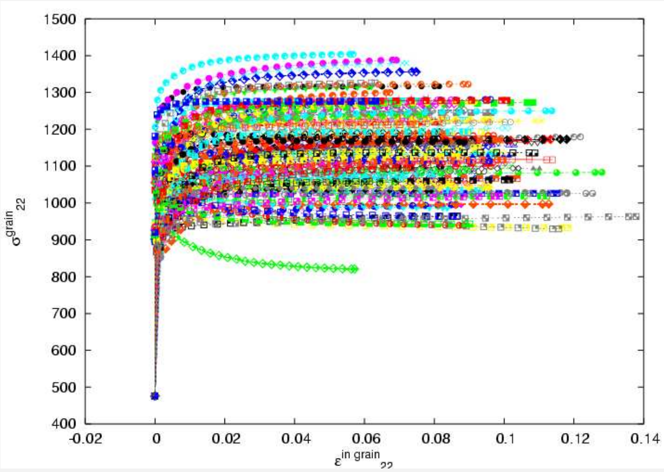
Computation settings	
mesh	*linear plane strain elements*
u3	*zero displacement on front and back planes*
u2	*set to cause vertical force* $P = 133$ N
u1	$\delta_{max} = 75\ \mu m$
friction coefficient	*0.8*
cycling frequency	5 Hz

- *element size in contact* $5.4\mu m$ x $5.4\mu m$ x $6.3\mu m$
- *small deformations formulation*

Crystal plasticity: identification strategy

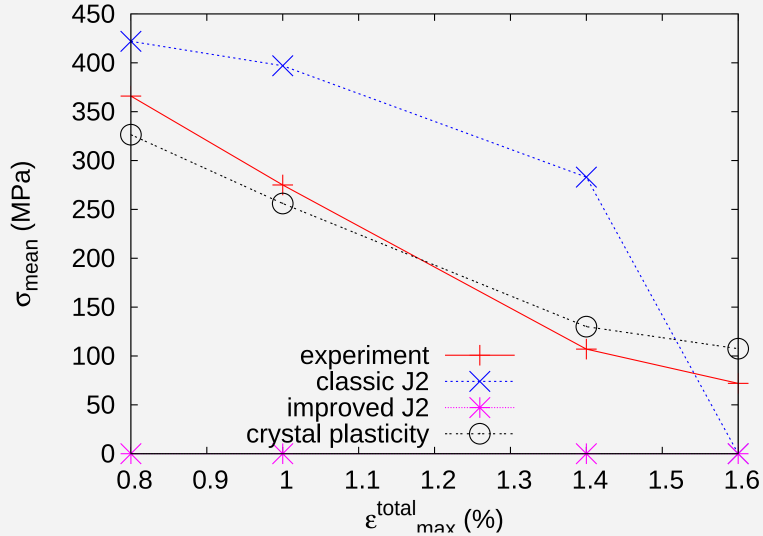
1. α *phase slip families: prism. , basal , pyramidal* $< a + c >$ *(Fundenberger et al.)*
2. *slip repartition: 50% prismatic, 30% basal slip, 20% pyramidal* $< a + c >$ *(Fundenberger et al.)*
3. *texture in Ta6V disk: c-directions parallel to disk-axis (Thesis Le Biavant-Guerrier)*
4. R_0 *and* R_1 *cyclic fatigue tests (Thesis Le Biavant-Guerrier)*

Average grain response in an FE aggregate



tensile test, aggregate with 15x15x15 el., 120 grains, periodic BC

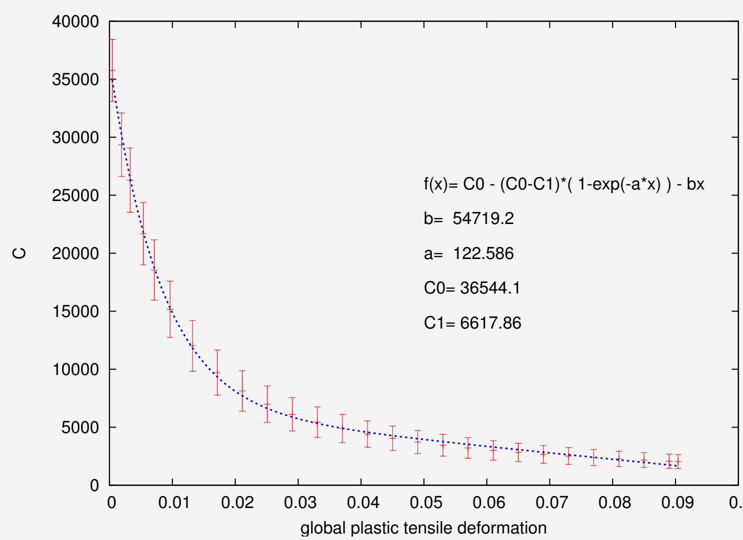
Mean stress relaxation in R_0 tests



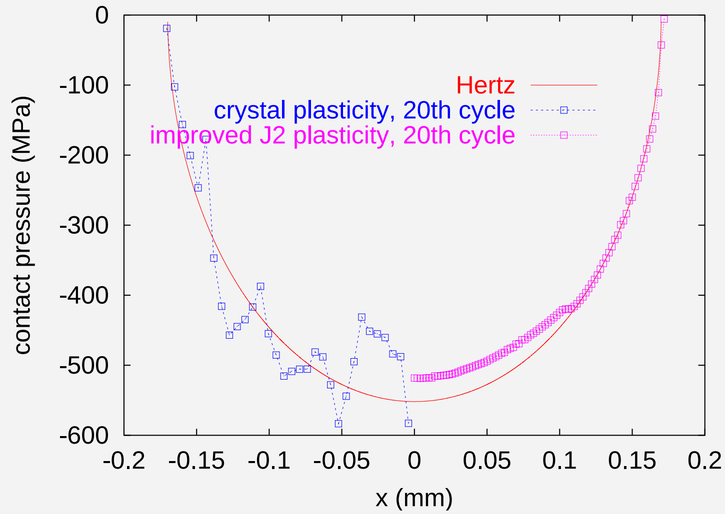
Crystal plasticity: model parameters

Model Parameters		*prismatic*	*basal*	*pyramidal a+c*
Viscosity	*K*	*20*	*20*	*20*
	n	*7.41*	*7.41*	*7.41*
Isotropic hard.	*R0*	*280*	*300*	*540*
	Q	*-49.4*	*-52*	*-83.2*
	b	*2*	*2*	*2*
Kinematic hard.	*C*	*30000*	*30000*	*30000*
	D	*300*	*300*	*300*

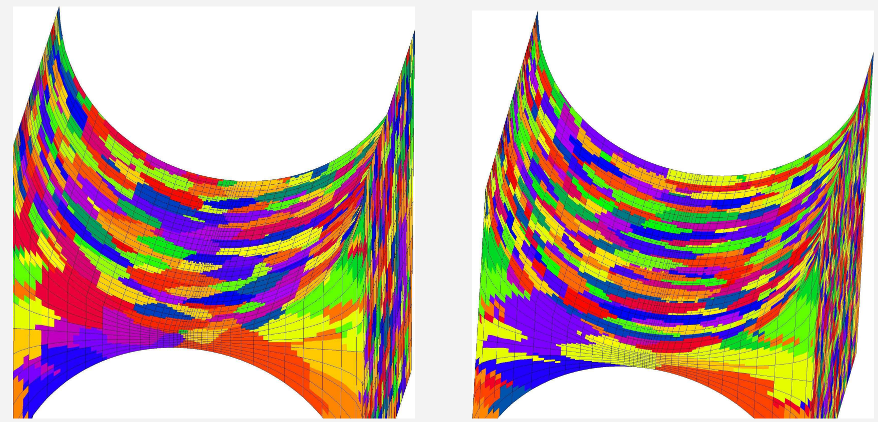
C evolution in a tensile test



Computation Results: contact pressure



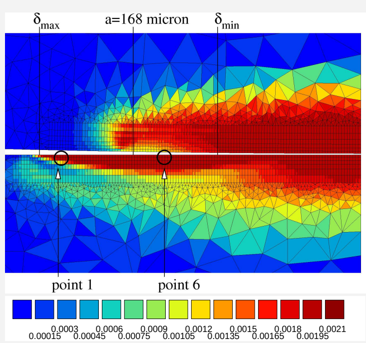
A millimetric sized component made of copper



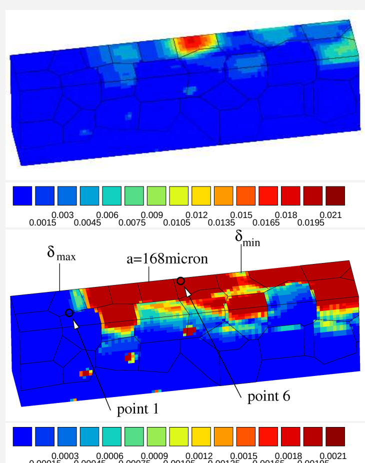
Post.doc El Houdaigui, 2004

Equivalent plastic strain after 20 fretting cycles

$\varepsilon^{in}_{eq} = \sqrt{\frac{2}{3}\varepsilon^{in}_{ij}\varepsilon^{in}_{ij}}$



improved J2 plasticity
$\varepsilon^{\rm in}_{\rm eq}(\max) = 0.34\%$

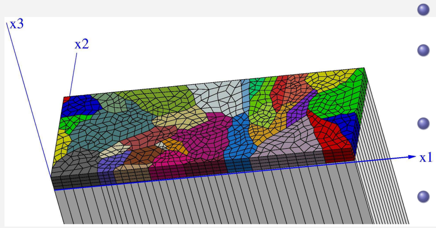


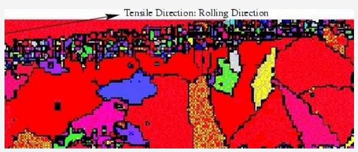
Crystal plasticity
$\varepsilon^{\rm in}_{\rm eq}(\max) = 1.8\%$

Conclusions and Outlook

- *Life is heterogeneous... soft and hard areas*
- *Crystal plasticity is now manageable, even in large meshes*
  - *it gives a good idea of the local stress and strain gradients related to microstructure*
  - *it is time to move from the* homogenization *to the* relocalization *process needed for damage modeling*
- *Future crystal plasticity computations:*
  - *higher spatial resolution*
  - *more loading cycles* $\rightarrow$ *steady state*
  - *micro scale damage measures*

Mechanical behaviour of a zinc coating on a galvanized steel sheet





- *Coating thickness 10 μm*
- *Orientation obtained by EBSD*
- *Biaxial stress state in the thin film*
- *Critical resolved shear stresses identified from a bulk specimen*
- *Plastic strain is mainly due to basal slip*
- *Presence of twinning* $\{10\bar{1}2\}\,\langle 10\bar{1}\,\bar{1}\rangle$

PhD R. Parisot

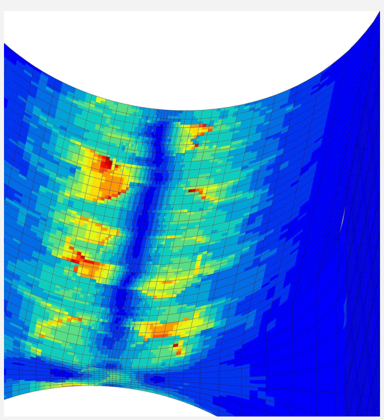
Cailletaud, G., Diard, O., and Musienko, A. (2002).
Damage, opening and sliding of grain boundaries.
In et al., S. A., editor, Multiscale Modelling of Engng. Materials, *Marrakech, Oct. 2002, pages 149–156. Kluüwer.*

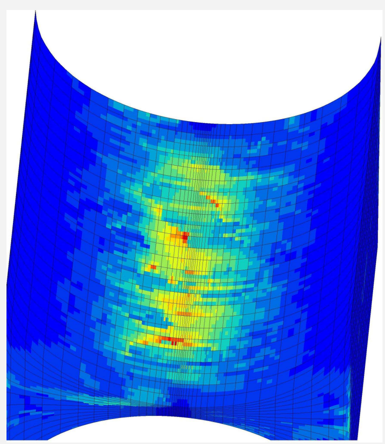
Parisot, R., Forest, S., Gourgues, A.-F., Pineau, A., and Mareuse, D. (2000).
Modeling the mechanical behavior of a multicrystalline zinc coating on a hot-dip galvanized steel sheet.
Computational Materials Science, *19:189–204.*

Tatschl, A. and Kolednik, . (2003).
A new tool for the experimental characterization of micro-plasticity.
Material Science and Engineering, *A339:265–280.*

Tatschl, A. and Kolednik, . (2004).
On the experimental characterization of crystal plasticity in polycrystals.
Material Science and Engineering, *A364:384–399.*

Von Mises stress for two realizations

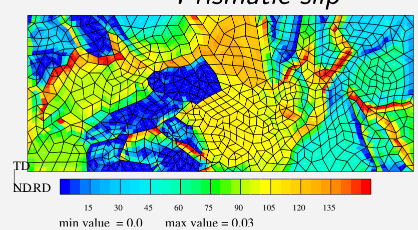




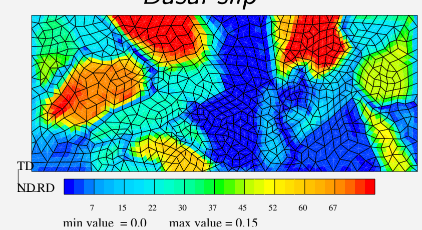
Post.doc El Houdaigui, 2004

Distribution of slip and twinning in the specimen

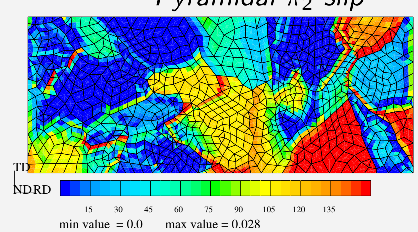
Prismatic slip



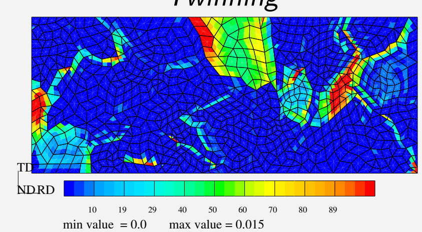
Basal slip



Pyramidal π_2 slip



Twinning



(more in [Parisot et al., 2000])