2137-50

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Multiscale modeling of thermal fatigue damage in austenitic steels

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United Nations
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Cultural Organization

IAEA
International Atomic Energy Agency

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12 – 23 April 2010
Miramare – Trieste, Italy

Christian Robertson
CEA-Saclay France
DEN/DMN/SRMA

Multi-scale modelling of thermal fatigue damage in austenitic steels

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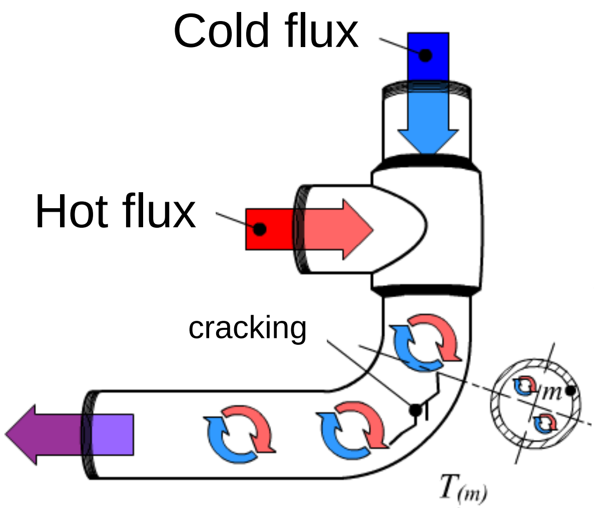
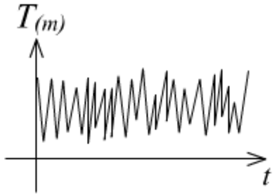
Motivation: predict thermal fatigue damage in PWR cooling lines

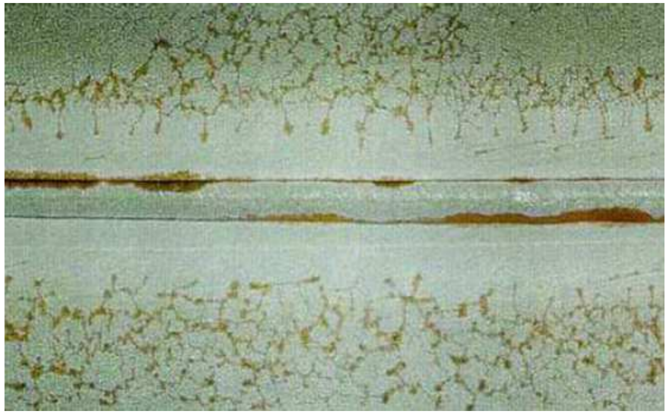


- Cracking in high ΔT fluid mixing zones

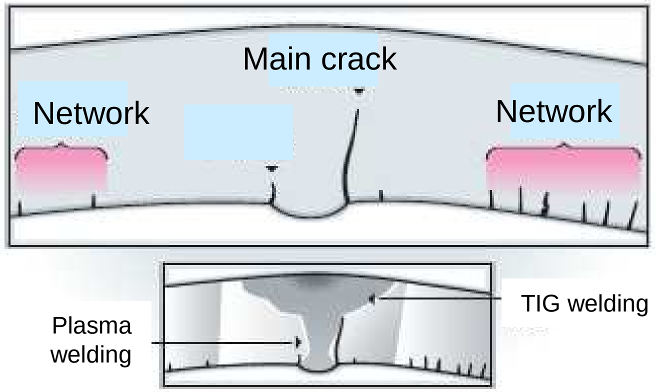


⚠ *May1998 : leak 30M³/h*

- Damage :
Trans-granular crack networks

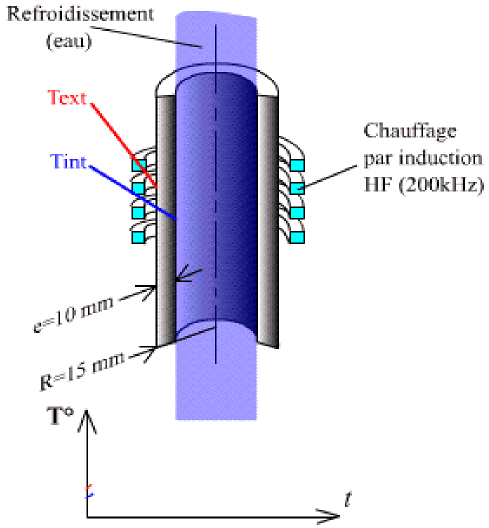


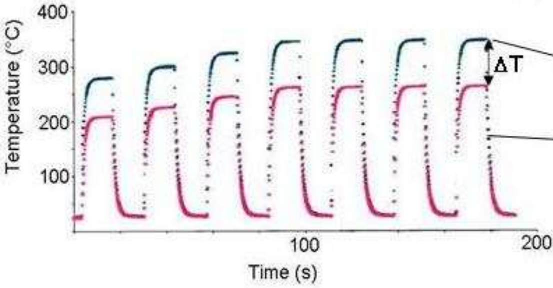
Tube wall

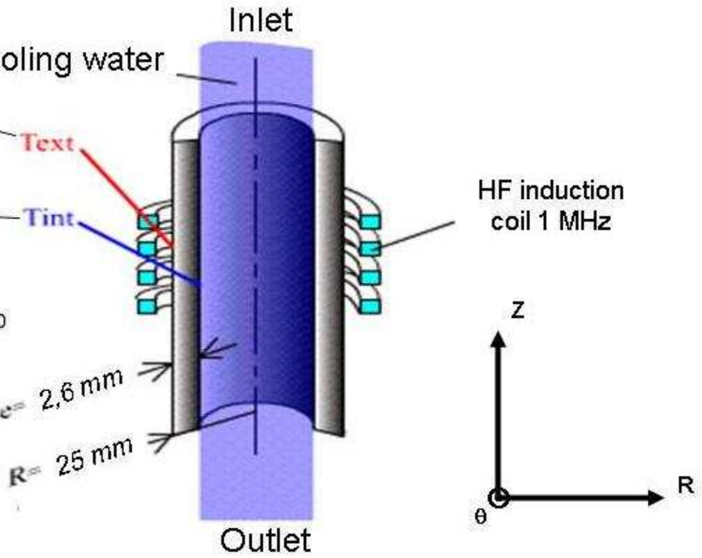


Cross-section

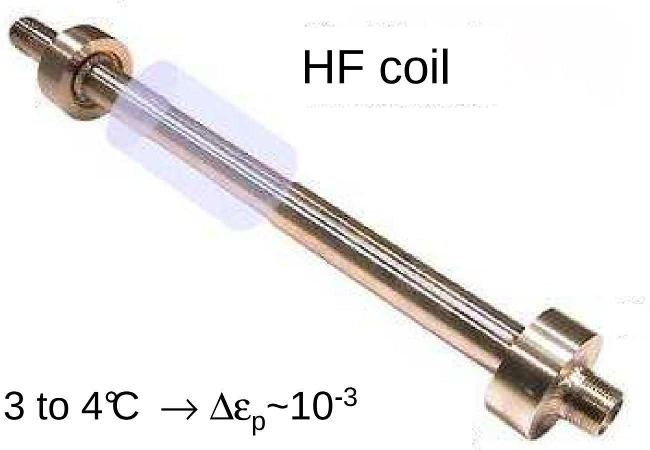
Crack initiation in thermal fatigue testing (BIAX test)





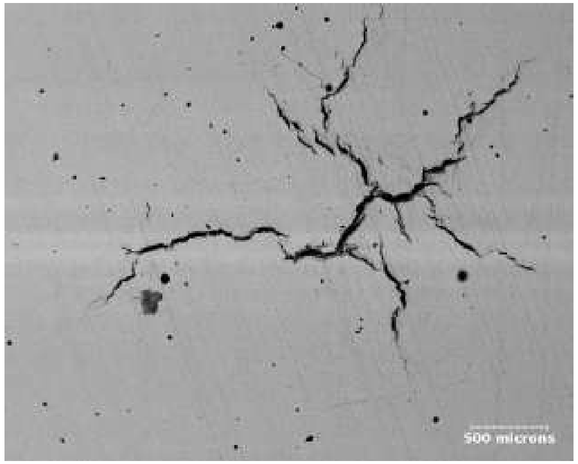


$$\Delta\theta = (T_{outlet} - T_{inlet})$$
$$\Delta T = (T_{ext} - T_{int})$$
$$\Delta\theta \propto \Delta T$$



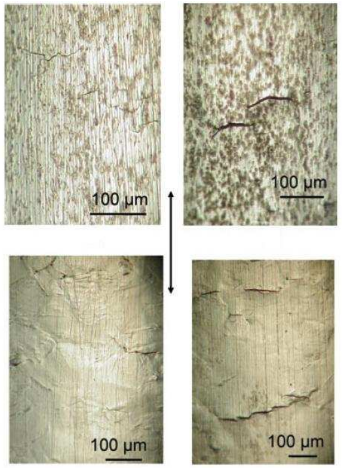
$\Delta\theta$ = 3 to 4℃ $\rightarrow \Delta\varepsilon_p \sim 10^{-3}$

Thermal fatigue



Equi-axial crack cells

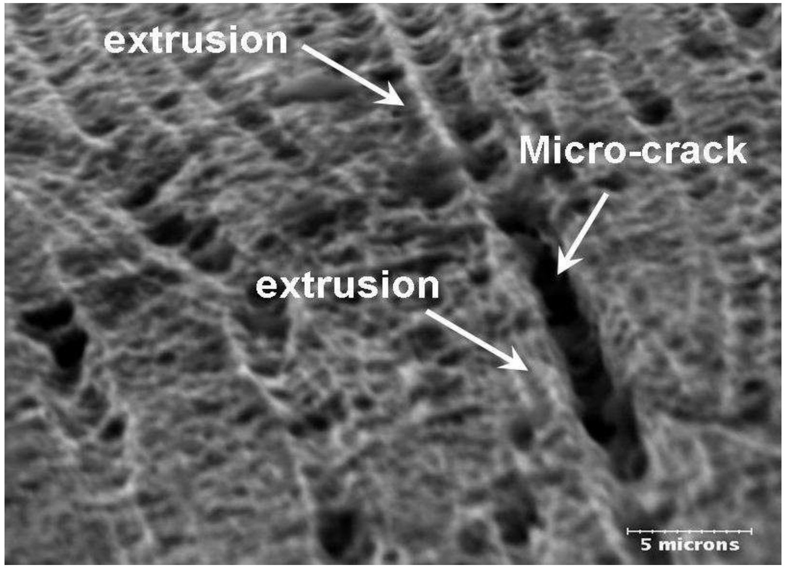
Uniaxial fatigue



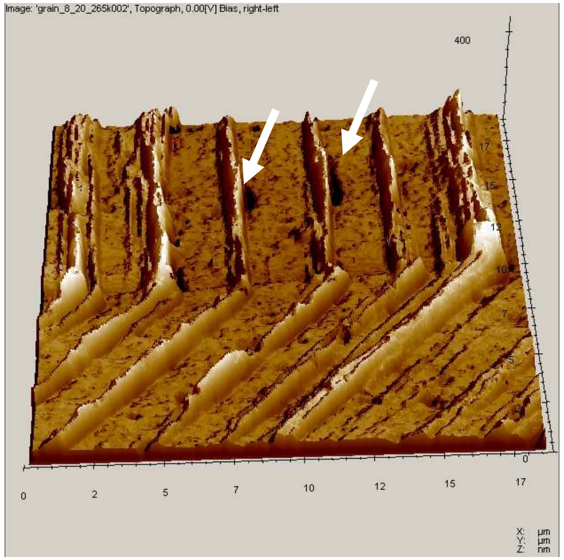
Parallel cracks

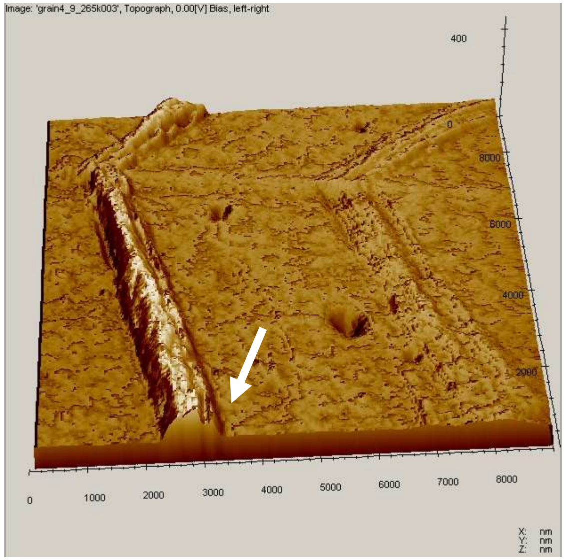
Crack initiation in fatigue: fcc metals & T < 300°C

X-section SEM



Micro-crack initiation is related to extrusion growth in fatigue & thermal fatigue





…in single & poly-crystals

Observations: summary

Thermal fatigue in PWR cooling lines

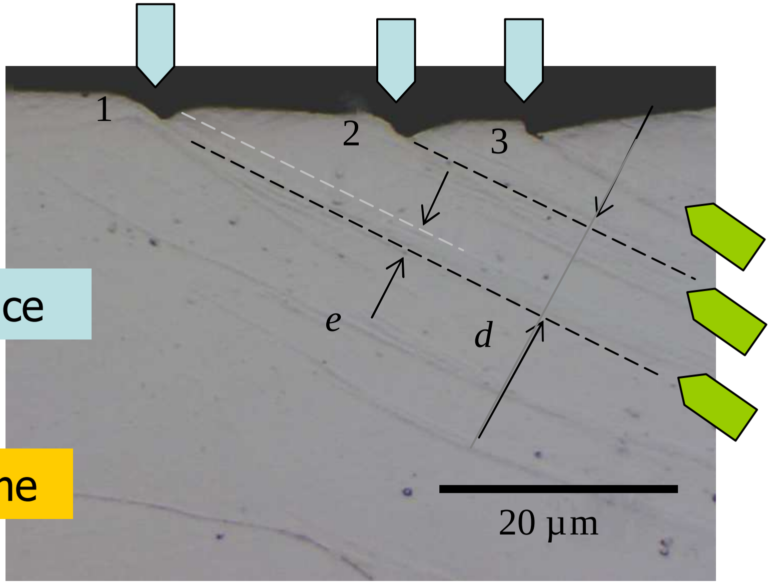
→ small plastic strain in surface grains

→ plastic strain localisation

visible in surface

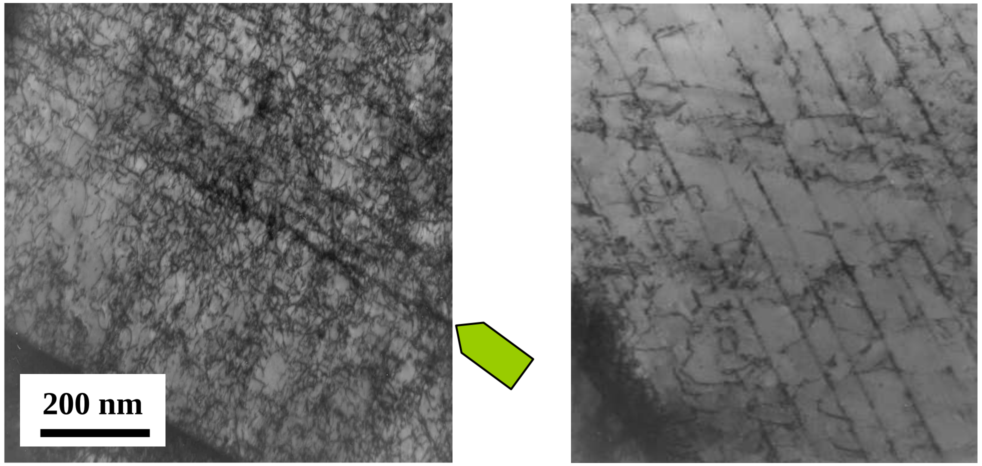
visible in volume

Surface displacements



cross-section

TEM



2 slip systems

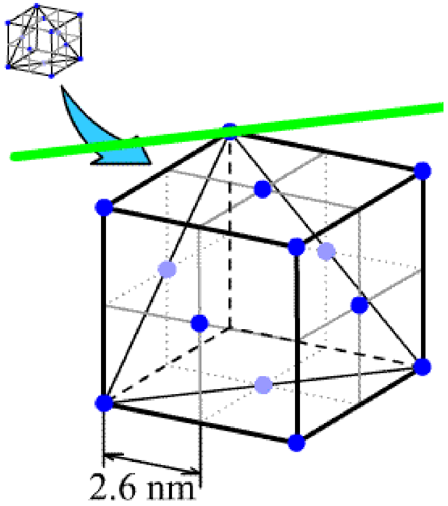
(primary and cross)

Origin strain localisation in the form of PSB ☞ collective dislocation effects

Dislocations Dynamics modelling in 3D

Dislocations model

- Discrete lines
- Discrete time step: 10^{-9} s
- Discrete lattice



Stress → **CFC material modelled by Dislocation Dynamics** →

- Dislocation microstructure
- Plastic Deformation

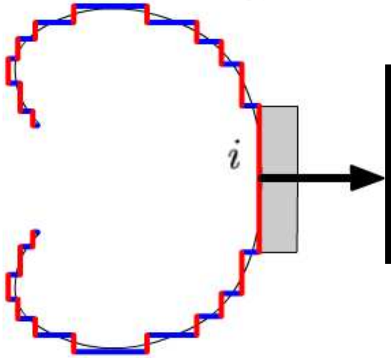
Dislocations Theory

→ Mobility rules
→ Dislocation/dislocation interactions
→ Cross-slip
⚠ No climb (⇒ no point defects)

3D Dislocations Dynamics modelling

Effective resolved shear stress

$$\begin{cases} \tau^{**} & = \left\{ \left[\frac{1}{b} \left(\sigma_{app} + \sigma_{int} + \sigma_{image} \right) \mathbf{b} \right] \times \mathbf{l} \right\} .\mathbf{g} + \tau_{tl} \\ \tau^{*} & = \tau^{**} - \mathrm{sign}(\tau^{**}) .\tau_{fr} \end{cases}$$



$$\boxed{\begin{cases} v^i & = \frac{\tau^* b^{(s_i)}}{B} \\ \mathrm{d}A^i & = l^i .v^i .\delta t \end{cases}}$$

Mobility rule:

Phonon drag

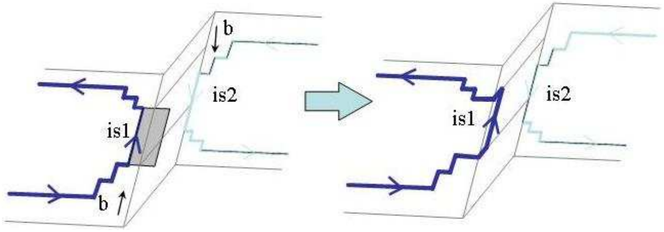
$$\mathrm{d}\gamma_p^i = b^{(s_i)} \frac{\mathrm{d}A^i}{V}$$

Plastic strain

$$\begin{cases} \mathrm{d}\epsilon_p^i & = \frac{1}{2} (\mathbf{b}^{(s_i)} \otimes \mathbf{n}^{(s_i)} + \mathbf{n}^{(s_i)} \otimes \mathbf{b}^{(s_i)}) \mathrm{d}\gamma_p^i \\ \mathrm{d}\epsilon_p & = \sum_{i=1}^{N} \mathrm{d}\epsilon_p^i \end{cases}$$

Thermally activated cross-slip

$$P = \beta \frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp\left(\frac{\tau^* - \tau_{III}}{kT/V} \right)$$

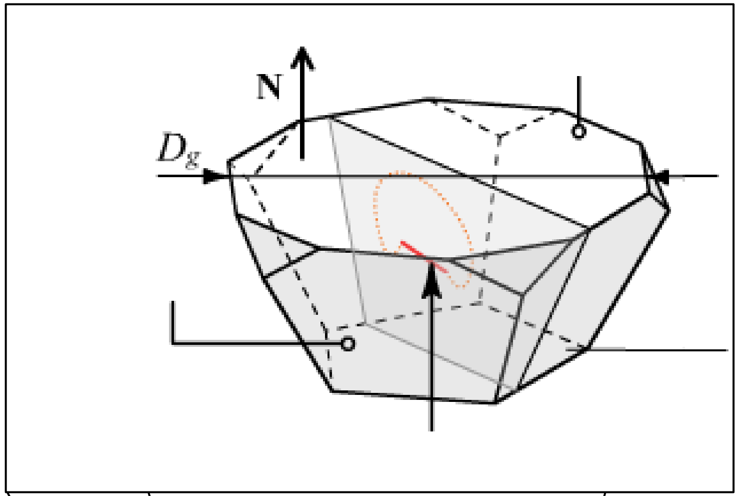


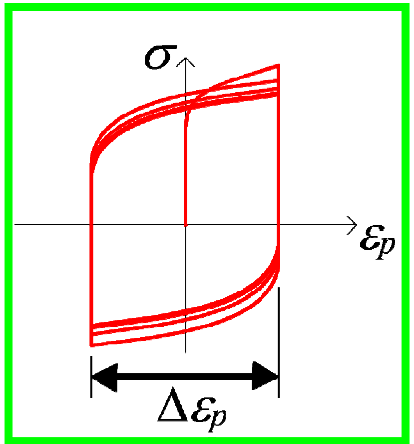
ONLY IN 3D!

Typical materials parameters for austenitic steels

Poisson's ratio ν	Young's modulus E (GPa)	Density ρ ($\mathrm{kg\,m^{-3}}$)	Burgers vector magnitude b (10^{-10} m)	Stacking-fault energy γ ($\mathrm{J\,m^{-2}}$)	Activation volume V/b^3	Viscous drag coefficient B (10^{-5} Pa s)	Threshold stress τ_{III} (MPa)
0.26	189	7870	2.54	30	1800	0.712	52

Thermal fatigue = biaxial fatigue





Stress

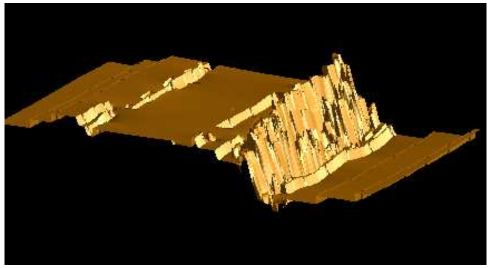
Code DD : mobility, multiplication, interactions, X-slip

Dislocation Microstructure

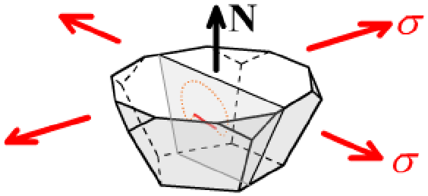
Plastic Deformation

Post-Traitement

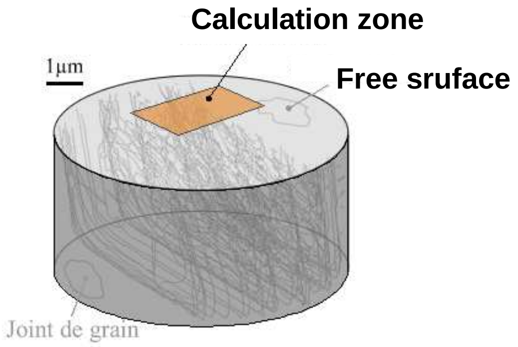
Surf. Displ.

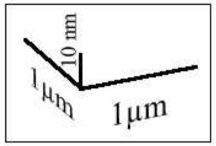


$$\sigma = \begin{pmatrix} \sigma & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & 0 \end{pmatrix}_{\{\bullet,\bullet,\,\mathbf{N}\}}$$



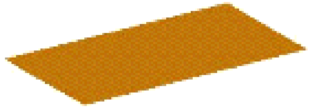
Evolution of surface slip markings

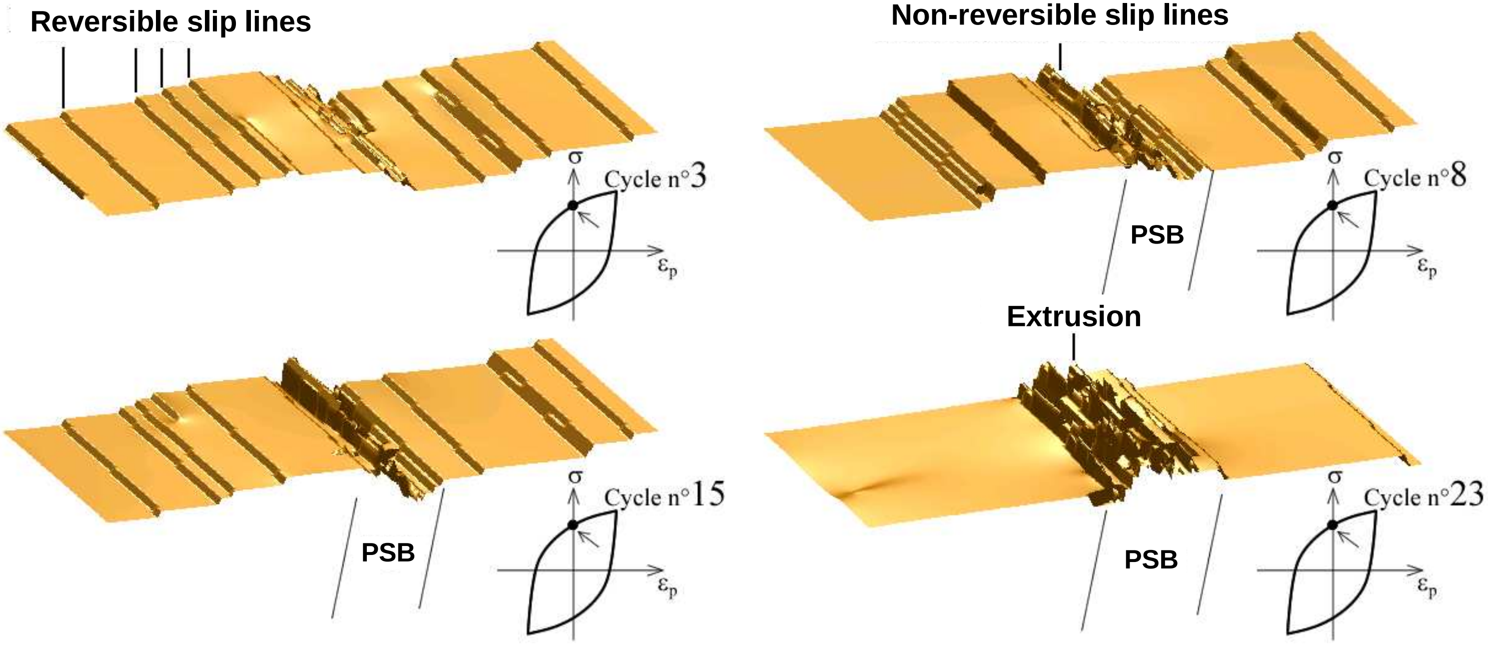


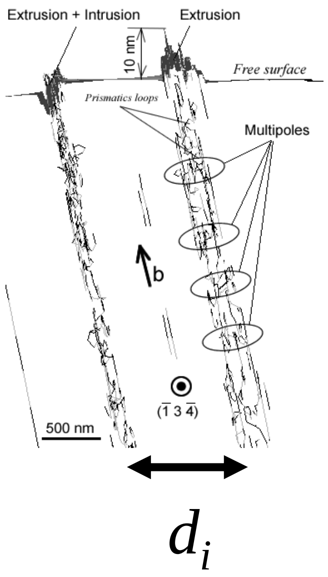


Single slip

$\Delta\varepsilon_p = 10^{-3}$

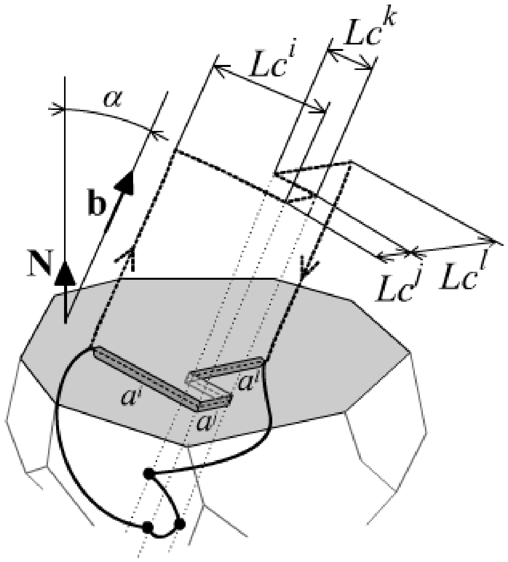






Calculation of cumulated irreversible slip

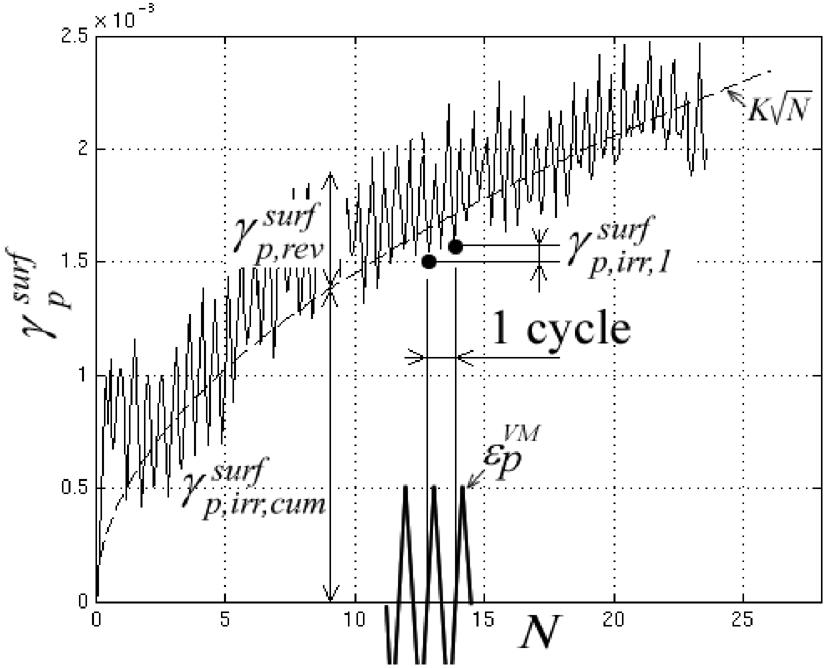
General description



$$a_{cum} = \sum_{n_{coin}} \frac{L_c^i}{\cos\alpha}$$

$$\gamma_p^{surf} = \frac{a_{cum}.b.\cos\alpha}{S}$$

Evolution of surface slip



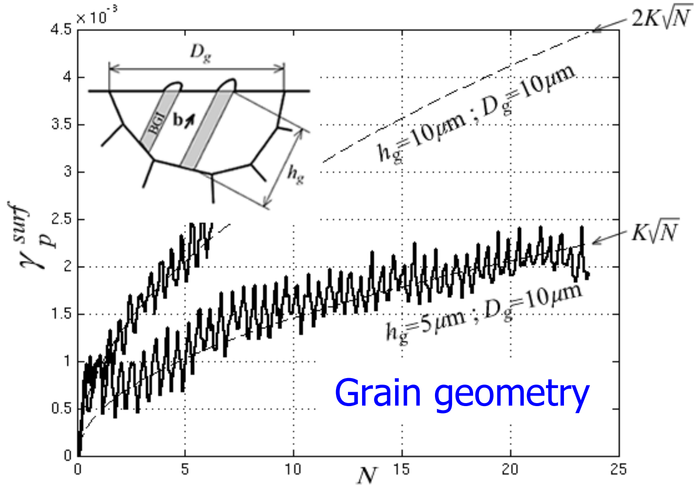
$$\gamma_p^{surf}(t) = \gamma_{p,rev}^{surf}(t) + \gamma_{p,irr,cum}^{surf}(t)$$

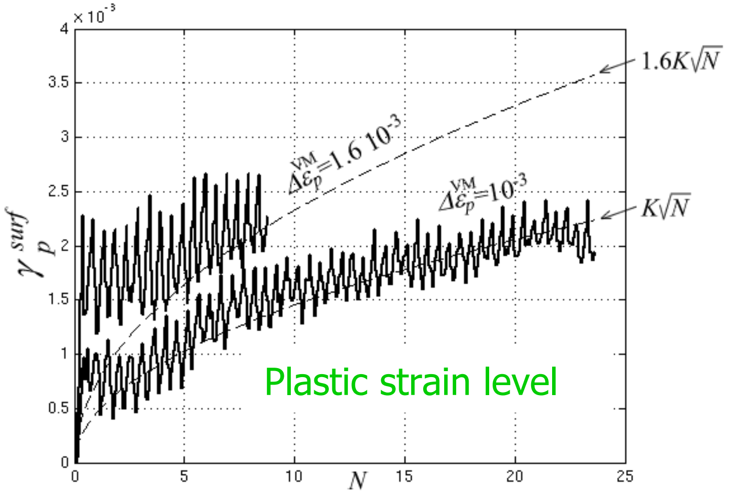
$$\boxed{\gamma_{p,irr,cum}^{surf}(N) = K\sqrt{N}}$$

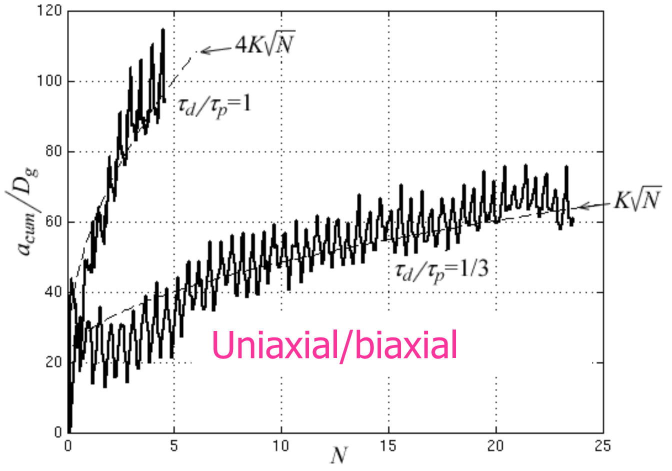
Square root of N : random-walk process

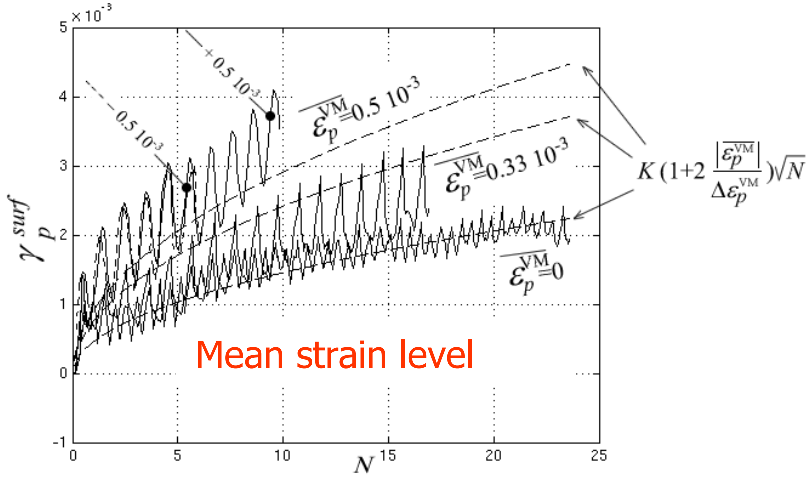
Prefactor K…

Construction of a general expression : extrusion growth





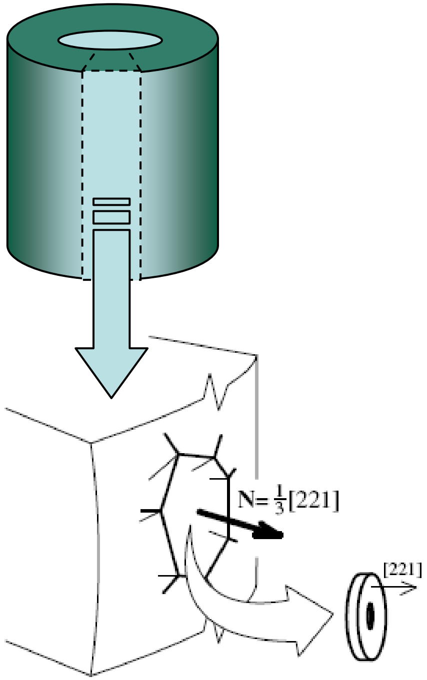


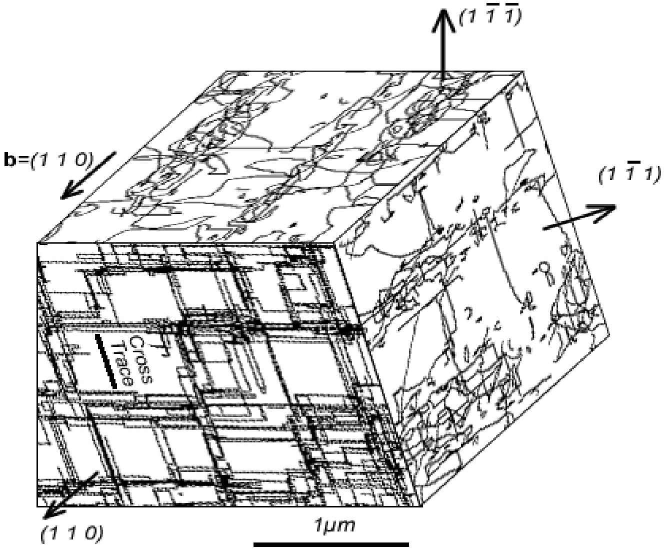


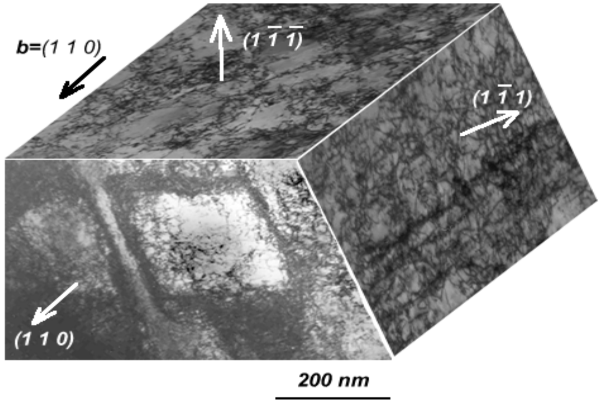
$$\gamma^{surf}_{p,irr,cum}(N) = K\overbrace{\frac{h_g}{D_g}}\overbrace{\Delta\epsilon_p^{VM}}\overbrace{f\left(\frac{\tau_{dev}}{\tau_{prim}}\right)}\overbrace{\left(1+2\frac{|\overline{\epsilon_p^{VM}}|}{\Delta\epsilon_p^{VM}}\right)}\sqrt{N}$$

Biaxial loading conditions: dislocation structures

BIAX specimen







4 times as many PSB as in single slip

If early propagation is due to coalescence, then probability ↑

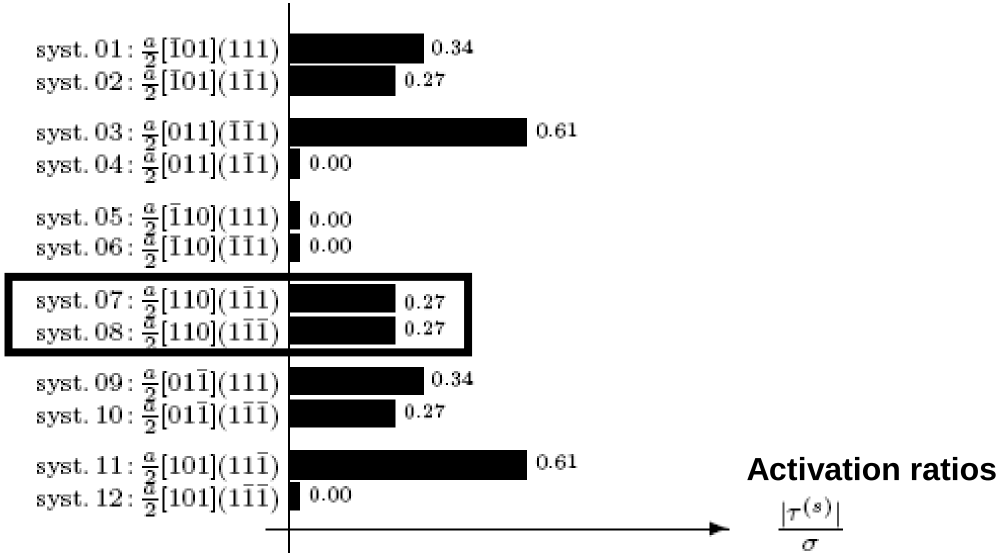
Other effect of biaxial loading: active slip system selection

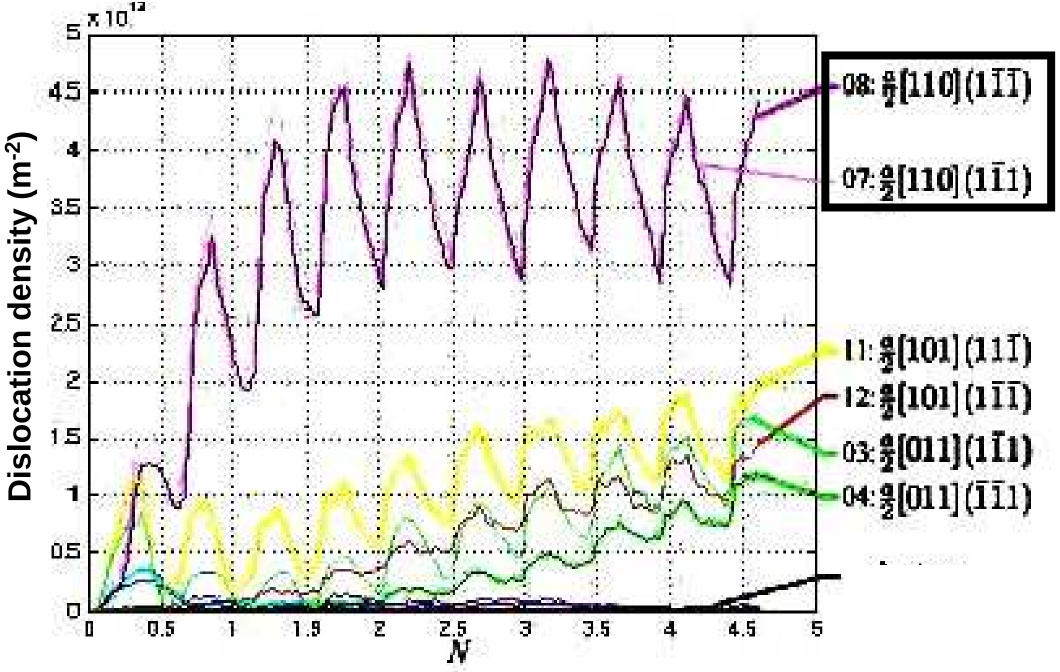
Development of dislocation densities: biaxial slip

$$\sigma \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{\{\bullet,\bullet,\mathrm{N}\}}$$

$$\downarrow$$

$$\sigma \begin{pmatrix} \frac{7}{12} & -\frac{5}{12} & -\frac{1}{3} \\ -\frac{5}{12} & \frac{7}{12} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{4}{3} \end{pmatrix}_{\{\mathrm{R_{cristallo}}\}} \longrightarrow$$

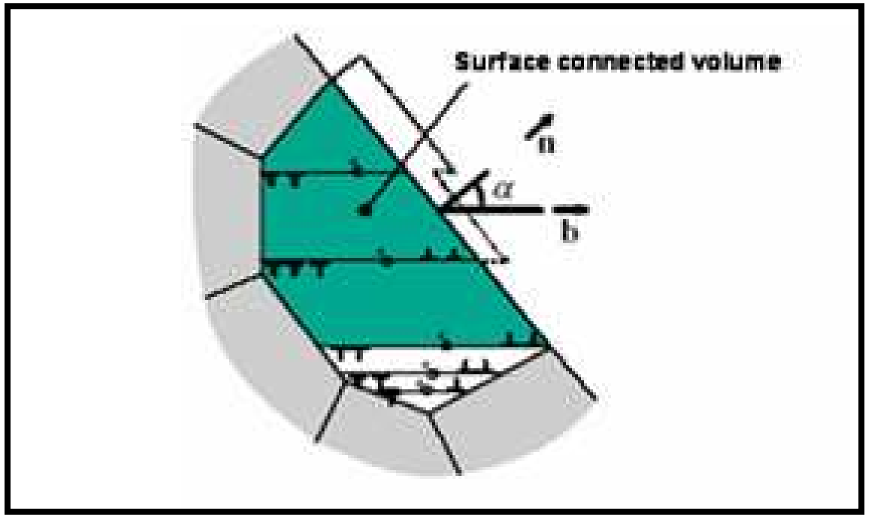




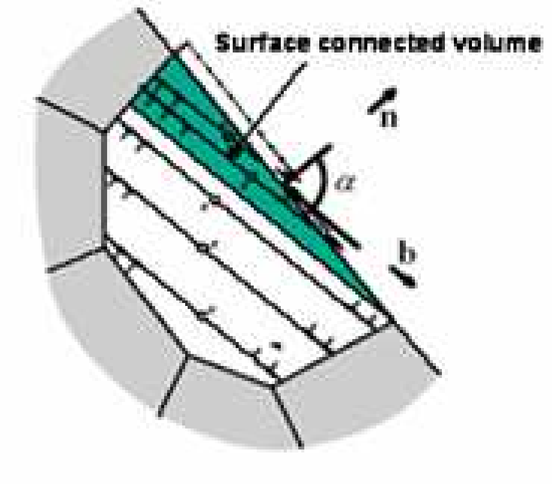
Development of dislocation densities: biaxial loading conditions

Specificity of slip systems 07, 08, 04, 12 ???

☞ Dot product (n.b) $\propto$ effective grain size



Active slip systems 07, 08, 04, 12 have largest (n.b) & effective grain sizes

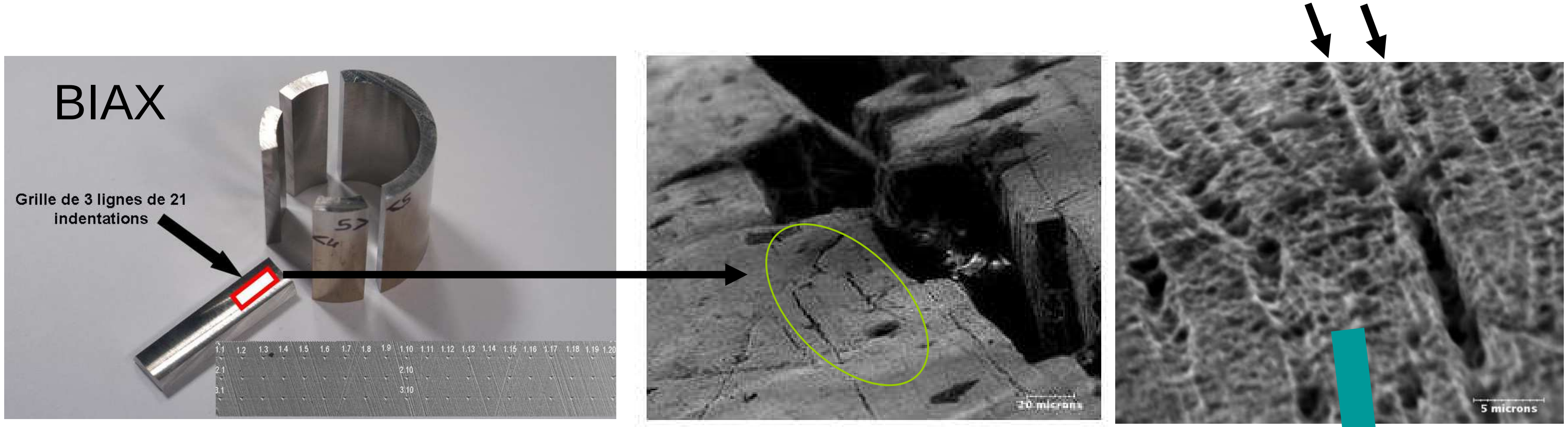


Other slip systems

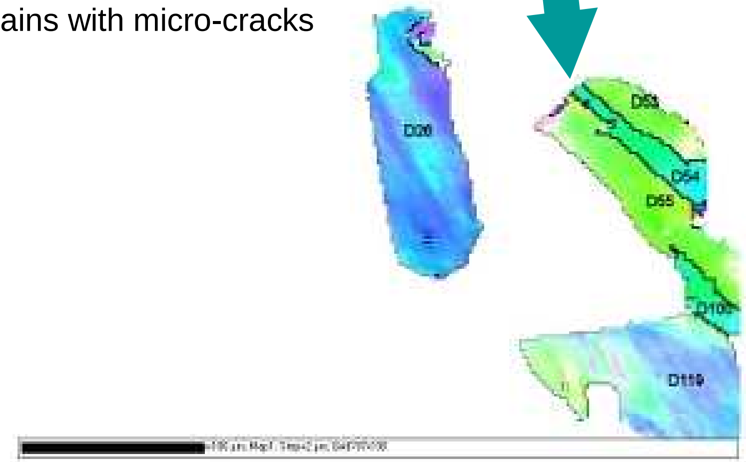
In biaxial loading conditions RSS is not the only cause for selective slip activity : sufficient effective D_g also needed to accomodate the slip & to form PSB structures (>dipoles)

Experimental evidence? Look for orientations of cracked grains!

Experimental evidence of active slip system selection effect



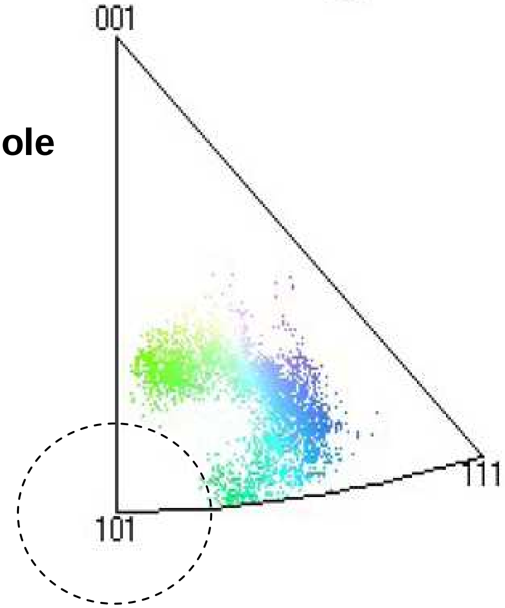
Grains with micro-cracks



Color code: orientation of n, normal to the grain surface

Each pixel = 1 orientation measurement

Reverse pole figure



n ∠ b [110] : 10-20°

Dot product (n.b) in cracked grains is maximal → DD prediction

Summary

2 effects of biaxial loading conditions (thermal fatigue) not predicted by continuum theory

i- there four times as many PSBs per grain as in uniaxial fatigue

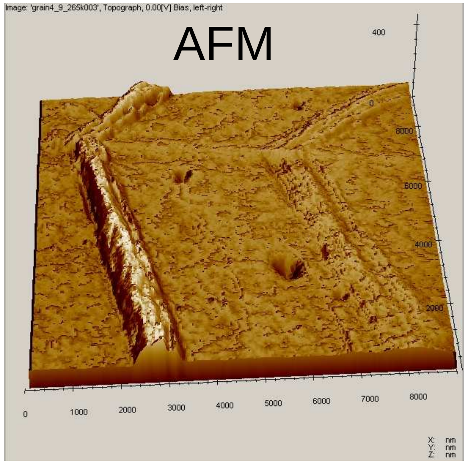
… PSB means micro-crack, linking is then 4 times more probable as in uniaxial fatigue

ii- active slip system selection depends on effective grain size thus, are present in grains with specific grain orientations (n close to b)

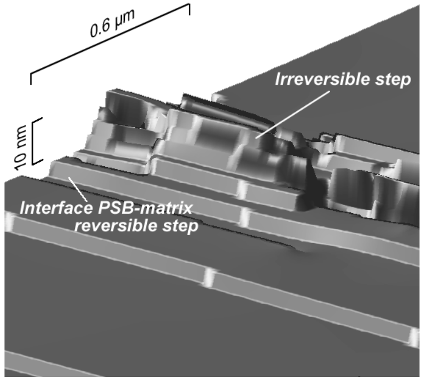
Max RSS is not the only cause for selective slip activity in biaxial loading conditions:
sufficient effective grain size also needed to accomodate the imposed slip

Scale change: from single grains to poly-crystals

$$\gamma^{surf}_{p,irr,cum}(N) = K\,\overbrace{\frac{h_g}{D_g}}\,\overbrace{\Delta\epsilon_p^{\mathrm{VM}}}\,\overbrace{f\left(\frac{\tau_{dev}}{\tau_{prim}}\right)}\,\overbrace{\left(1+2\frac{|\overline{\epsilon_p^{\mathrm{VM}}}|}{\Delta\epsilon_p^{\mathrm{VM}}}\right)}\,\sqrt{N}$$


AFM

DD simulation



Initiation → critical extrusion size $\gamma^{surf}_{p,irr,cum} = \gamma_{\lim}$

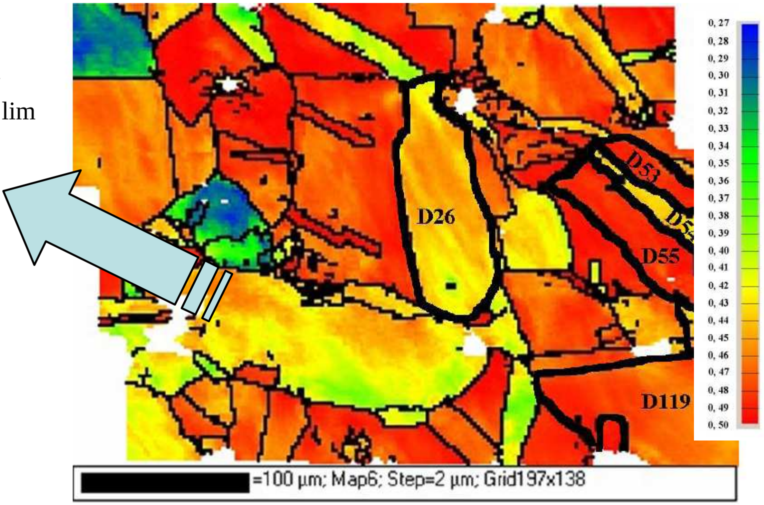
$$\gamma_{\lim} = \sqrt{2}\,\frac{h_b}{d_b} \approx 0.7$$

Symmetrical tension-compression

Single extrusions

$$\sqrt{N_i} = \frac{D_g}{h_g}\,\frac{1}{\sqrt{K}\,\boxed{\Delta\varepsilon_{p,eq}}}\,\gamma_{\lim}$$

$\Delta\varepsilon_p$ in grains: alternate method to grain-by-grain measurement ?



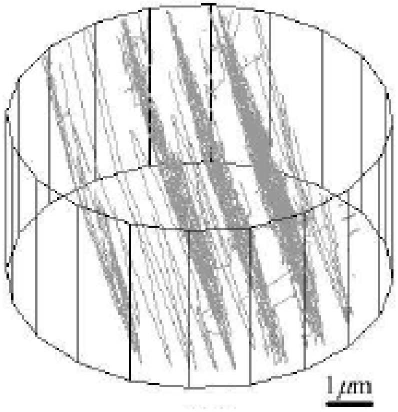
Grain stress-strain: orientation-dependent **(EBSD)**

Realistic?

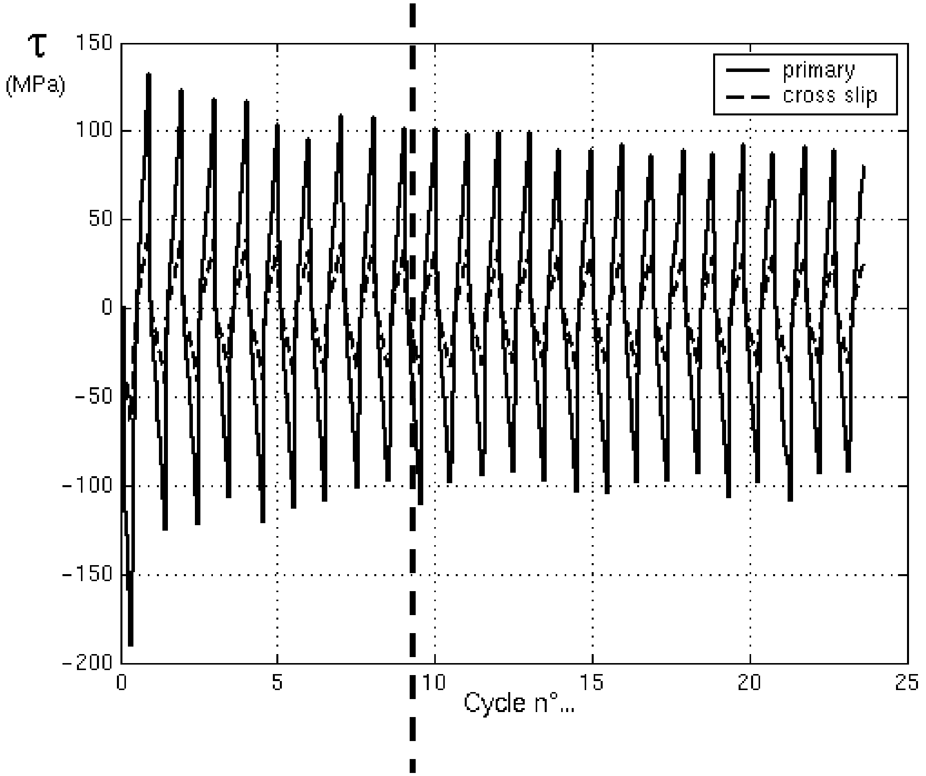
DD calculations yield $K \sim 0.5$ hence,

$N_i \sim 2.5\times10^5$ cycles with $D_g/h_g = 1$ and $\Delta\varepsilon_{p,eq} = 2\times10^{-3}$

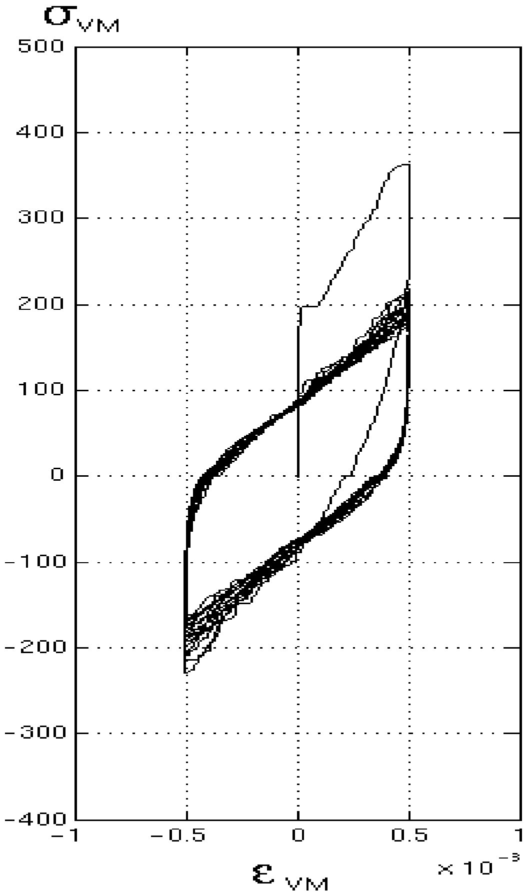
Cyclic stress-strain behaviour at grain scale



$\Delta\varepsilon_p$: standard DD simulation predictions…

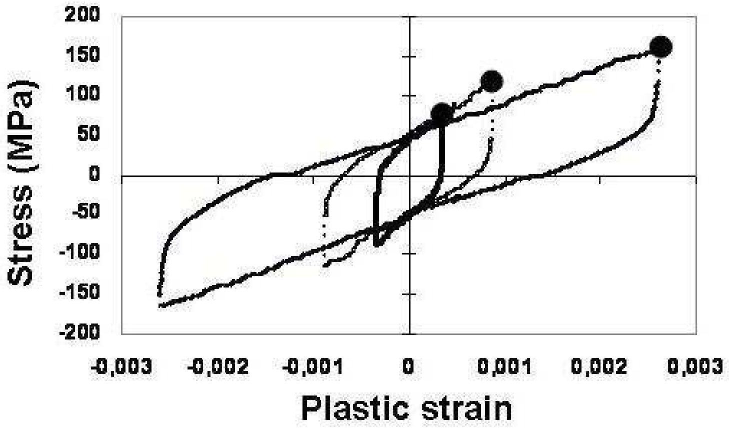


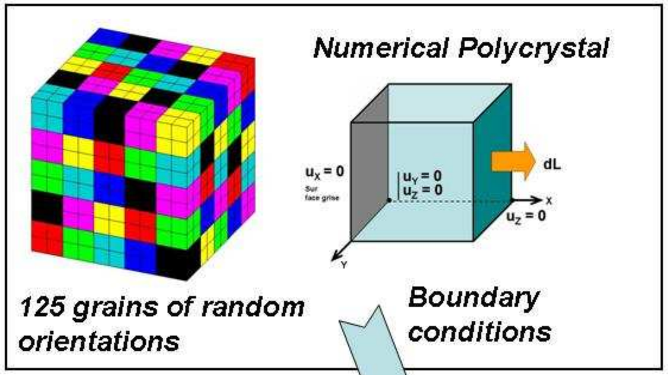
$N_{sat} \approx 10$

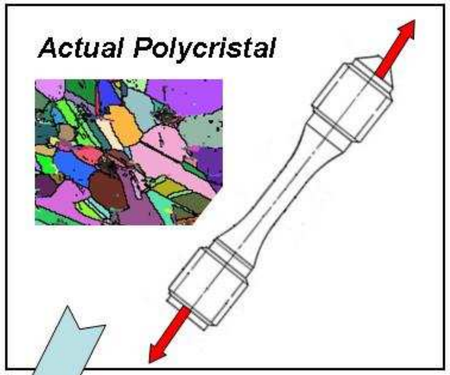


Cyclic stress-strain behaviour: from single grain to polycrystal

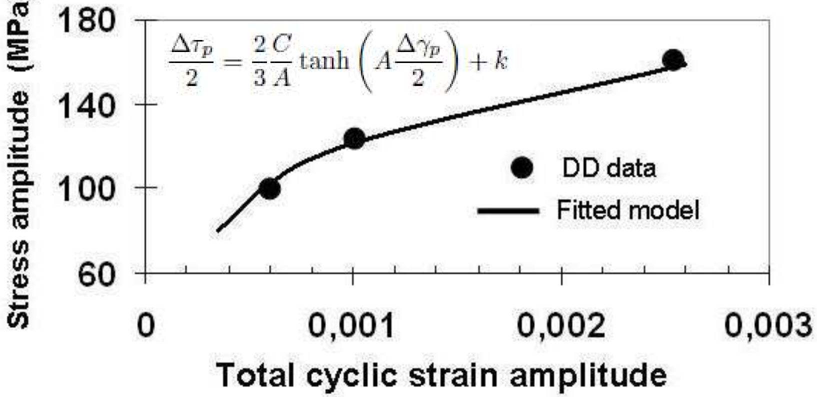
DD data



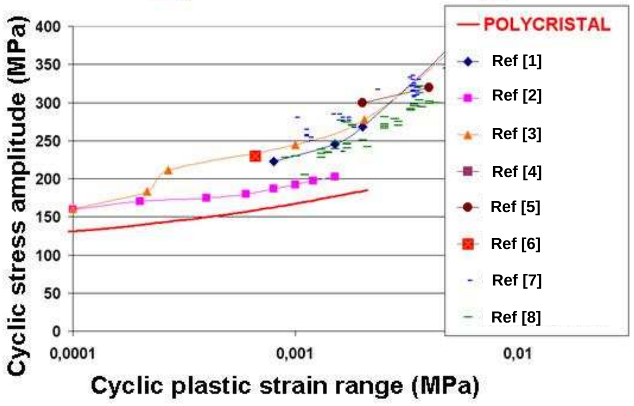




Fit FEM (linear kinematics) model to DD data



$$\frac{\Delta\tau_p}{2} = \frac{2}{3}\frac{C}{A}\tanh\left(A\frac{\Delta\gamma_p}{2}\right) + k$$



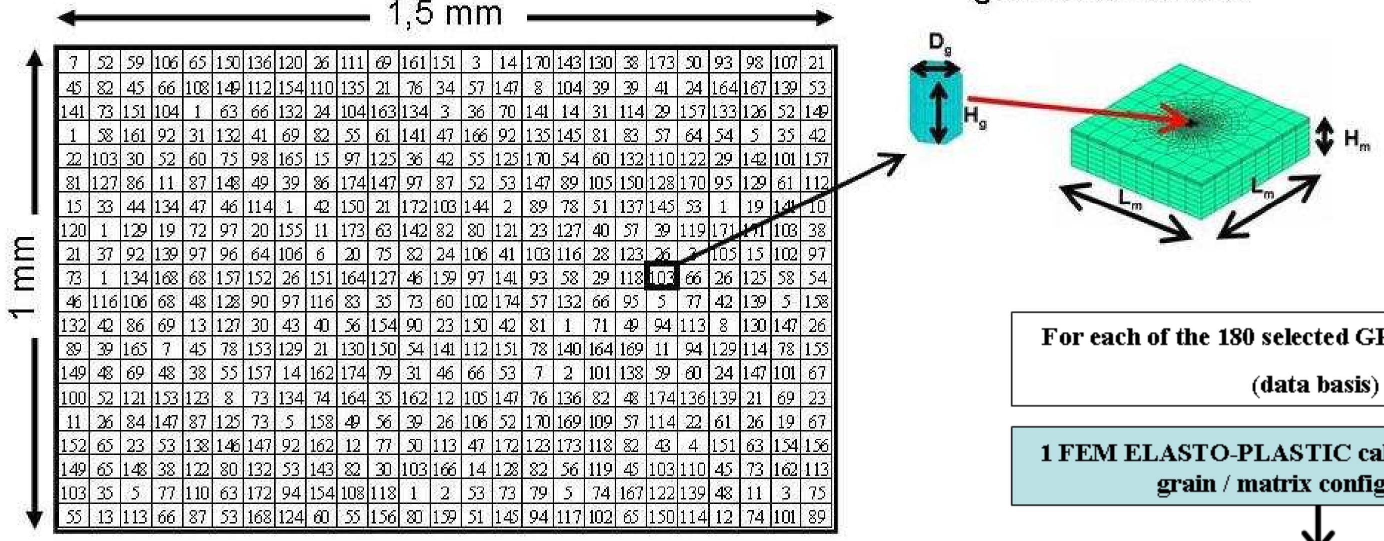
$$dX = \frac{2}{3}C \cdot \gamma_p - AX\,dp$$

C : isotropic hardening X : kinematic hardening k : tensile yield stress

Grain behaviour from DD → stress-strain behaviour of poly-crystals

Polycrystal made of 500 grains

Data basis: 180 different grain orientations



7	52	59	106	65	150	136	120	26	111	69	161	151	3	14	170	143	130	38	173	50	93	98	107	21
45	82	45	66	108	149	112	154	110	135	21	76	34	57	147	8	104	39	39	41	24	164	167	139	53
141	73	151	104	1	63	66	132	24	104	163	134	3	36	70	141	14	31	114	29	157	133	126	52	149
1	58	161	92	31	132	41	69	82	55	61	141	47	166	92	135	145	81	83	57	64	54	5	35	42
22	103	30	52	60	75	98	165	15	97	125	36	42	55	125	170	54	60	132	110	122	29	142	101	157
81	127	86	11	87	148	49	39	86	174	147	97	87	52	53	147	89	105	150	128	170	95	129	61	112
15	33	44	134	47	46	114	1	42	150	21	172	103	144	2	89	78	51	137	145	53	1	19	141	10
120	1	129	19	72	97	20	155	11	173	63	142	82	80	121	23	127	40	57	39	119	171	171	103	38
21	37	92	139	97	96	64	106	6	20	75	82	24	106	41	103	116	28	123	26	2	105	15	102	97
73	1	134	168	68	157	152	26	151	164	127	46	159	97	141	93	58	29	118	103	66	26	125	58	54
46	116	106	68	48	128	90	97	116	83	35	73	60	102	174	57	132	66	95	5	77	42	139	5	158
132	42	86	69	13	127	30	43	40	56	154	90	23	150	42	81	1	71	49	94	113	8	130	147	26
89	39	165	7	45	78	153	129	21	130	150	54	141	112	151	78	140	164	169	11	94	129	114	78	155
149	48	69	48	38	55	157	14	162	174	79	31	46	66	53	7	2	101	138	59	60	24	147	101	67
100	52	121	153	123	8	73	134	74	164	35	162	12	105	147	76	136	82	48	174	136	139	21	69	23
11	26	84	147	87	125	73	5	158	49	56	39	26	106	52	170	169	109	57	114	22	61	26	19	67
152	65	23	53	138	146	147	92	162	12	77	50	113	47	172	123	173	118	82	43	4	151	63	154	156
149	65	148	38	122	80	132	53	143	82	30	103	166	14	128	82	56	119	45	103	110	45	73	162	113
103	35	5	77	110	63	172	94	154	108	118	1	2	53	73	79	5	74	167	122	139	48	11	3	75
55	13	113	66	87	53	168	124	60	55	156	80	159	51	145	94	117	102	65	150	114	12	74	101	89

For each of the 180 selected GRAIN orientations (data basis)

1 FEM ELASTO-PLASTIC calculation using the grain / matrix configuration

Calculation of the mechanical stress-strain state at each Gauss point, for a fixed macroscopic loading level. Calculation of the mean grain stress and strain levels

Calculation of the (grain-averaged) resolved shear stresses on each of the 12 slip systems

Calculation of the $\tau_i / \tau_{cross,\,i}$ ratios in each slip system

Identification of the slip system pair having the smallest $\tau_i / \tau_{cross,\,i}$ ratio (≥ 1)

Identification of the primary and cross-slip systems and calculation of the number of cycles to crack initiation

Fix N

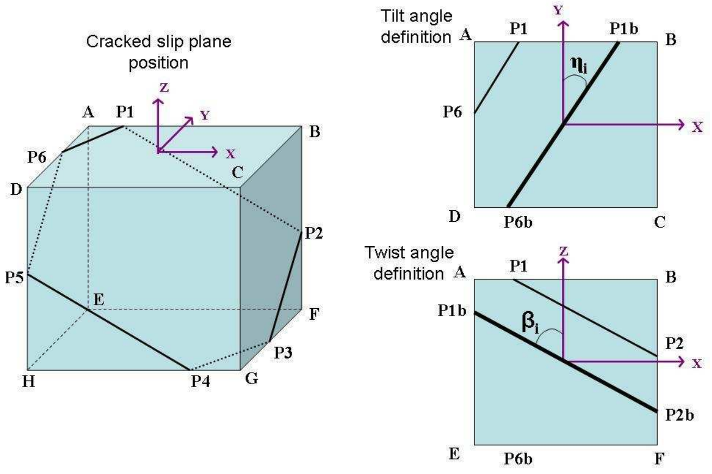
Check, in each grain, N > N_i

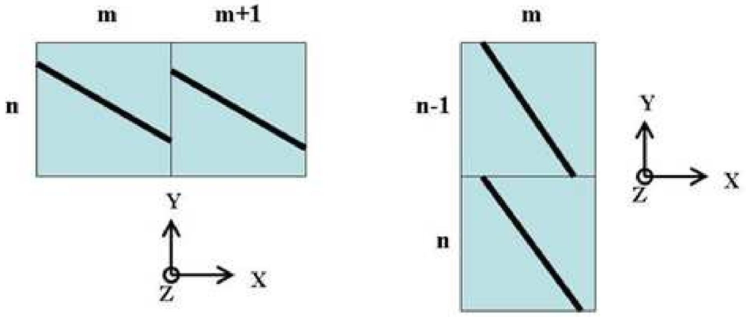
$$\sqrt{N_i} = \frac{D_g}{h_g}\frac{1}{\sqrt{K}\,\Delta\varepsilon_{p,eq}}\gamma_{lim}$$

N = N + ΔN

EBSD data: micro-crack habit planes maximizes (N.b) ∝ effective D_g

Fatigue damage: from grain to polycrystal

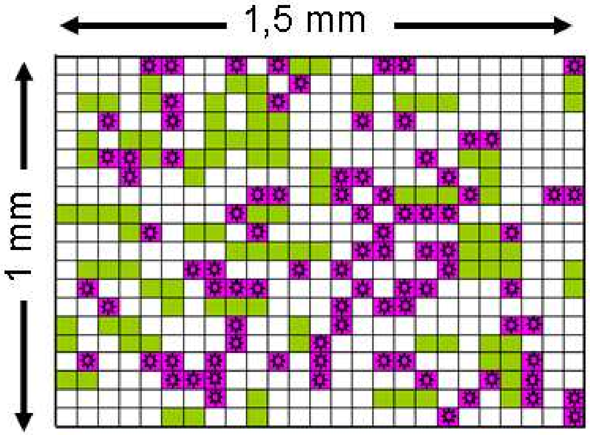




Crack coalescence: 2 possible directions

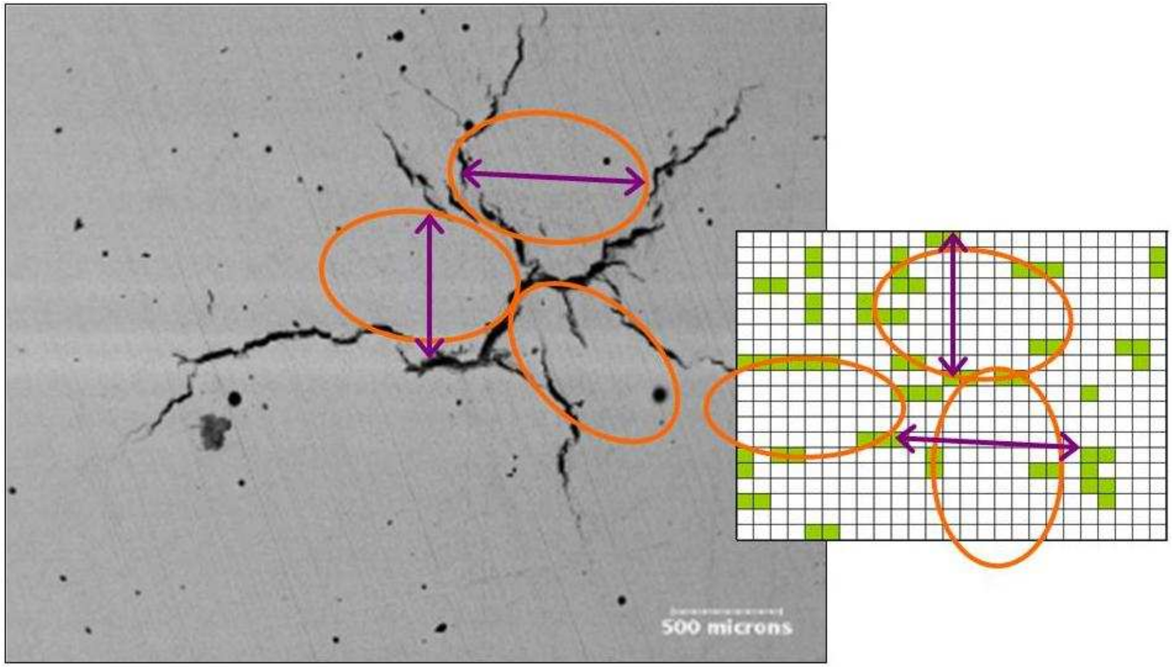
$N = 10\times10^{6}$ cycles

$\Delta\varepsilon^{VM} = 2{,}5\times10^{-3}$



☼ Grains where crack coalescence is not possible

🟩 Grains where crack coalescence is possible



Slip plane	Primary plane	Secondary plane	Total
(111)	43	49	92
(-111)	44	50	94
(1-11)	42	37	89
(-1-11)	51	44	95
Total	180	180	360

Intersection	Primary plane	Secondary plane	Total
GB || X	88	96	184
GB || Y	92	84	176
Total	180	180	360

Conclusions

DD predictions

- Slip (alone) is capable to generate extrusions
- If R = -1, average extrusion growth rate $\propto N^{1/2}$
- Slip is a sizable fraction of early extrusion growth (50%+), at low $\Delta\varepsilon_p$
- Probability of micro-crack initiation is higher, in thermal fatigue
- Stress-strain behaviour at the grain scale
- Scale change from single to poly-crystals

THE END