FROM MODELLING OF PLASTICITY IN SX SUPERALLOYS TO HIGH RESOLUTION X-RAYS TCD PEAKS SIMULATION

Alain JACQUES

IJL-CNRS/Labex DAMAS

Outline

- A rather long introduction
- A bit of Physics
- Some Mechanics
- A few results
- Add crystal defects
- Some results with plasticity
- Conclusion

HT mechanical behavior of SX superalloys

- γ corridors (fcc):

  a/2.<110> dislocations

  σ_{VM} > Orowan stress

- γ' rafts (Ni_3Al):

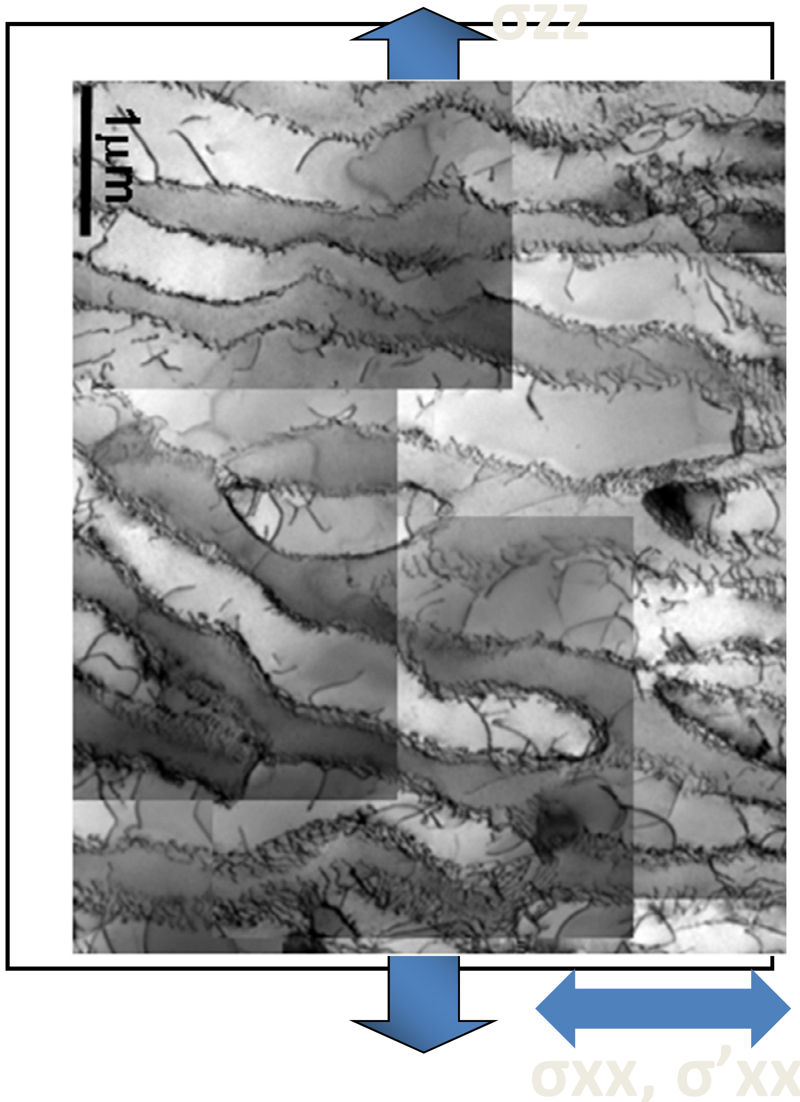
  climb of dislocations

  a'.[001] ($\sigma_{zz} = \sigma_a$) +Vac.

  a'.[100] (σ_{xx})

  -Vac

  a'.[010] (σ_{yy})



Stresses? Strains?

In situ Three Crystal Diffractometry

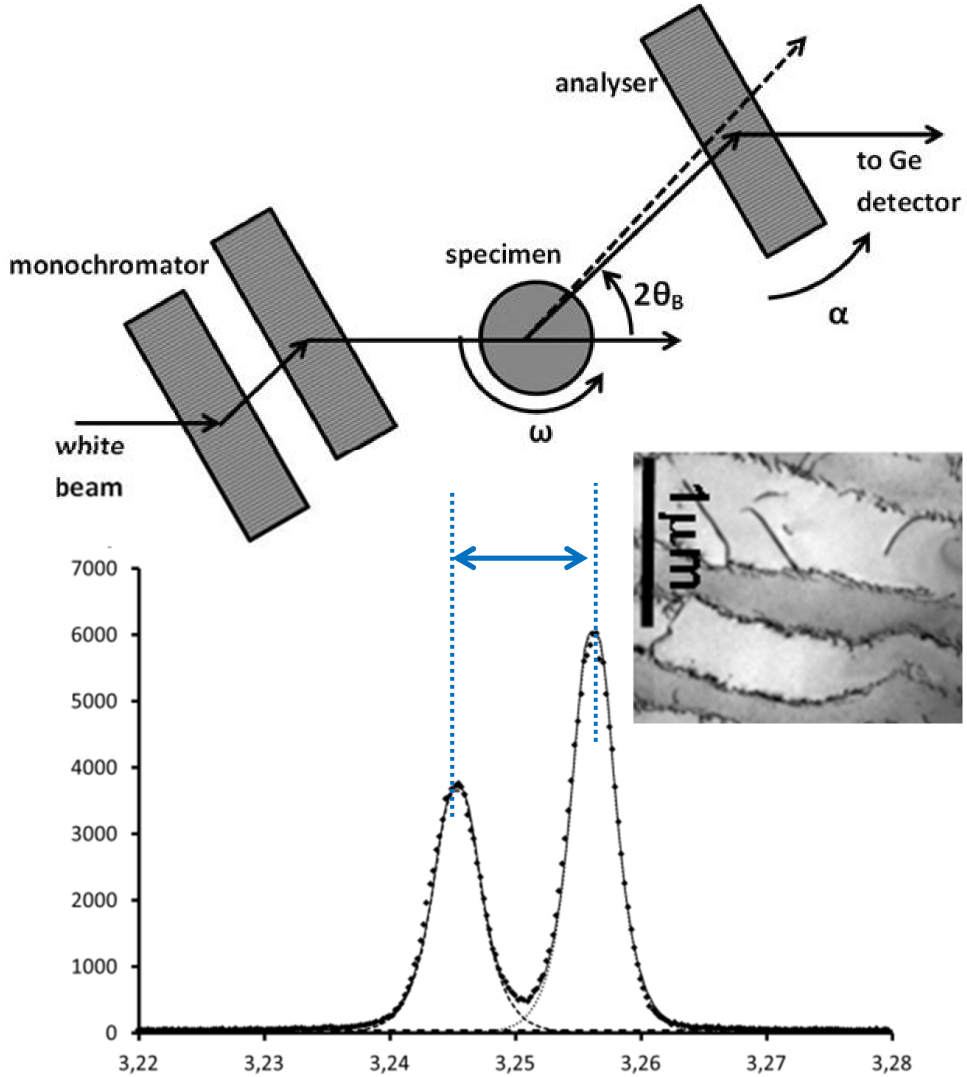
BW5, P07 (DESY) and
ID15 (ESRF)

100 to 150 KeV
(Transmission)

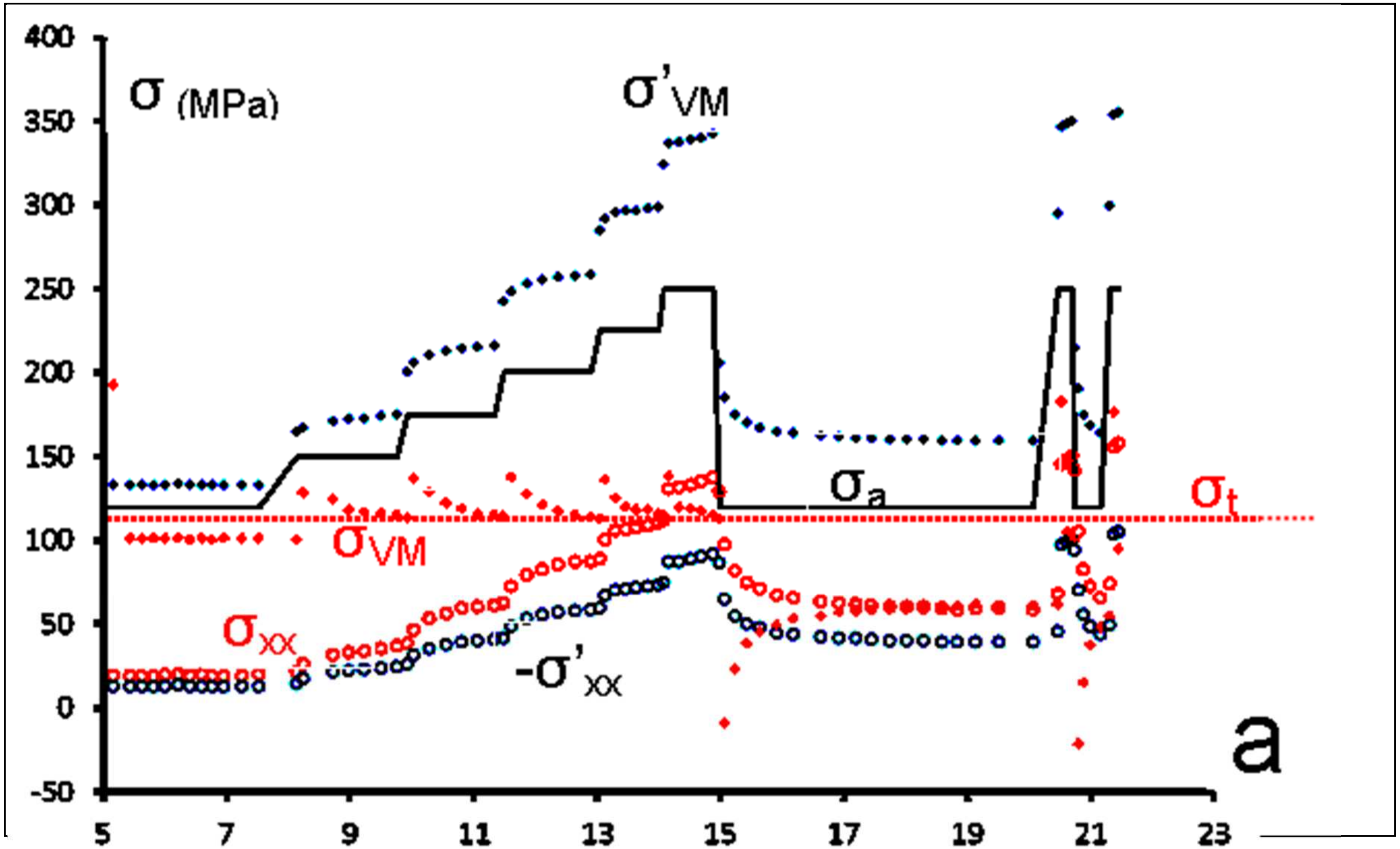
G = (200)

scan: (200 pts): 300 s

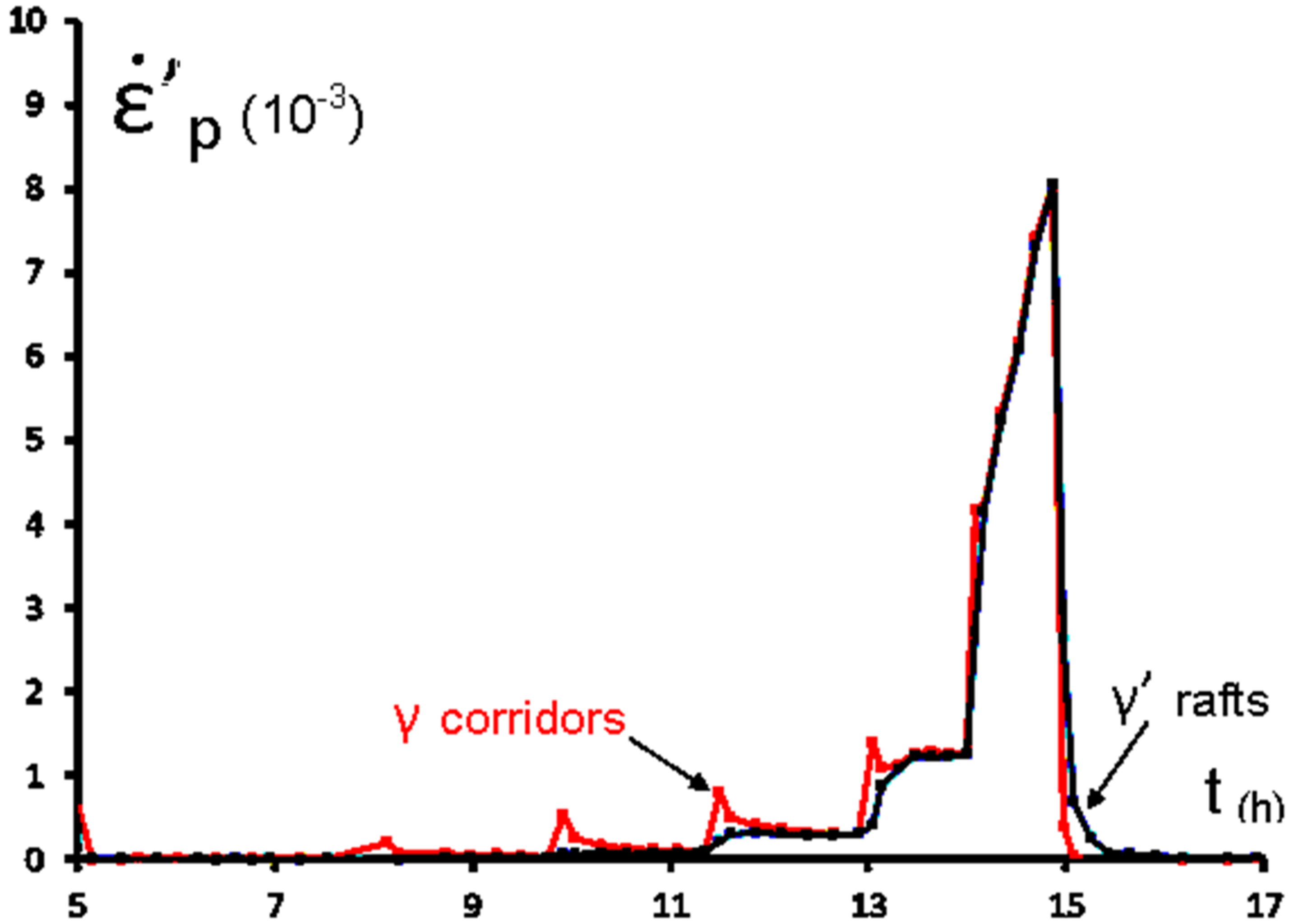
Precision: ± 2 MPa



From peak positions: stresses

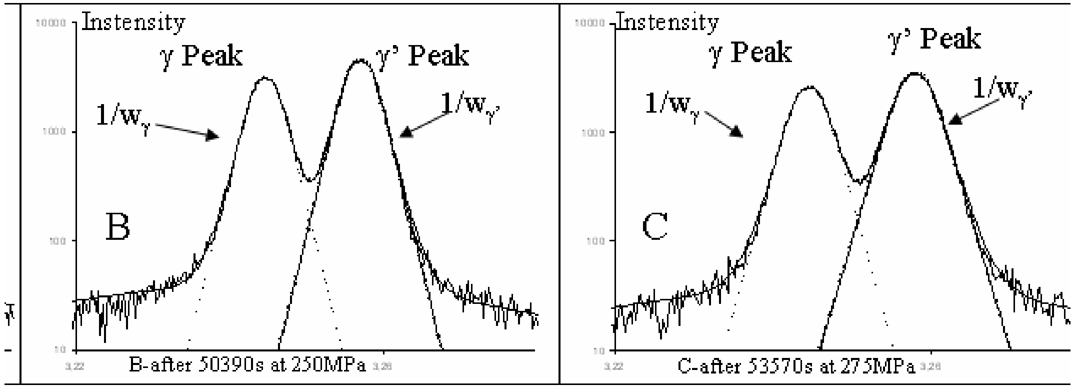


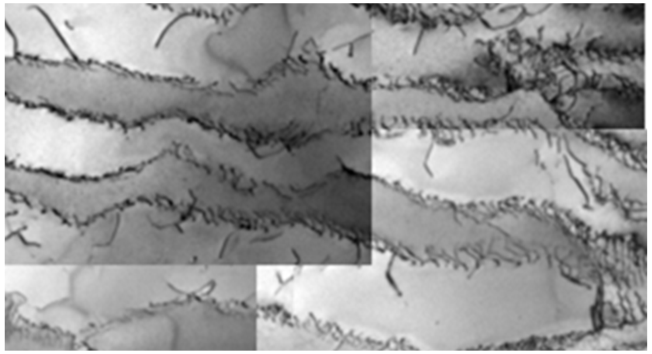
From peak positions: strain rates

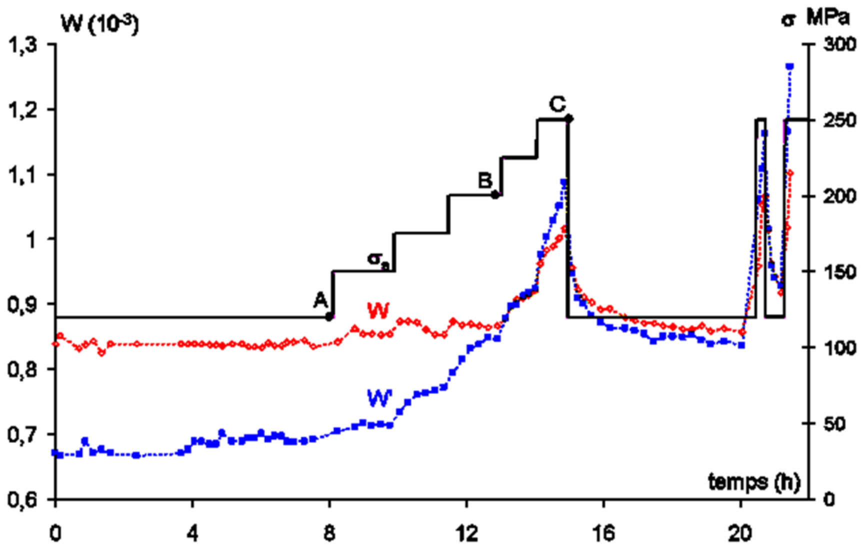


Questions:

- Missing ingredient:
  - How do dislocations densities within the γ’ phase vary with time?





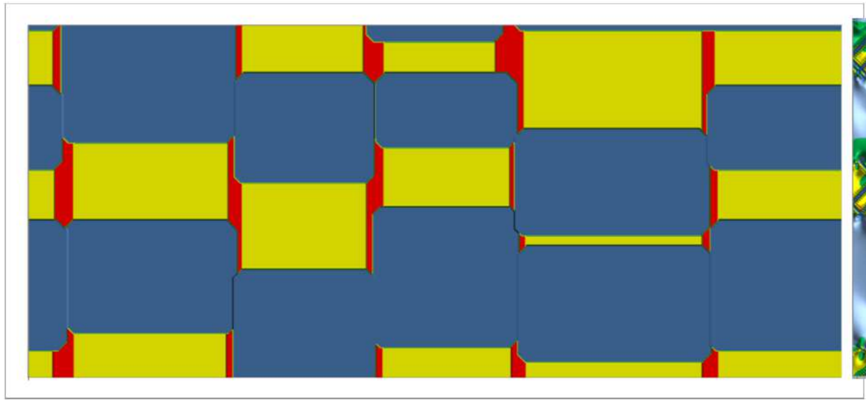
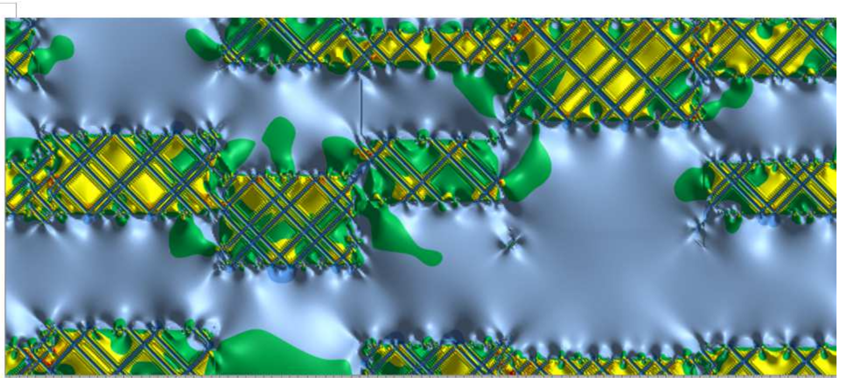


•Relation between a’.[100] and a’.[010] dislocation densities within the γ’ rafts and the peaks shapes?

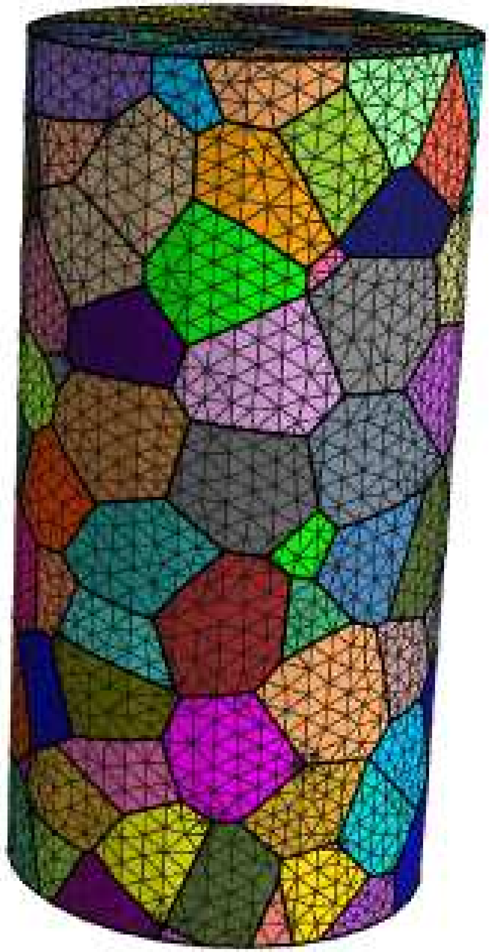
Questions:

- Missing ingredient:
  - How do dislocations densities in γ' vary with time?

- Modelling of plasticity: Experimental tests?

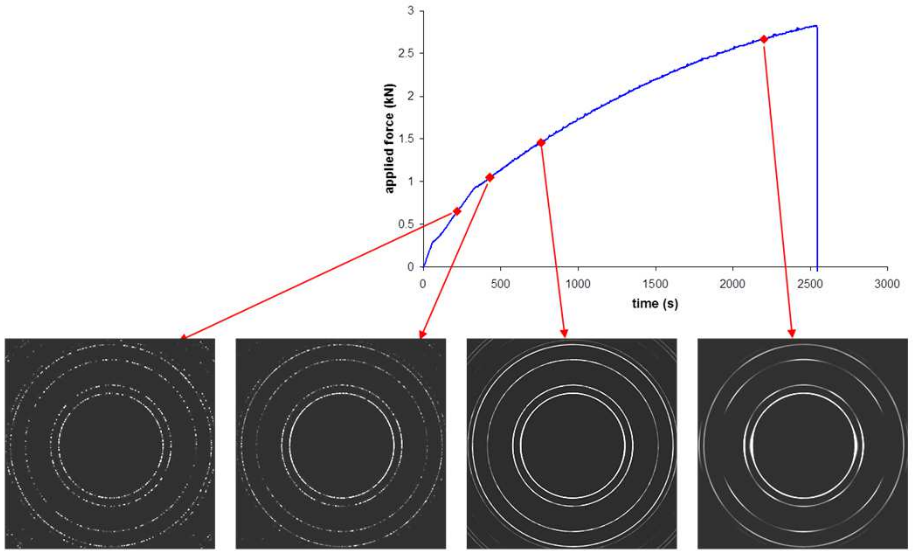



Polycrystals



- Distribution of strains between grains in an elastically strained material?

- During plastic strain: distribution of stresses between grains with different orientations/neighbourhood?



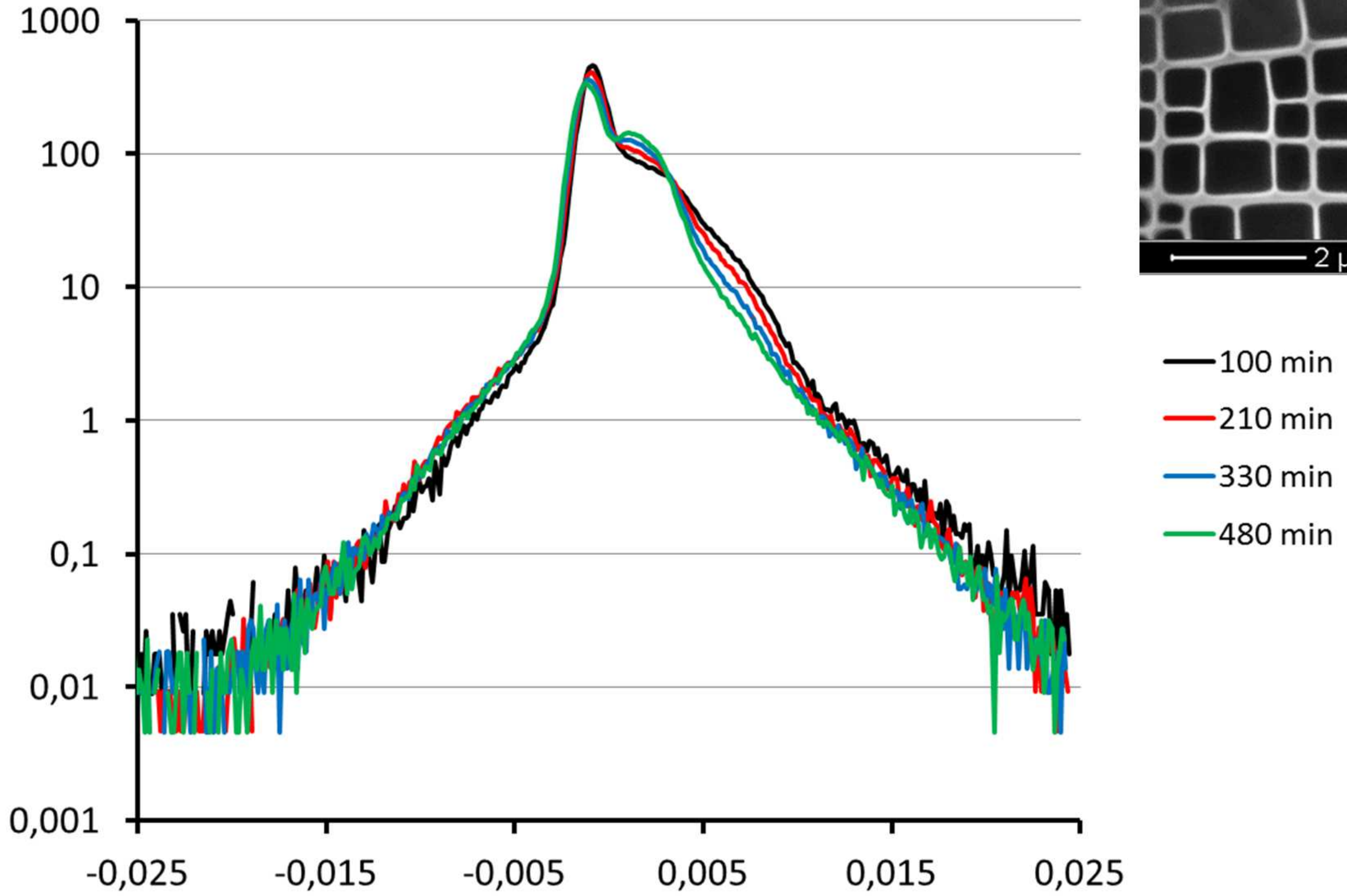
Questions:

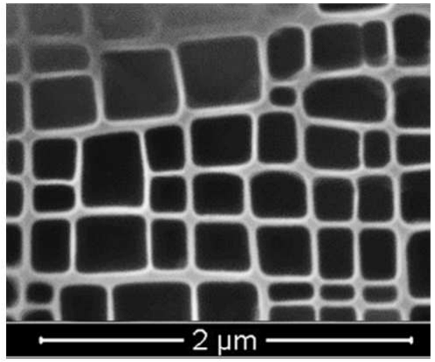
- Missing ingredient:
  - How do dislocations densities vary with time?

- Modelling of plasticity: Experimental tests?

Can we simulate diffraction peaks
To compare with experimental ones?

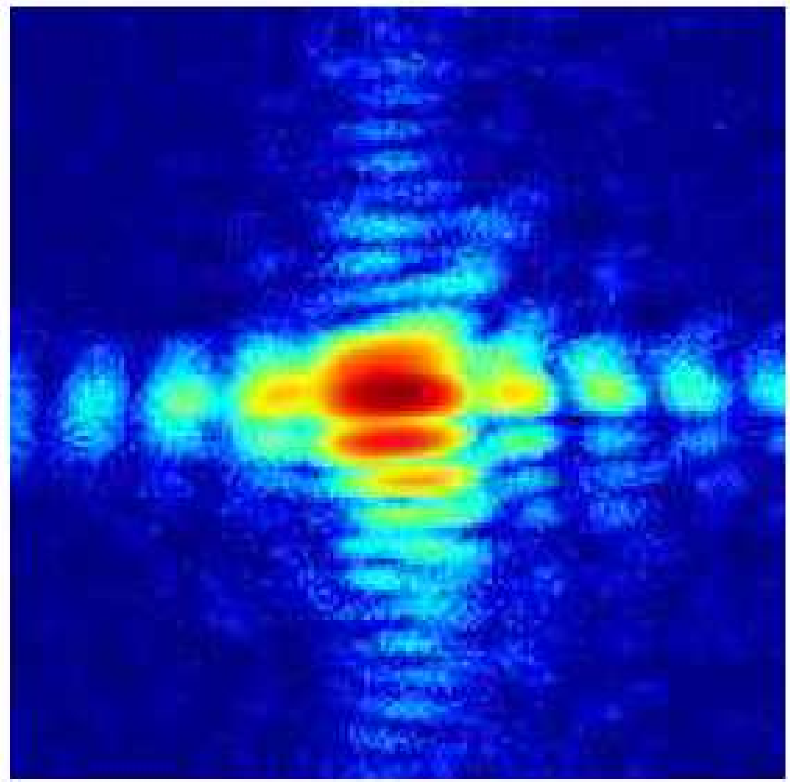
High resolution diffraction peaks





Modelling of diffraction peaks

- Coherent beam
- Small grains
- Strained Crystal lattice



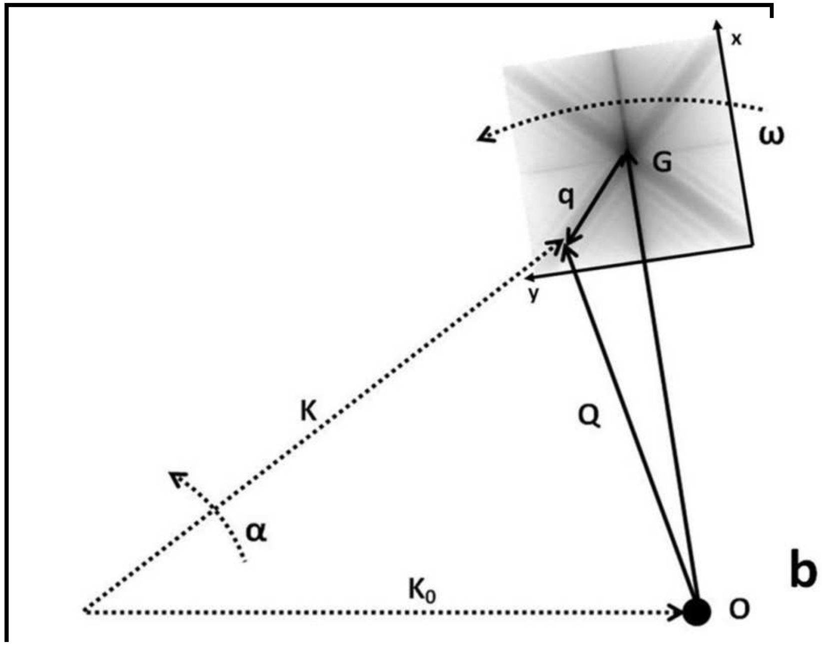
Simulation de la diffraction cohérente d'un film polycristallin

H. Proudhon[a], N. Vaxelaire[b,c], S . Labat[b,c], S. Forest[a], O. Thomas[b,c]

Modelling of diffraction peaks

- **Coherent beam**
- **Small grains**
- **Strained Crystal lattice**

  U(r): Displ. Field



Scattered amplitude:

$$A(K) = \sum_{vol} \boxed{A_0(r).F(\mathbf{G},r).exp(\boxed{-2i\pi.\mathbf{G}.U(r)})}.exp(-2i\pi.\mathbf{q}.r)$$

Fourier transform

•Phase

Recipe

- Generate a microstructure
- Calculate the displacement field
- Get the phase
- Take a Fourier Transform or FFT

  (taking coherence into account)
- Calculate and plot intensities

Recipe

- Generate a microstructure
- Calculate the strain (stress) field
- Calculate the displacement field
- Get the phase
- Take a Fourier Transform or FFT
- Calculate and plot intensities

- Model plasticity
- Put dislocations

Fourier Methods for calculating U(r)

- Periodic microstructure $(2\mu m)^3$
- Periodic Fields (displacement, strain, stress)
- Eigenstrain (plastic strain, coherence strain, defects…)
- Calculation in Real and Reciprocal spaces (Mura)
- Efficient algorithms even for inhomogeneous and anisotropic elasticity (Suquet, Anglin and others)

Fourier Methods for calculating U(r)

B.S. Anglin et al./Comput. Mat. Science 87 (2014) 209–217

Polarization tensor

$$\tau^{i}{}_{ij}(r) = \left(C_{ijkl}(r) - C^{0}{}_{ijkl}\right).\varepsilon^{i}{}_{kl}(r) - C_{ijkl}(r).\varepsilon^{p}{}_{kl}(r)$$

Iteration

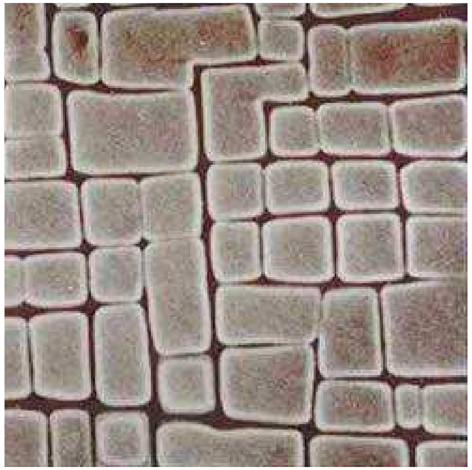
$$\varepsilon^{i+1}{}_{ij}(r) = E^{i}{}_{ij} + TF^{-1}\left[\Gamma^{0}{}_{ijkl}(\boldsymbol{k}).TF\left(\tau^{i}{}_{kl}(r)\right)(\boldsymbol{k})\right]$$

Rewritten for FFT instead of TF

Γ operator in Fourier space

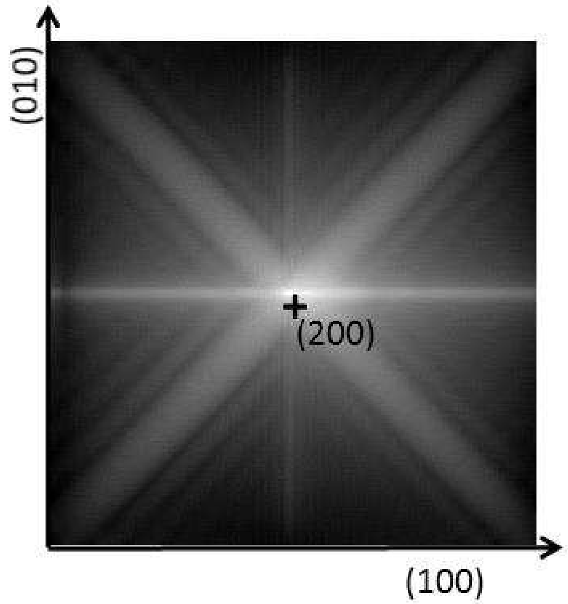
(TF of the Green function)

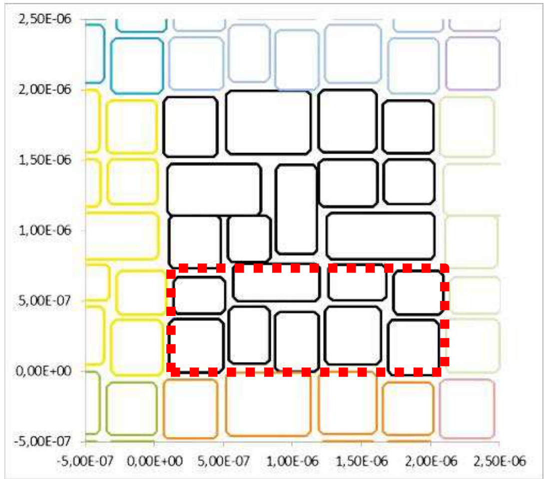
Recipe

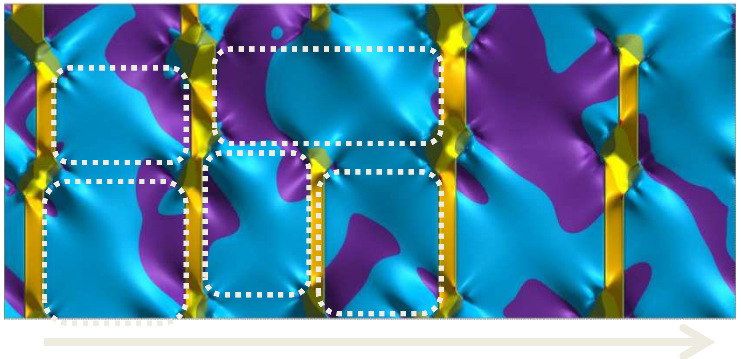


Calculate the stress, strain and displacement fields

(lattice mismatch between phases)

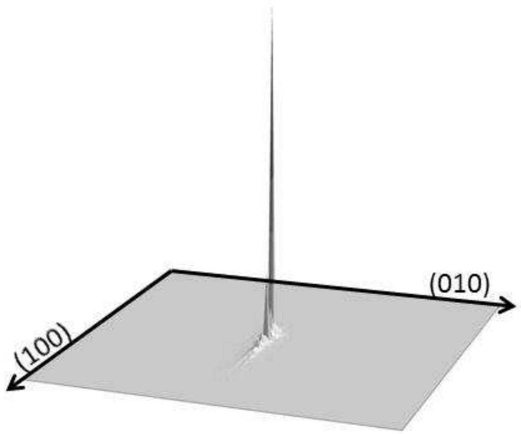






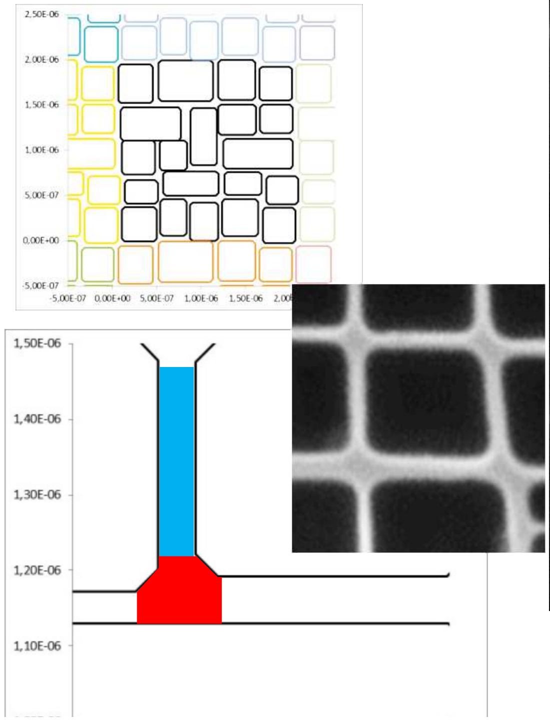
Design a microstructure

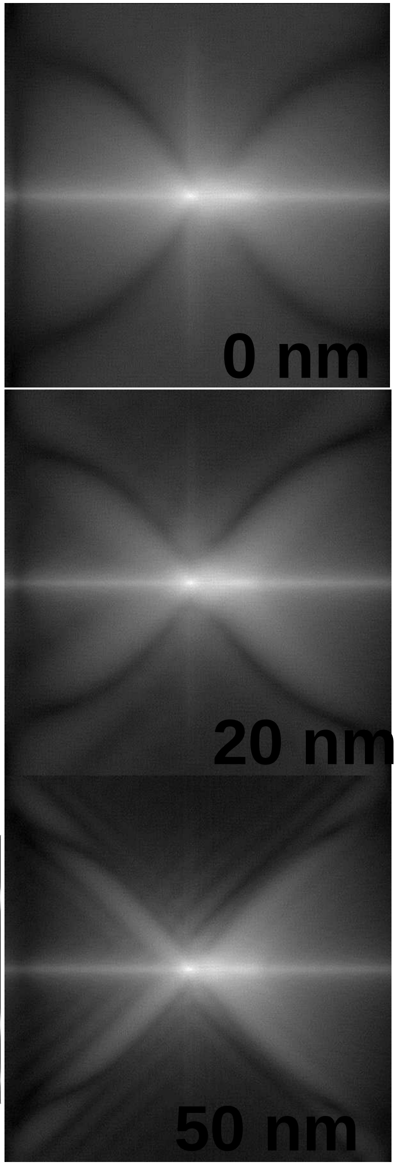
$(2\mu m)^3$, 512^3 voxels

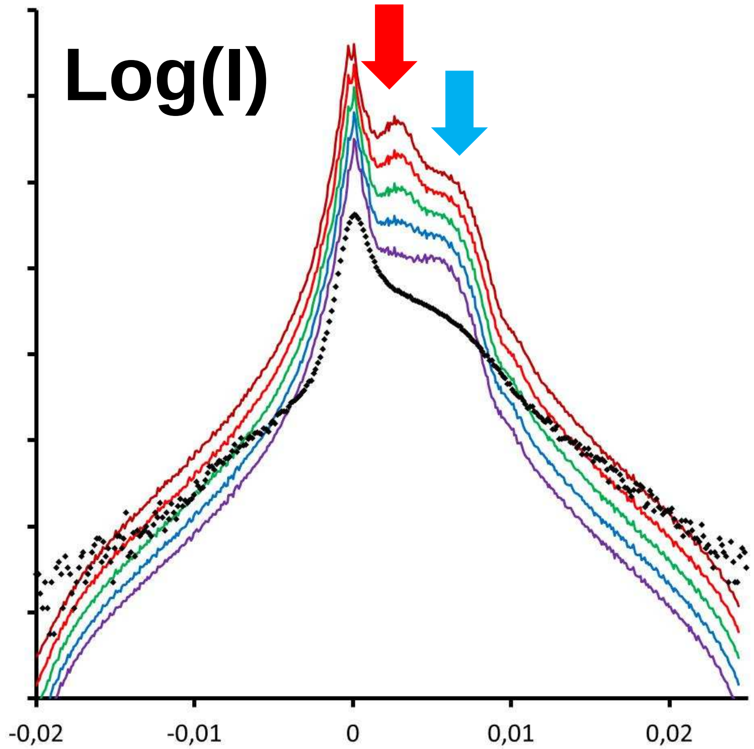


Comparison with Experiment

- T ≈ 1160°C
- f ≈ 50%
- Mismatch ≈ -0,003
- 1 fit parameter



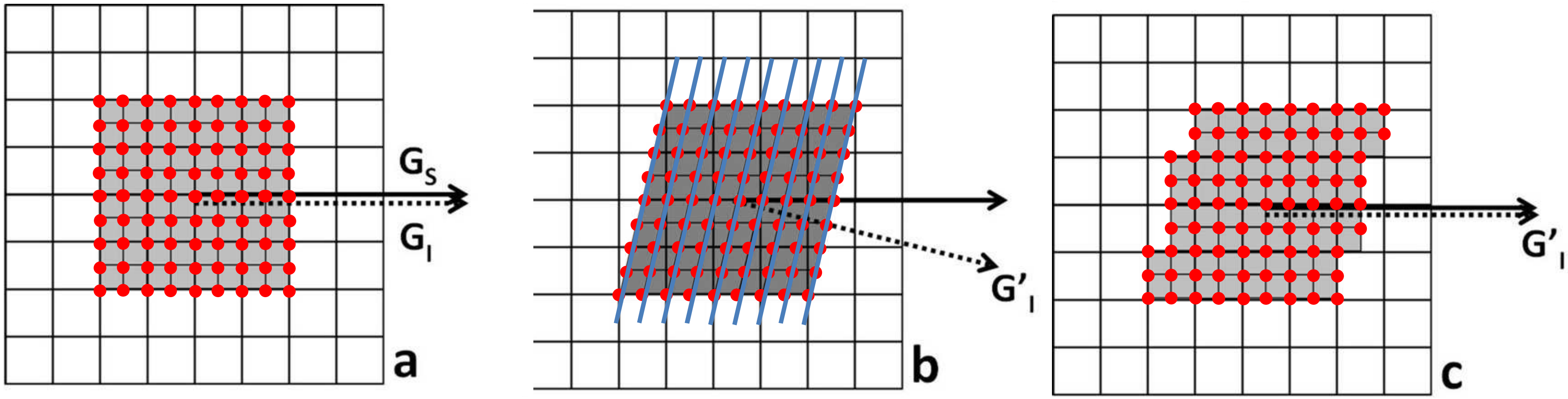




- Statistics of corridor widths
- Chemical inhomogeneity
- Dendritic solidification

Diffraction and plasticity:

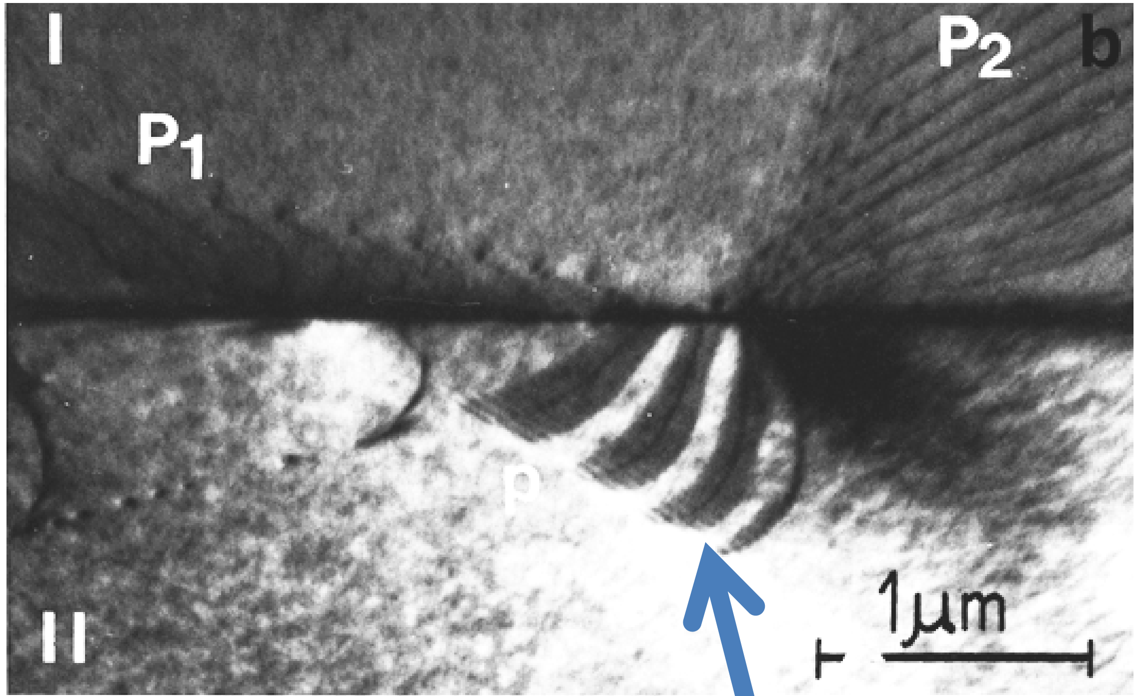
continuous vs. discontinuous



continuous stepwise

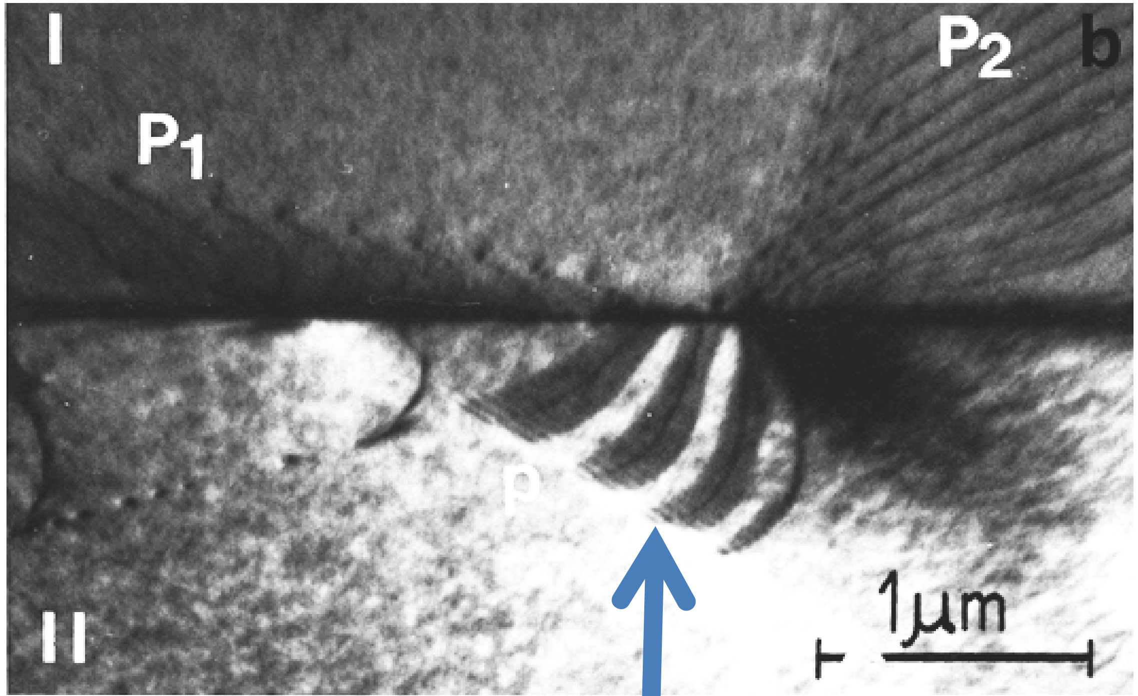
G.ΔU integer

Two beams bright field TEM: Diffraction contrast



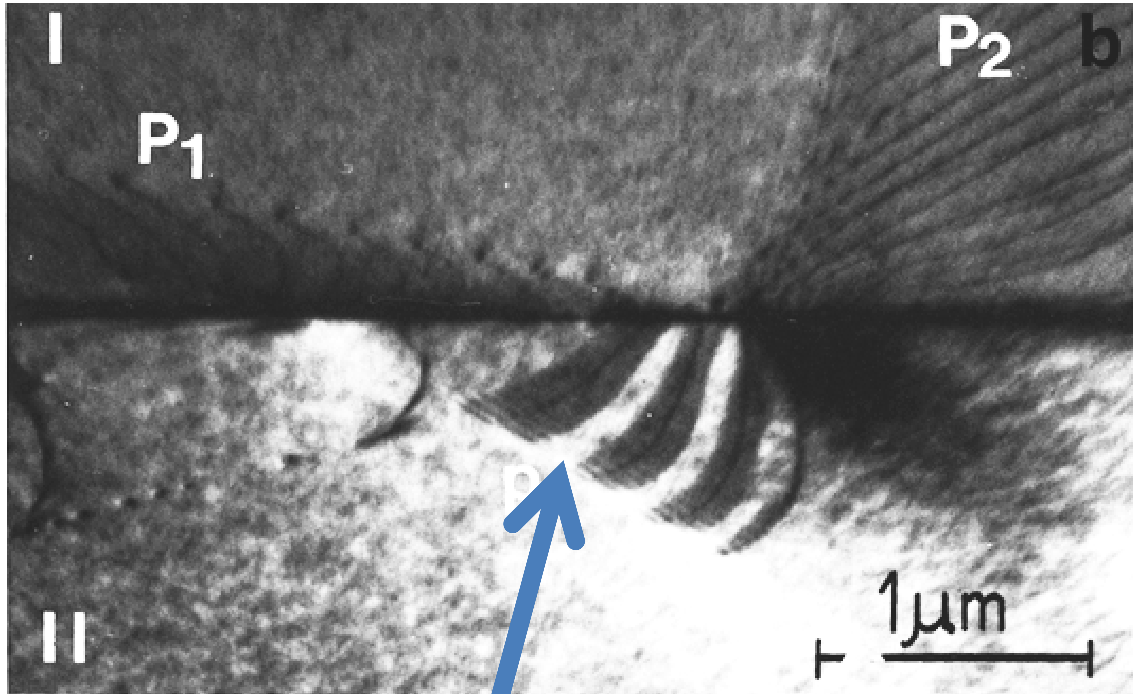
G.ΔU = (3n+1)/3

Two beams bright field TEM: Diffraction contrast



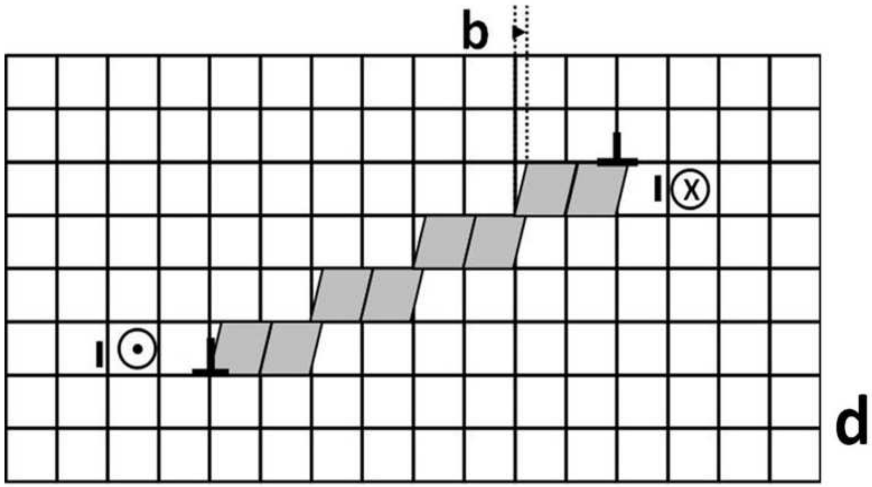
$G.\Delta U = (3n+2)/3$

Two beams bright field TEM: Diffraction contrast



G.ΔU = (3n+3)/3

With plasticity: continuous vs. stepwise



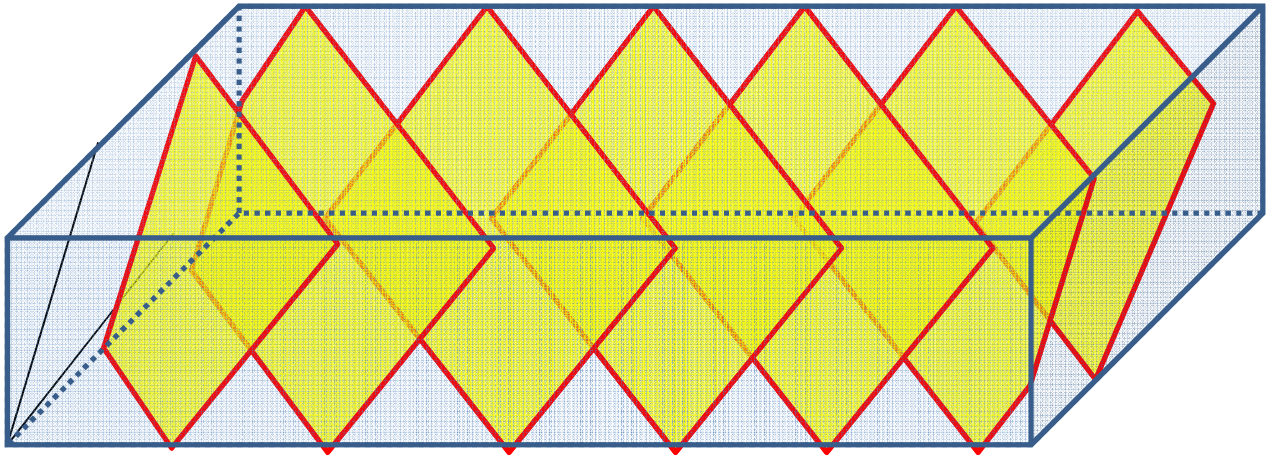
Dislocation **loops** as platelets with eigenstrain

Shift: $\Delta U = n.b$

$$\exp(2i\pi.G.\,\Delta U) = 1$$

(Restricted random distribution)

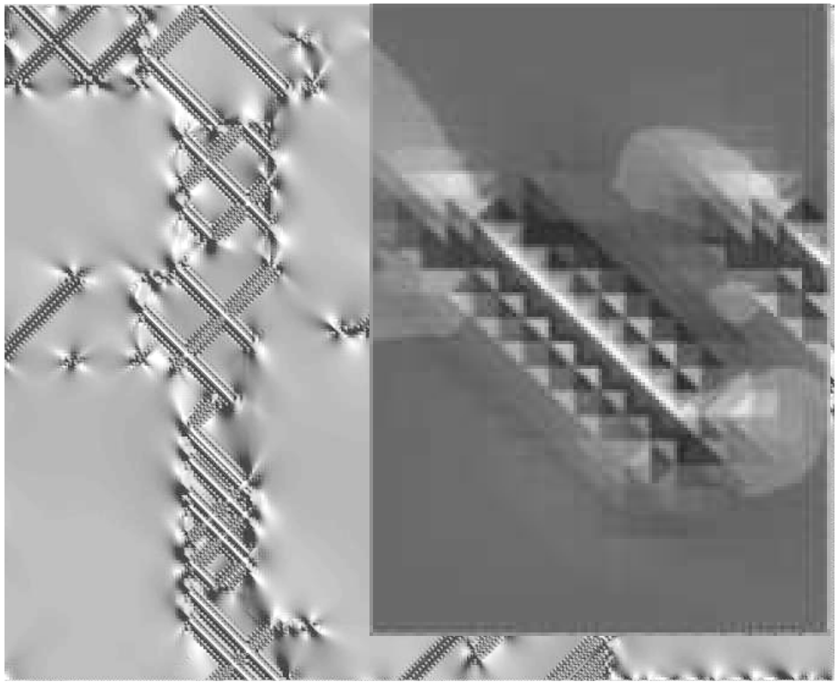
For each slip system (γ)

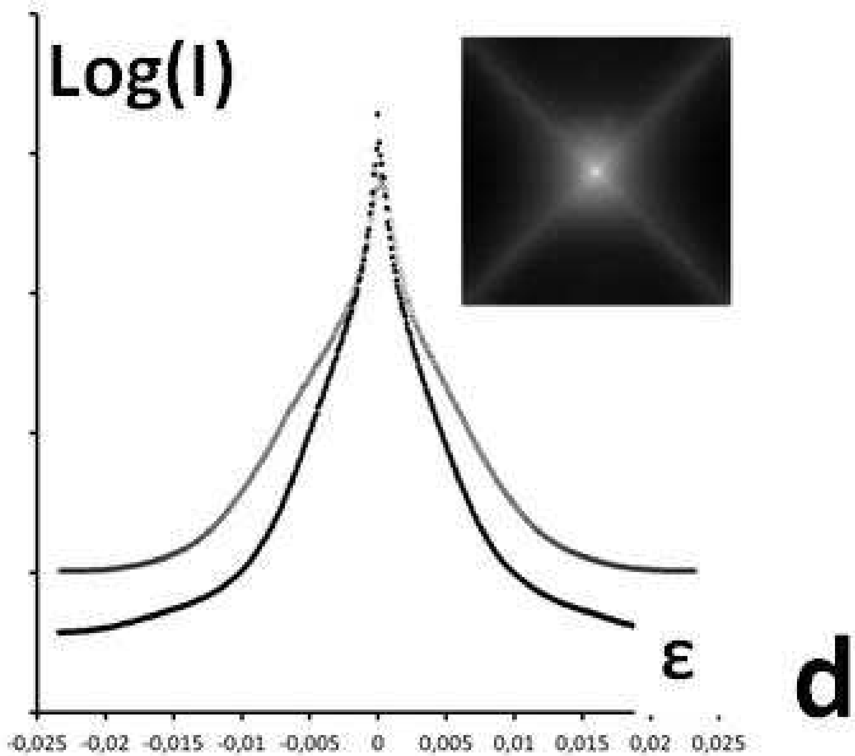


Array of dislocation loops

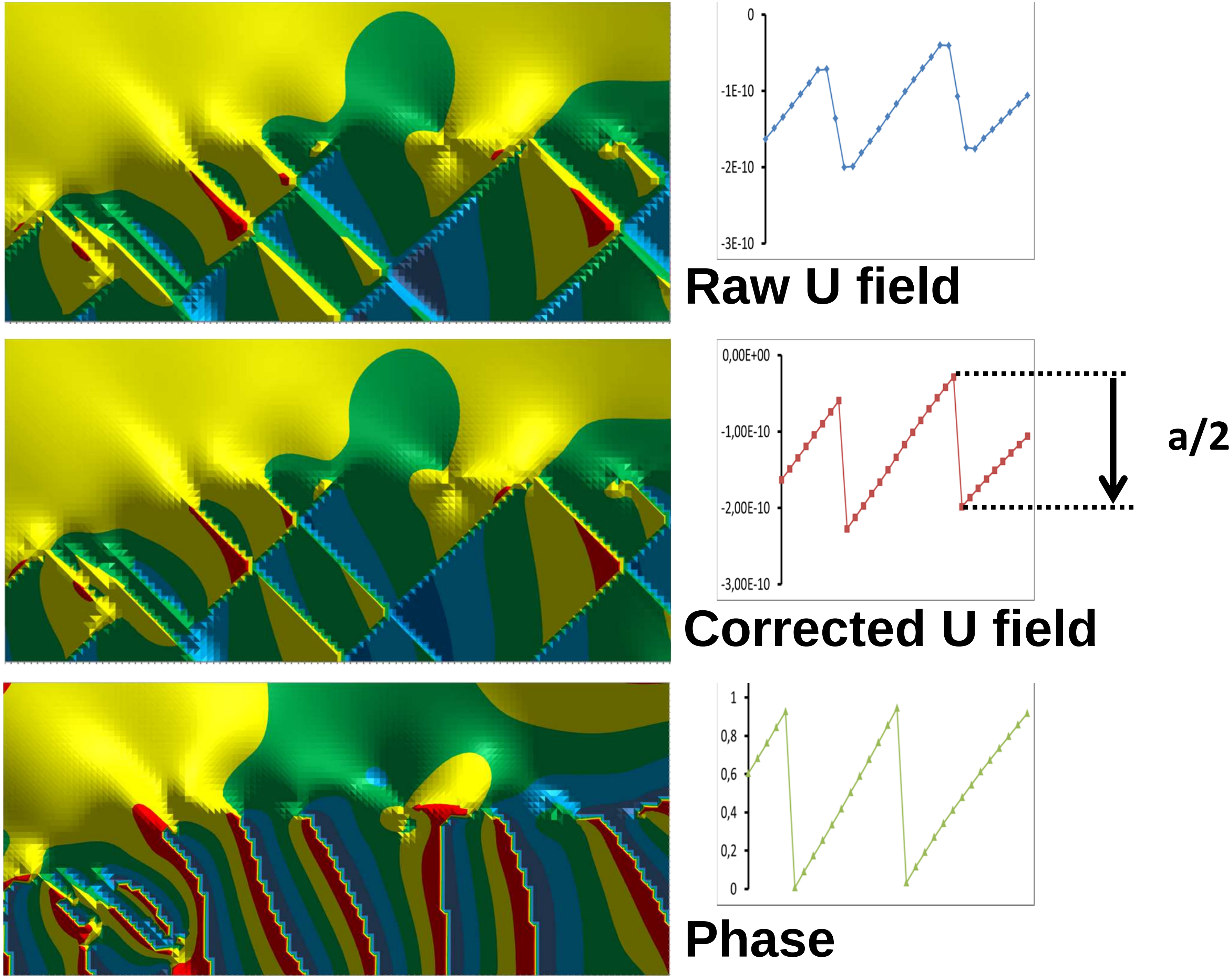
Eigenstrain: ε_{pij} = n.b/l*f(h,k,l)

Dislocations: peaks

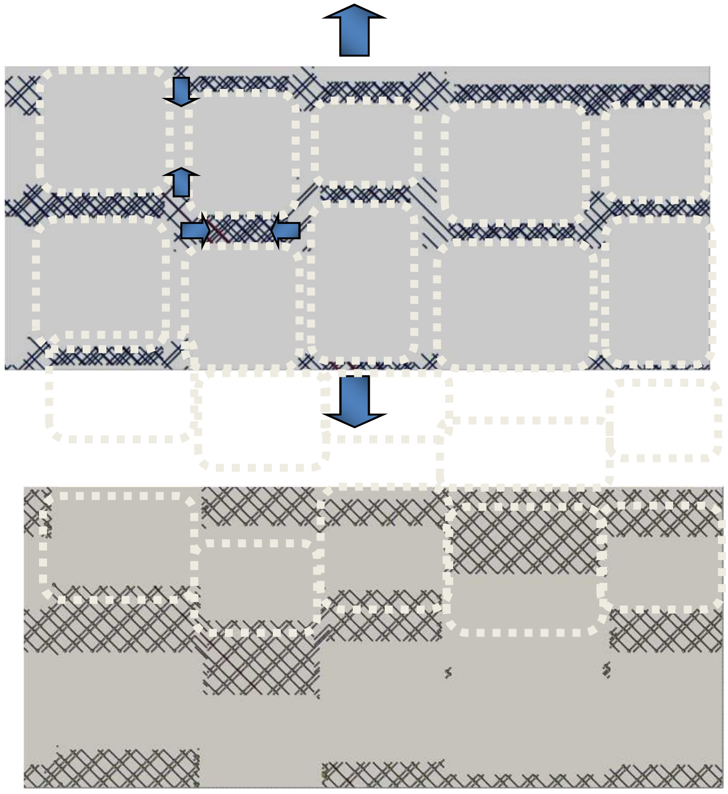


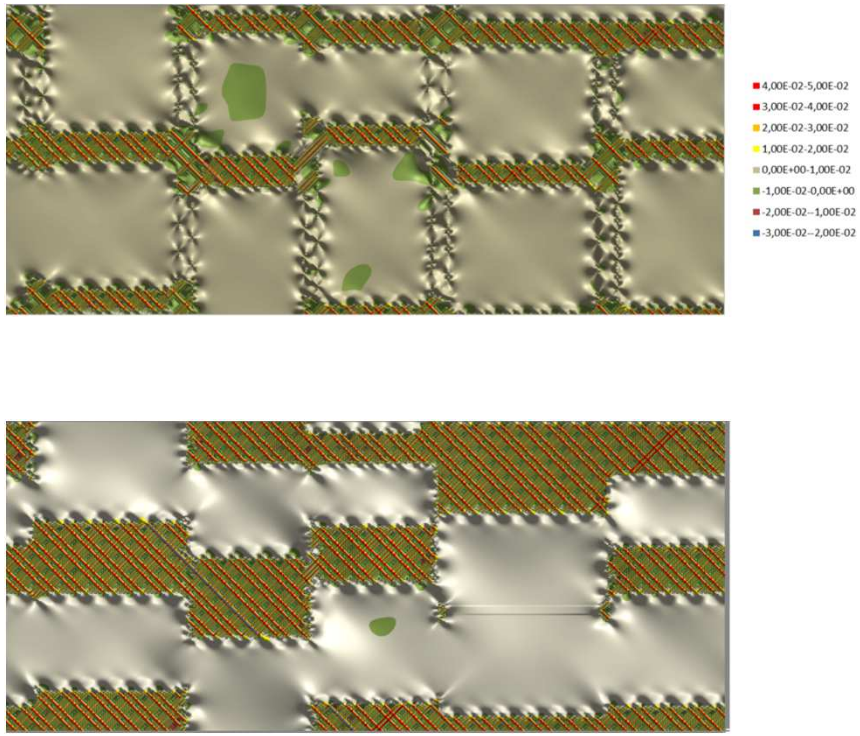


Dislocations loops in the γ phase


0
-1E-10
-2E-10
-3E-10
Raw U field
0,00E+00
-1,00E-10
-2,00E-10
-3,00E-10
a/2
Corrected U field
1
0,8
0,6
0,4
0,2
0
Phase

Tensile creep test





Recipe

- Generate a microstructure
- Calculate the strain (stress) field
- Calculate the displacement field
- Get the phase
- Take a Fourier Transform or FFT
- Calculate and plot intensities

- Model plasticity
- Put dislocations

Plastic strain within γ

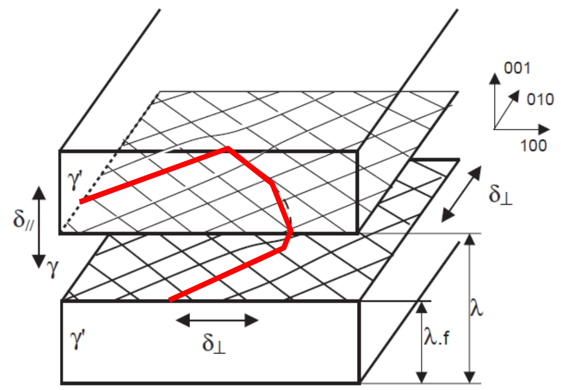
- The γ phase is divided in 875 « platelets » of various sizes and positions
- Each platelet has its own Orowan stress σO = (**A**/d)*LN(d/b)
- We can compute the “external stress”, the coherence stresses, the contribution of dislocations, and the total average resolved shear stress on different slip systems within a platelet
- The shear increment for each slip system of a platelet is proportional to the difference between its resolved shear stress and the Orowan stress
- Dislocation loops are defined. Their contribution is recomputed
- Stop after equilibrium is reached

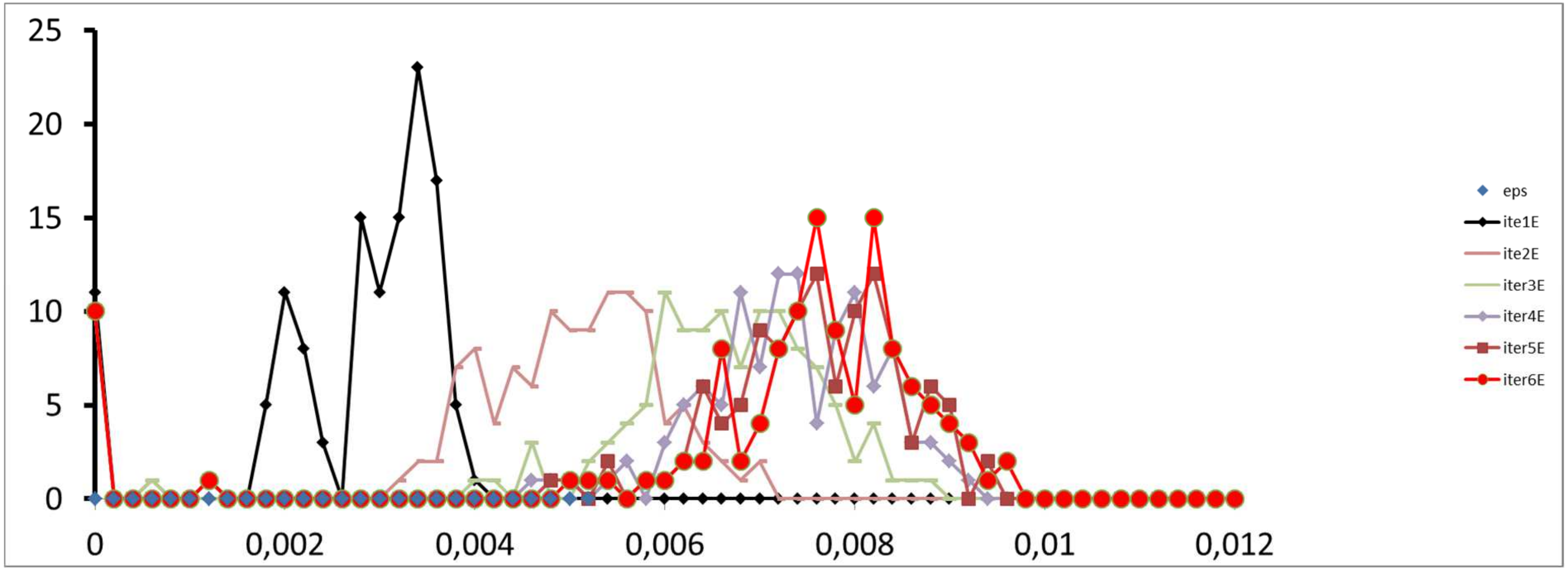
T = 1000°C

65% γ’

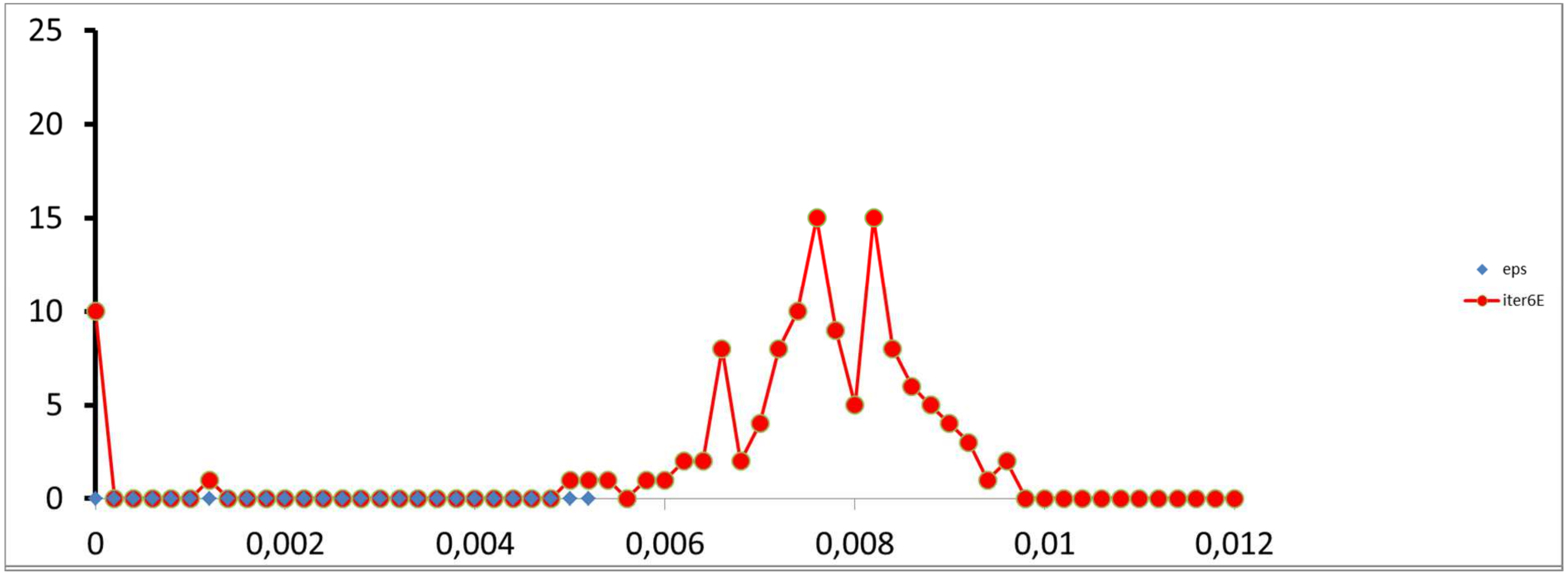
0.4 factor on elastic constants vs. RT

A Orowan: isotropic

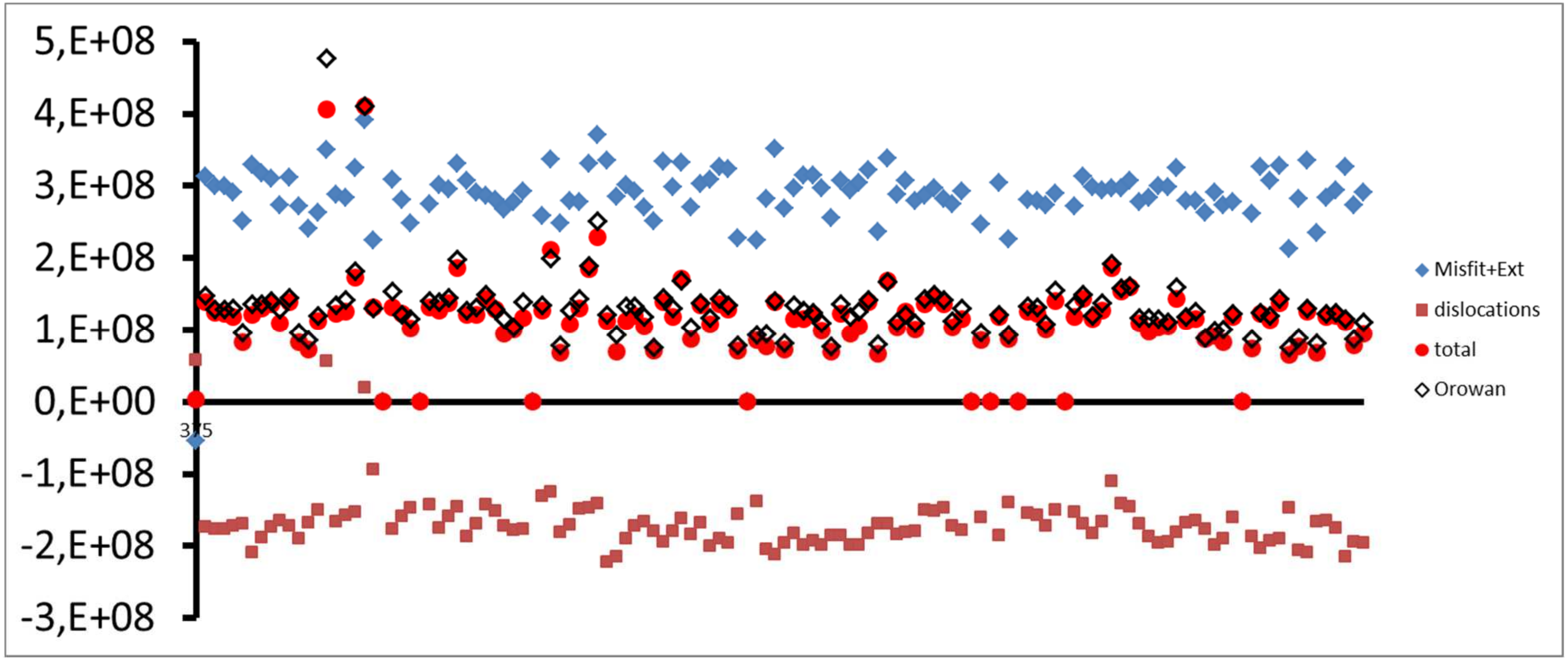




25
20
15
10
5
0
0
0,002
0,004
0,006
0,008
0,01
0,012
eps
ite1E
ite2E
iter3E
iter4E
iter5E
iter6E

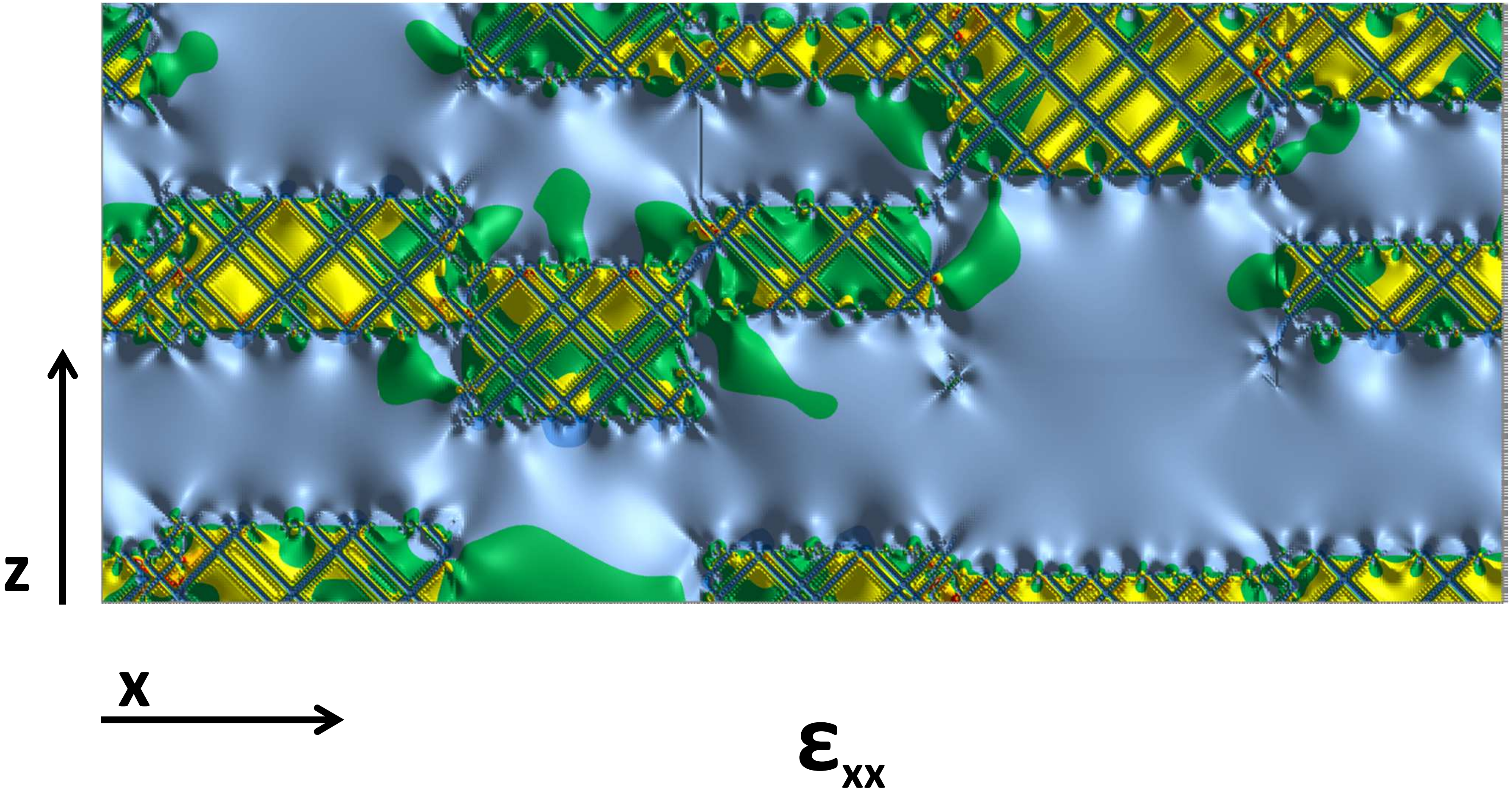


25
20
15
10
5
0
0
0,002
0,004
0,006
0,008
0,01
0,012
eps
iter6E

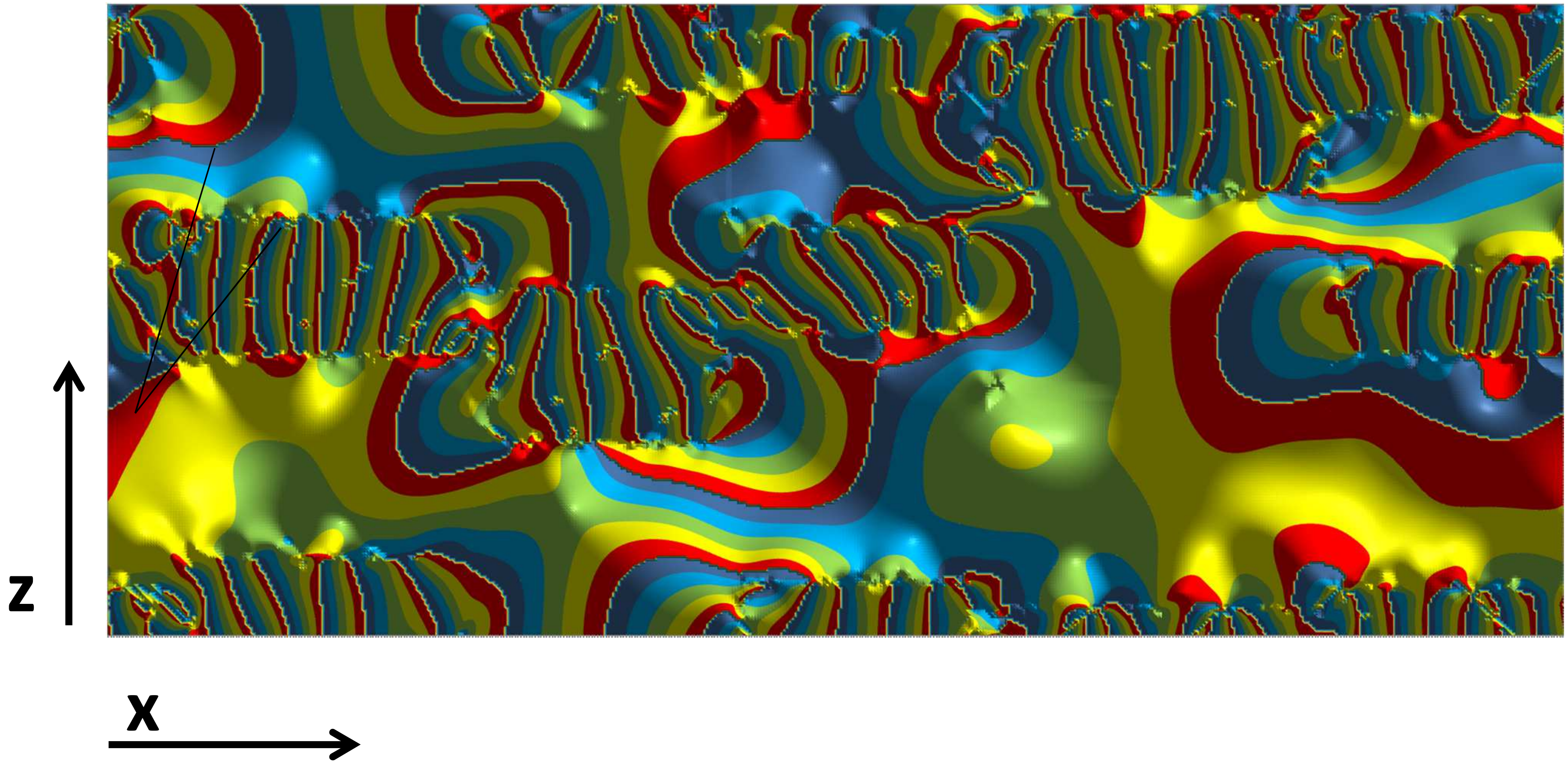


5,E+08
4,E+08
3,E+08
2,E+08
1,E+08
0,E+00
-1,E+08
-2,E+08
-3,E+08
Misfit+Ext
dislocations
total
Orowan

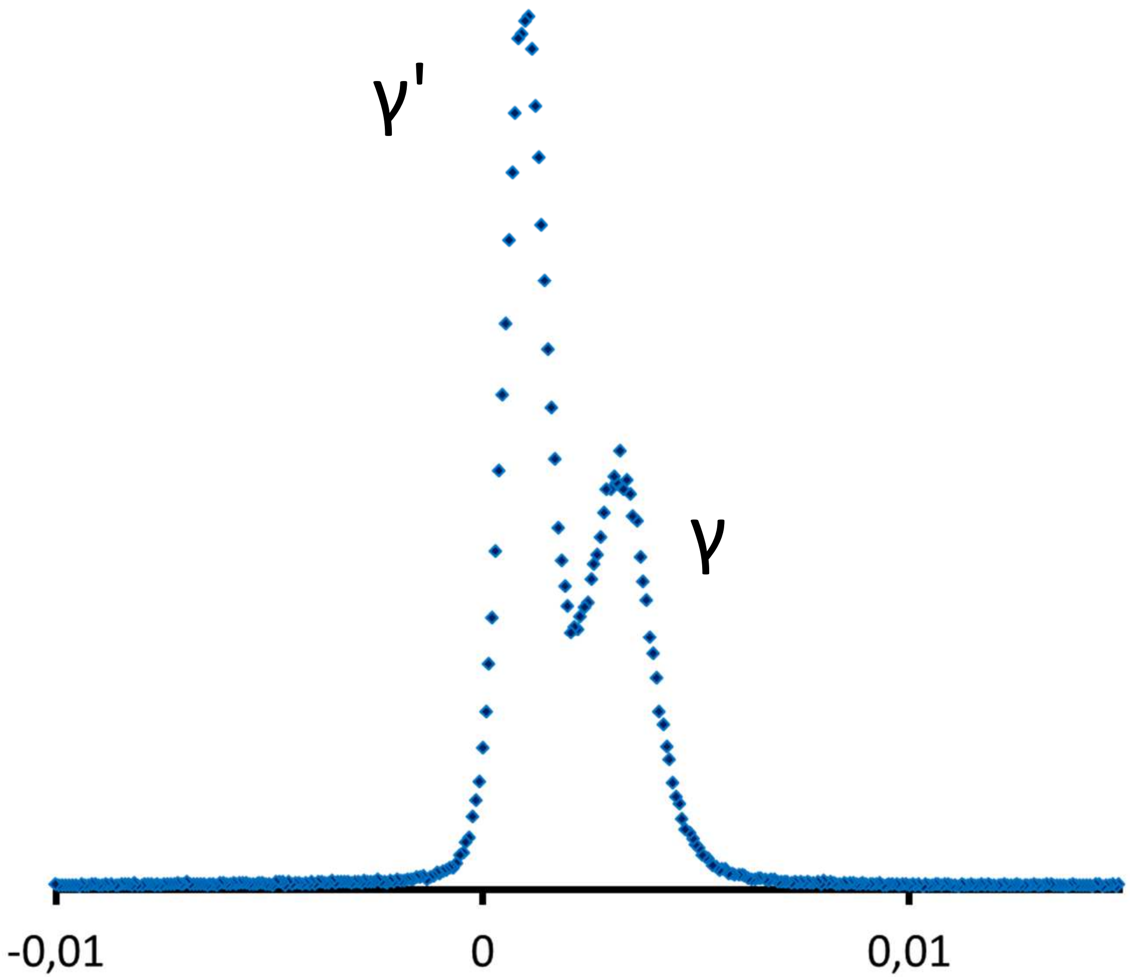
With plasticity



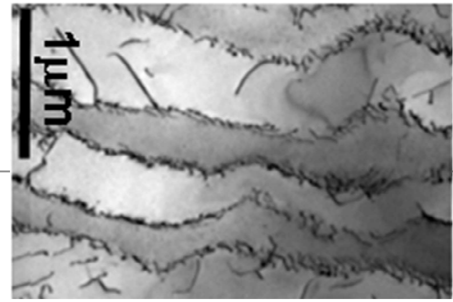
Phase

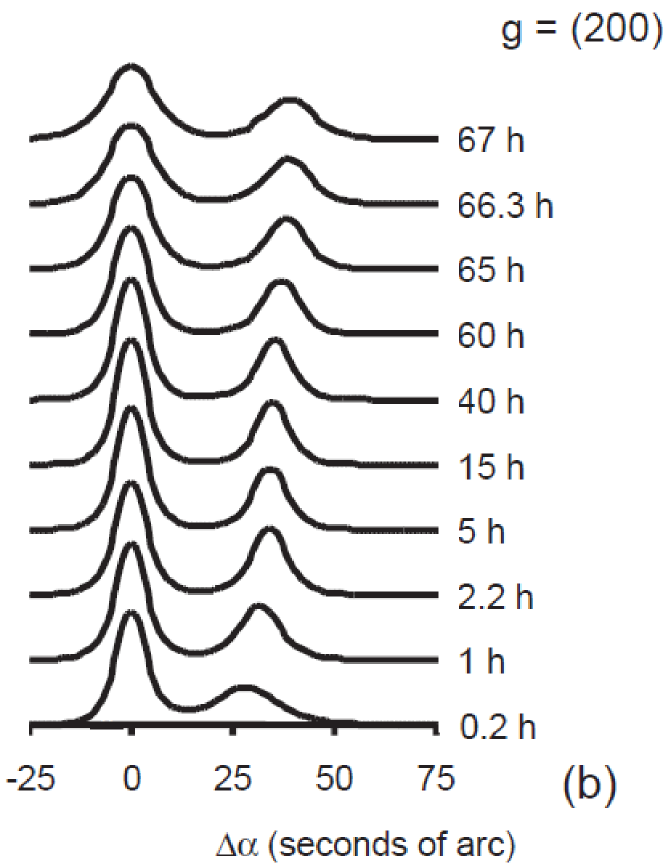


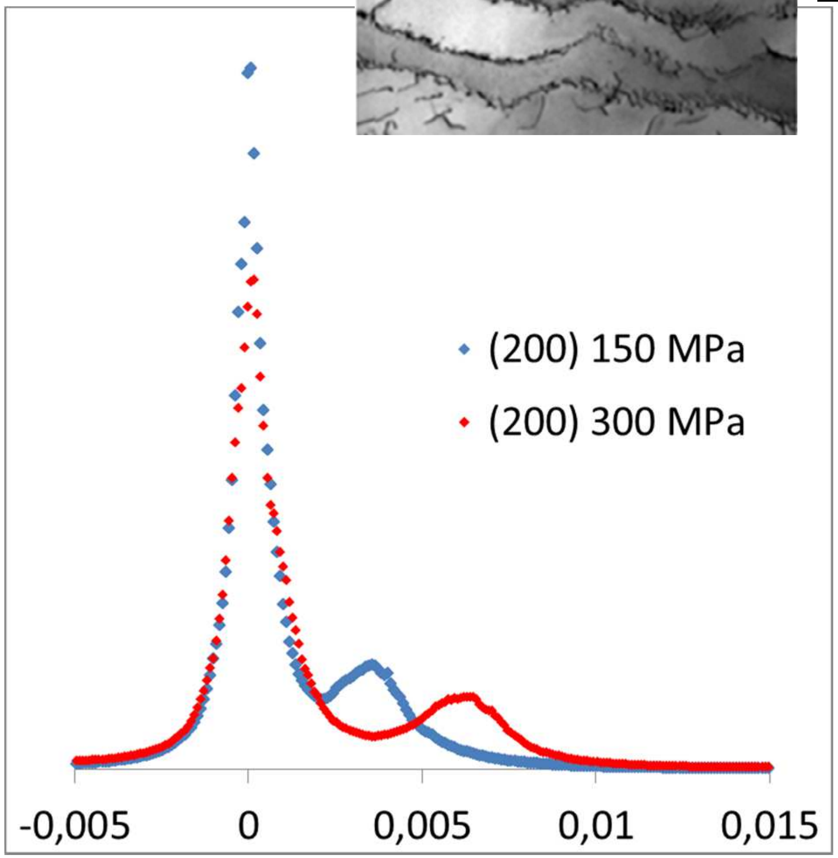
Tensile creep test



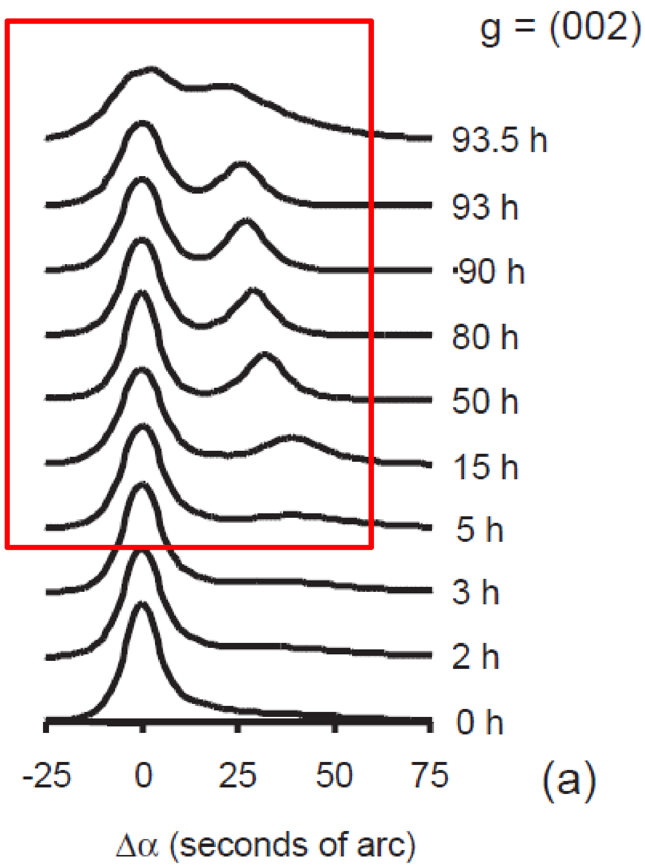
Tensile creep test

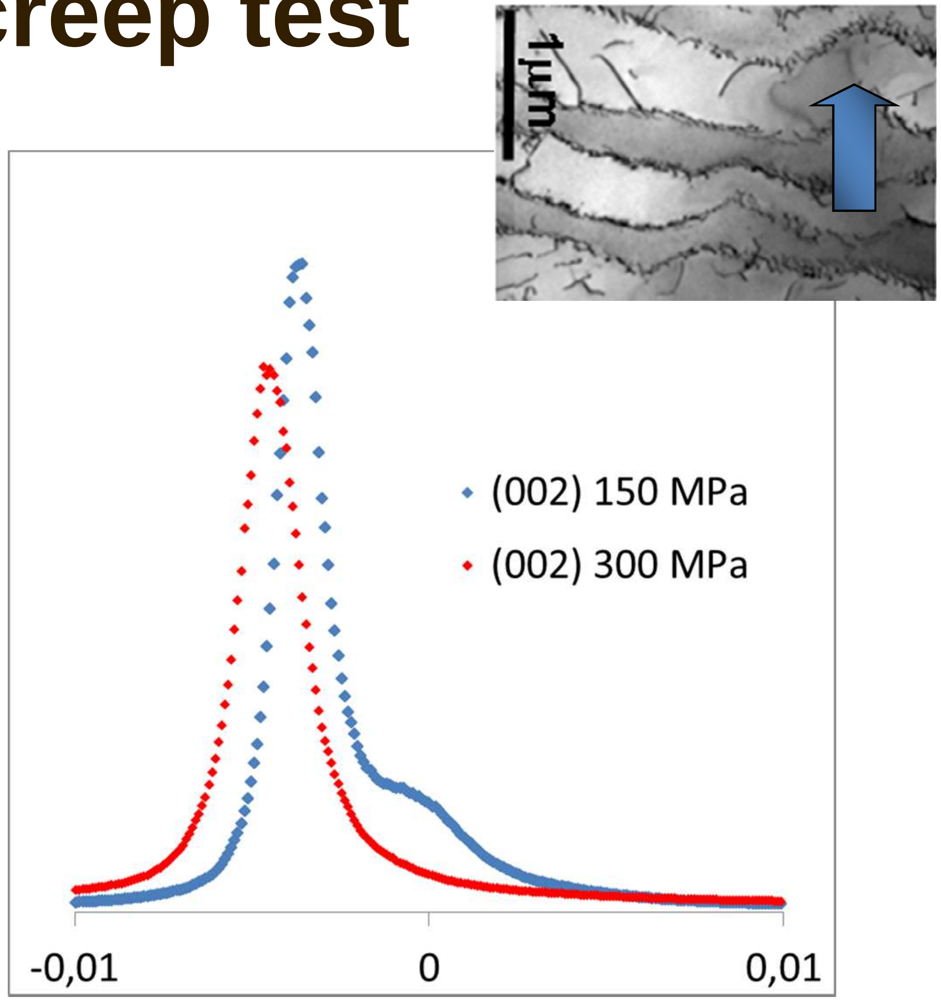




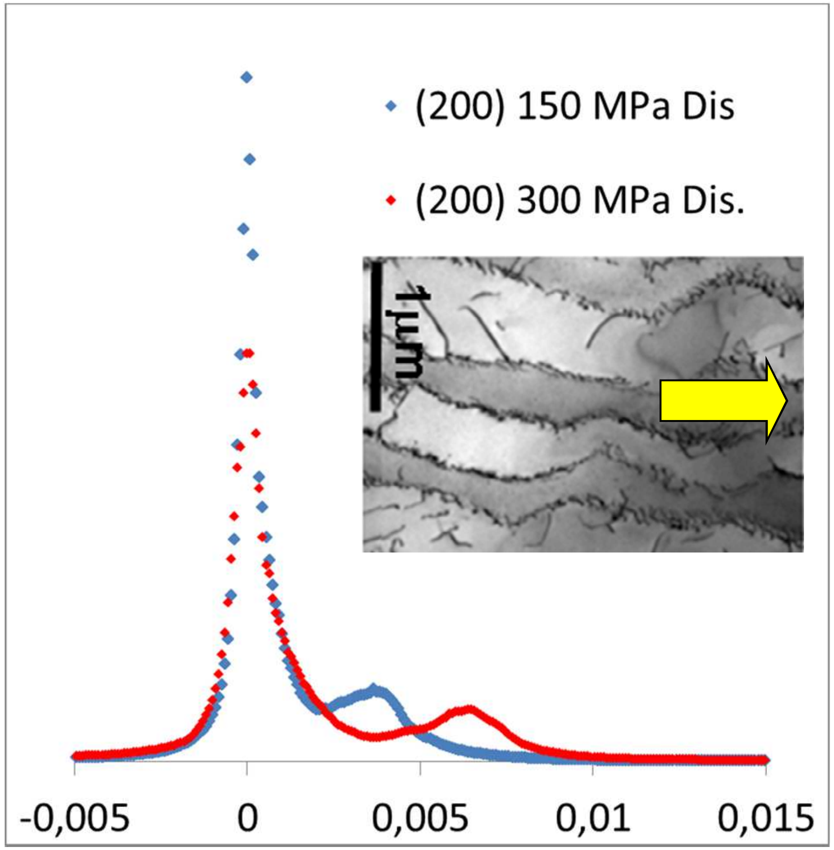


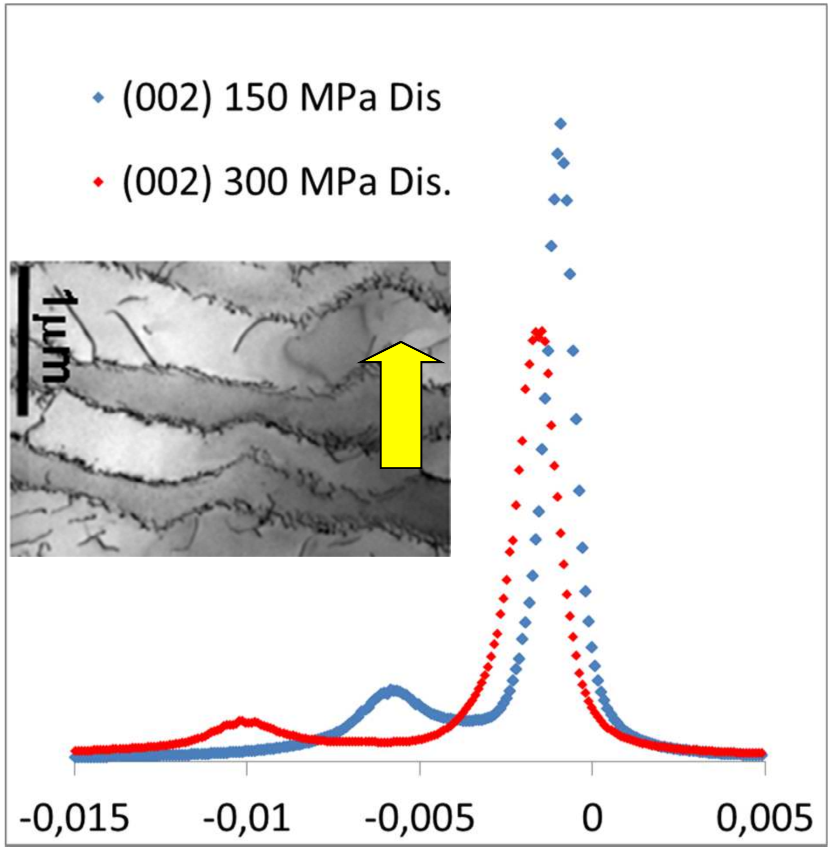
Tensile creep test



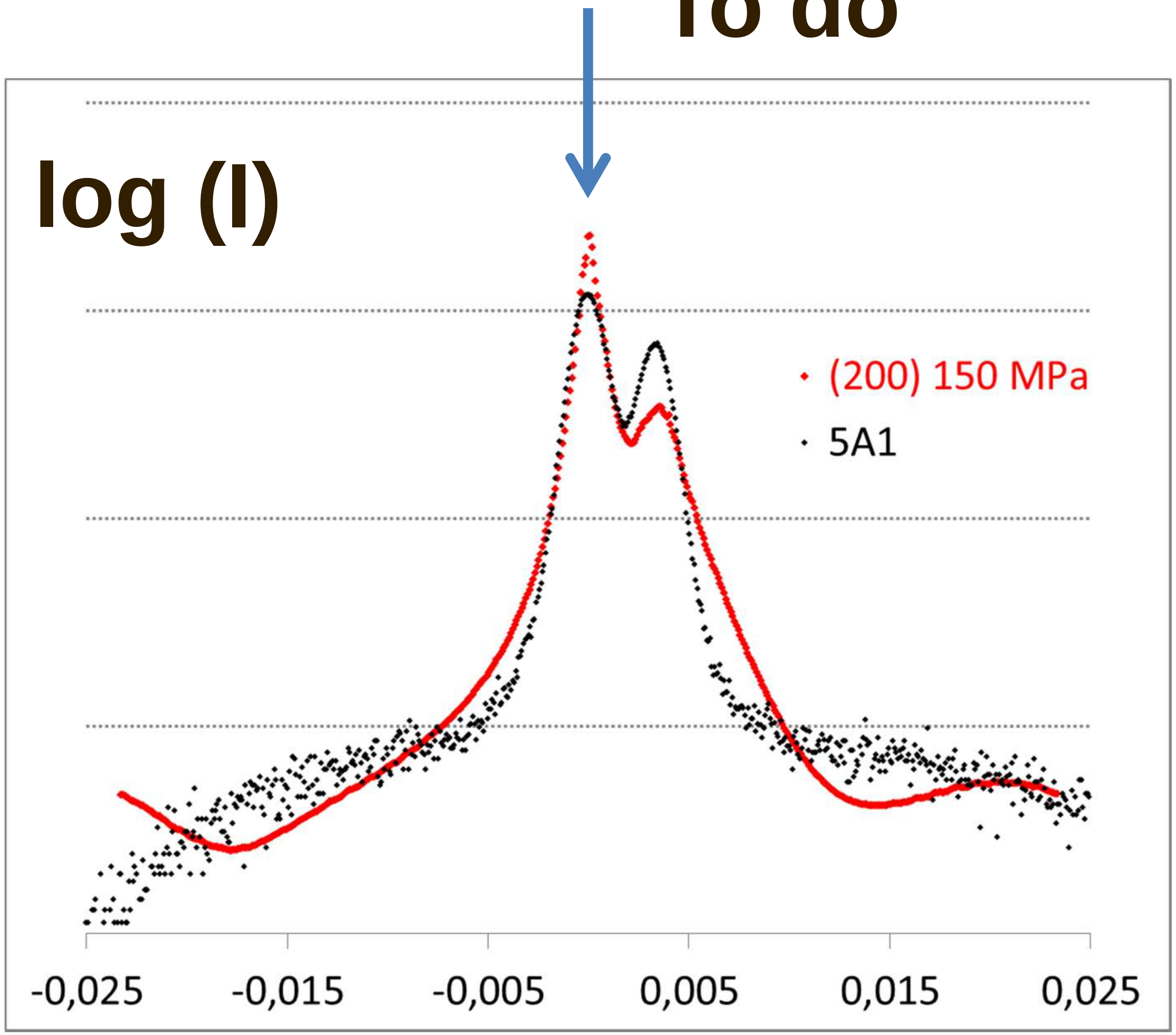


After cooling: dislocations only



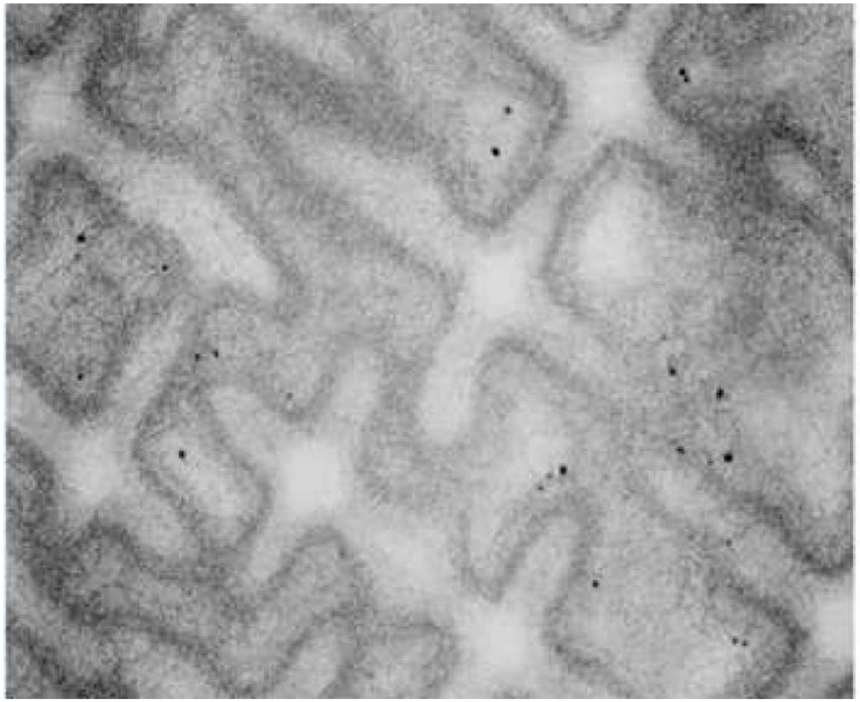


To do



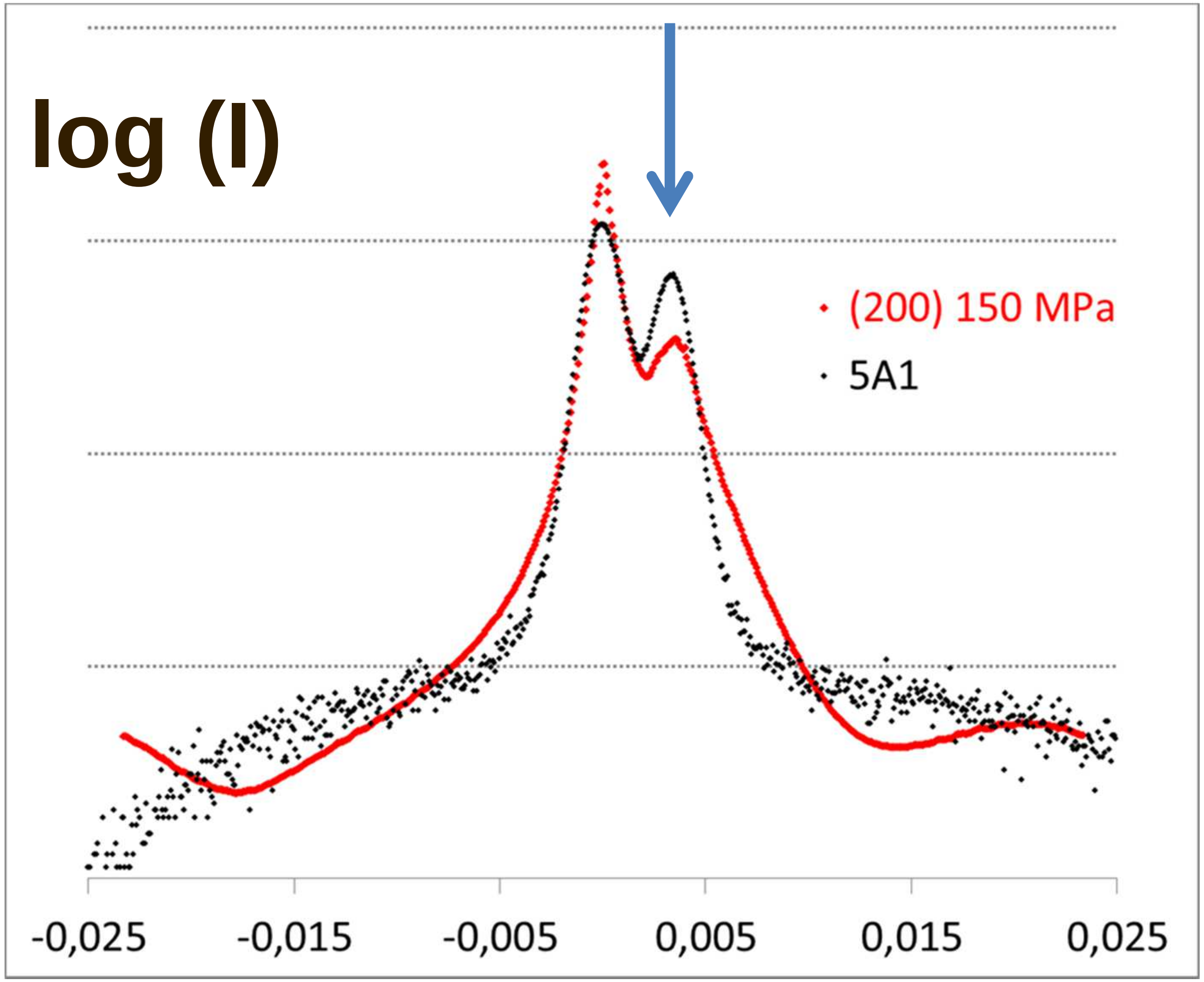
γ‘ peak too thin: Segregation

Dendritic solidification

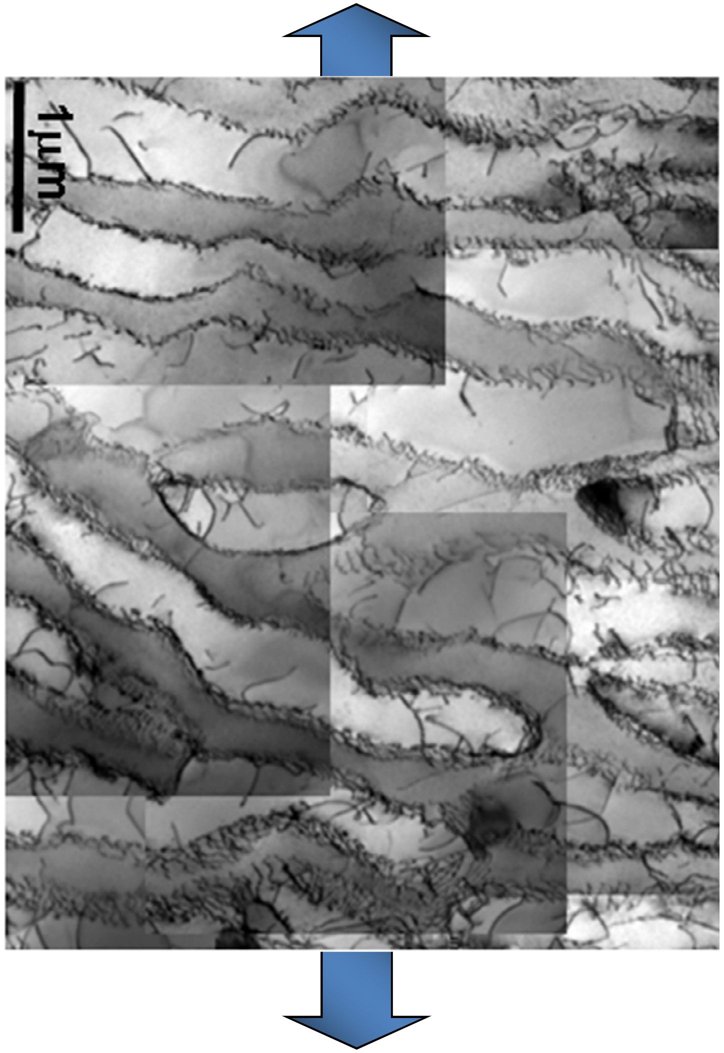


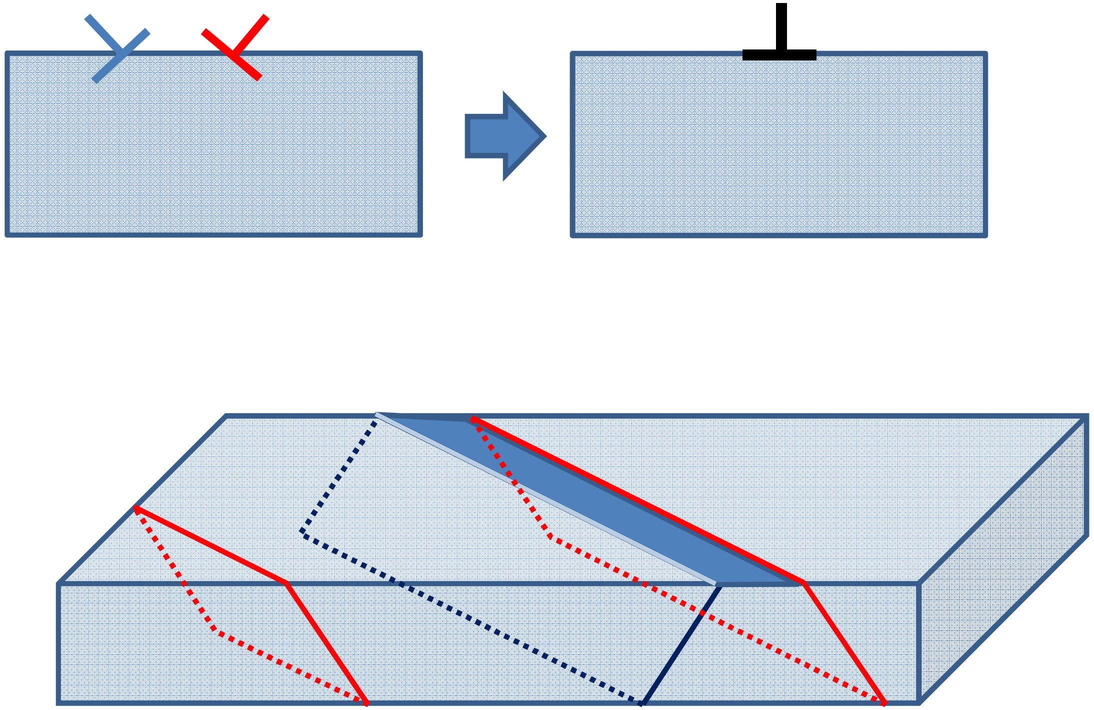
- Different compositions
- Different volume fractions
- Different lattice mismatchs

To do



γ too wide:
Dislocations
at interfaces





New dislocation loops at interfaces

Conclusion

- A FFT-based tool to calculate the elastic fields within a complex microstructure
- Possibility to introduce crystal defects
- Simulation of HR XRD peaks for comparison to experimental data.
- The peaks' shapes are realistic and quite sensitive to details.
- The only fit parameters are Material parameters:

A discriminating test for constitutive laws