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

12 - 23 April 2010

Application of DD modeling to plastic deformation of RPV steel in the ductile to brittle transition regime

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12 – 23 April 2010
Miramare – Trieste, Italy

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CEA-Saclay France
DEN/DMN/SRMA

Plastic deformation of RPV steel in ductile to brittle transition regime

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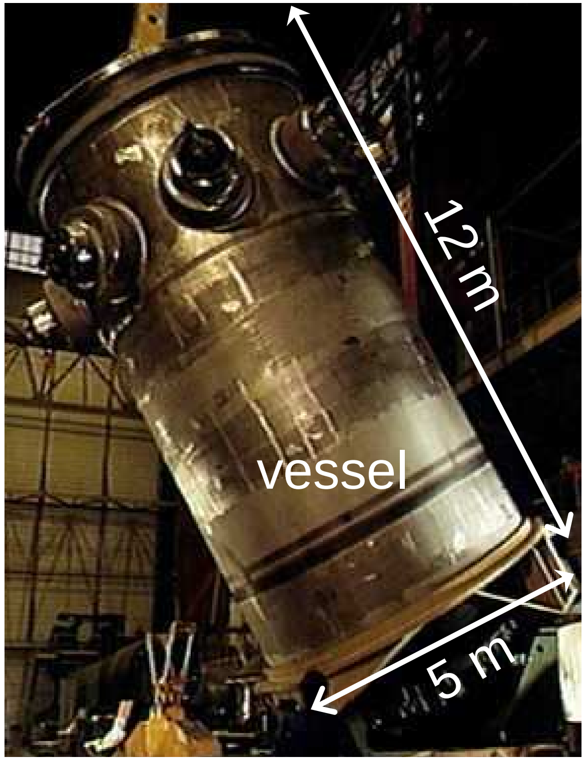
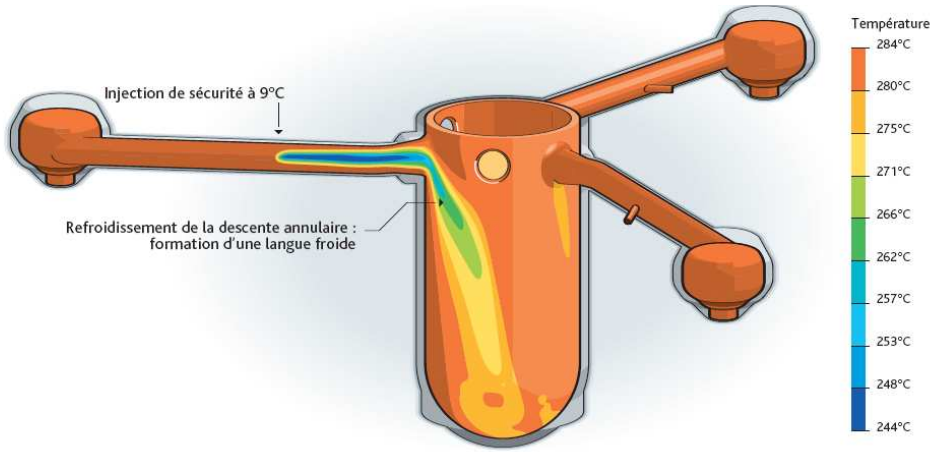
Introduction: motivations

➢ **Pressure vessel: the only part of a PWR that cannot be changed**

Safety issue: emergency procedures in case of core fusion



➡ Cold water injection in the vessel

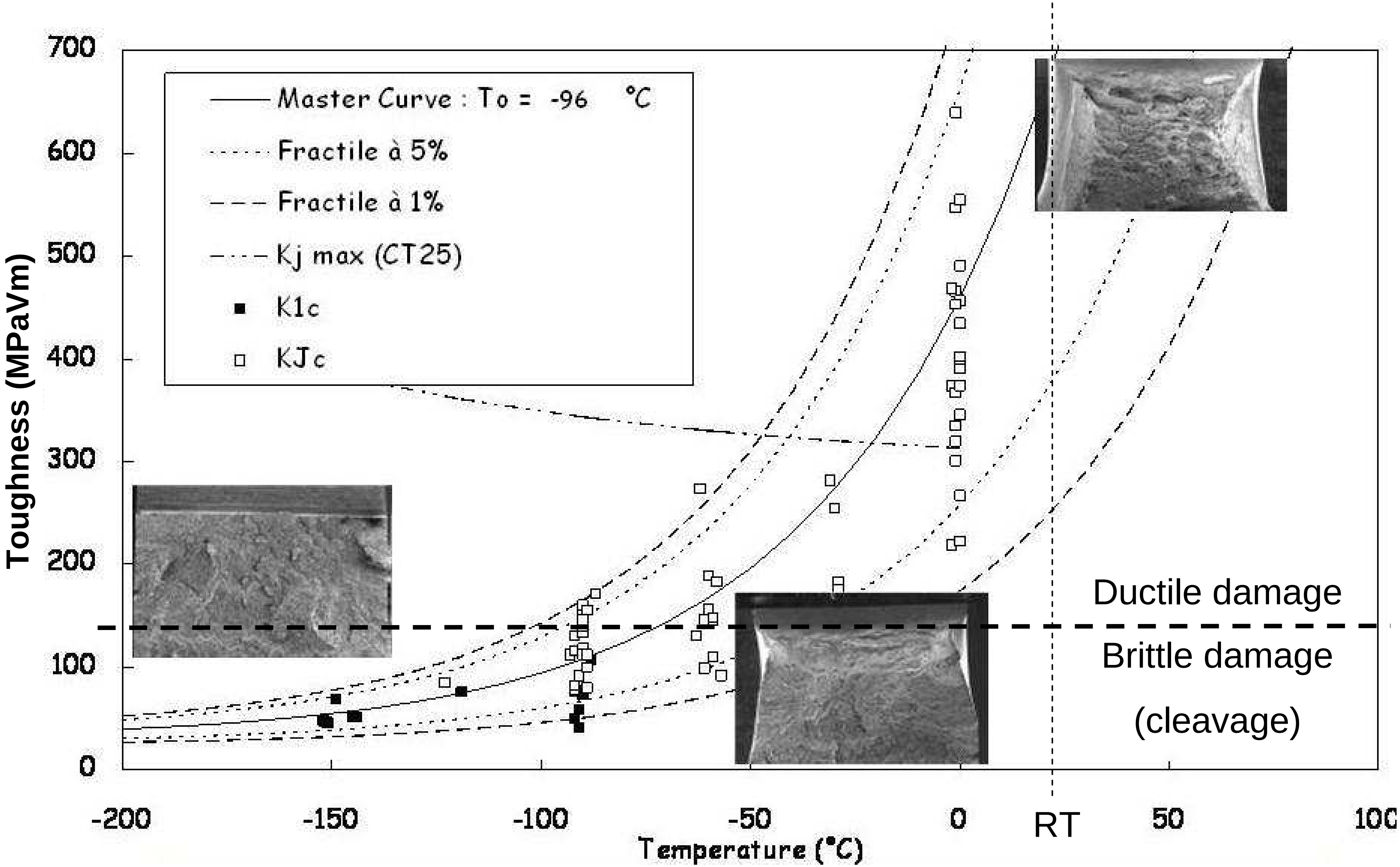


➡ Generation of thermo-mechnical stresses & T° falls down to the ductile/brittle regime

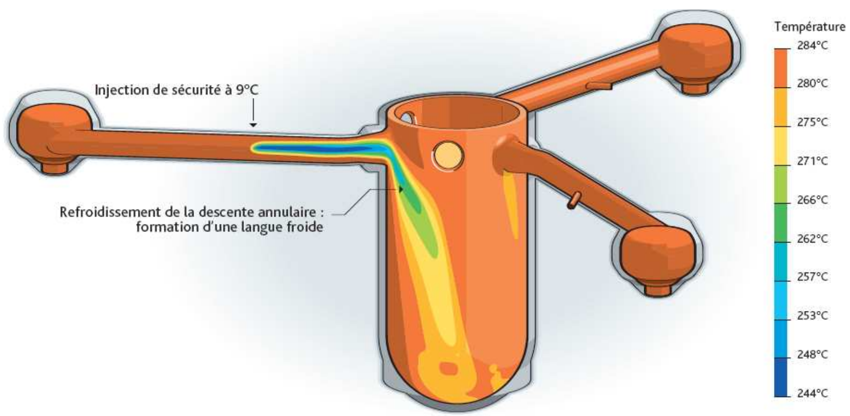
➡ Rupture of the vessel

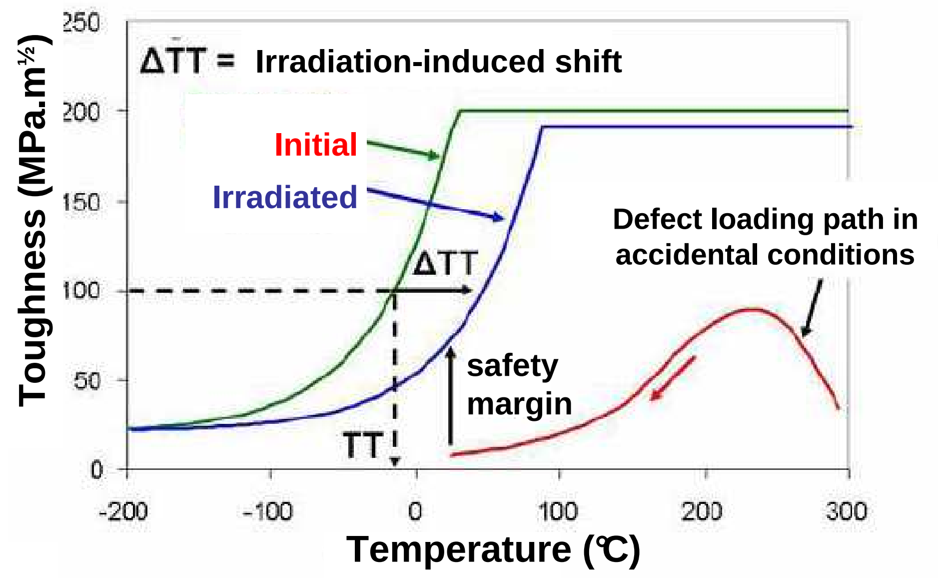
Brittle damage at RT (low toughness) = cleavage cracking

RPV steel toughness: temperature effect



RPV steel toughness: temperature and dose effects





Standard toughness prediction apploach is local approach of fracture

Reliability of this approach in accidental conditions?

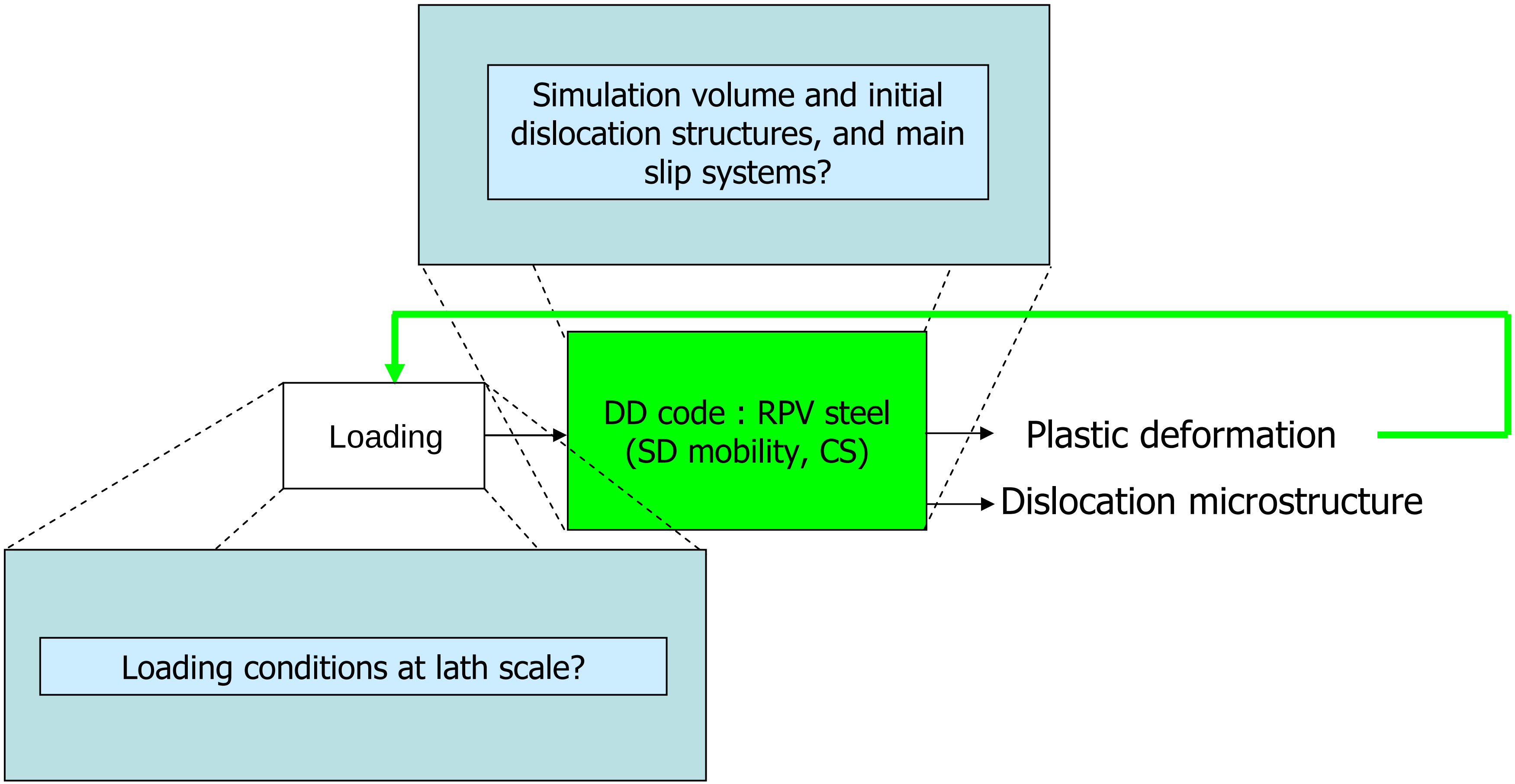
↓

Physical origin of dose and <u>temperature</u> dependences

Ductile-brittle is not a material parameter

Nucleation and motion of dislocation away from crack tip region is the rate limiting process

DD simulation of plastic deformation of RPV steel



Mobility rules adapted bcc at RT

FCC models (Cu, FCC Fe)

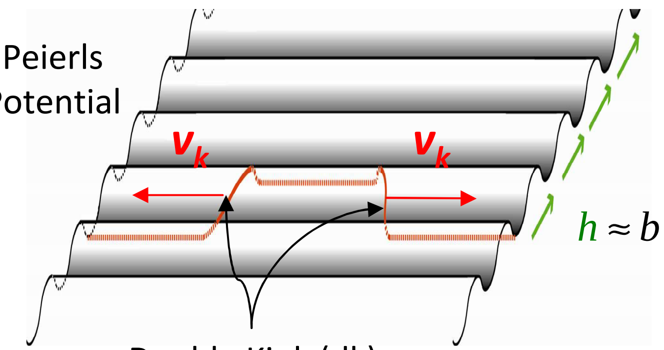
Screw ~ Edge

Negligible Peierls barrier (τ_p~x10 MPa)

Phonon-drag mechanism

$$v_{screw}(\tau) = v_{edge}(\tau) = \frac{\tau b}{B}$$

- τ : applied stress >> τ_p
- ***B*** : Viscous drag coefficient
- ***b*** : Burgers vector module
- τ_p : Peierls Stress



BCC Fe

Screw ≠ Edge

Velocity anisotropy depends on T°

Low temperature

Significant Peierls barrier (τ_p~1GPa)

Thermally activated mobility

$$v_{screw}(\tau, T) \ll v_{edge}(\tau) = \frac{\tau b}{B}$$

Room temperature

Athermal regime

$$v_{screw} \approx v_{edge}$$

On dislocation dynamics : "**Double Kink** Mechanism"

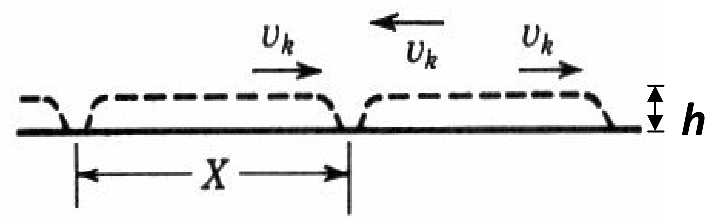
- **Nucleation** of a double kink (thermally activated)
- Kink **propagation** : $v_k \approx v_{edge}$

Kink pair mechanism and screw mobility

Guyot & Dorn [1967] – Hirth & Lothe [1982] hybrid model

General expression

$$v_{screw} = hXJ\alpha_{corr}$$



- ***h*** : distance between Peierls valleys
- ***J*** **[m^{-1}s^{-1}]** : kink pair (dk) **nucleation rate** per unit length
- ***X*** **[m]** : kp's **mean free path** before annihilation with another dk [increases with kinks velocity (v_k), and decreases with *J*]

G&D

$$J = \frac{\nu_D b}{l_c^2}\cdot\exp\left(-\frac{\Delta G(\tau^*)}{k_B T}\right)$$

H&L

$$X = X_\infty \cdot \frac{L}{X_\infty + L}$$

$$v_k = v_{edge} = \frac{\tau^* b}{B}$$

$$X_\infty = 2\left(\frac{v_k}{J}\right)^{1/2}$$

$$l_c^2 = \frac{\mu b h}{8\pi\tau^*}$$

- X_∞ : X for an infinite dislocation

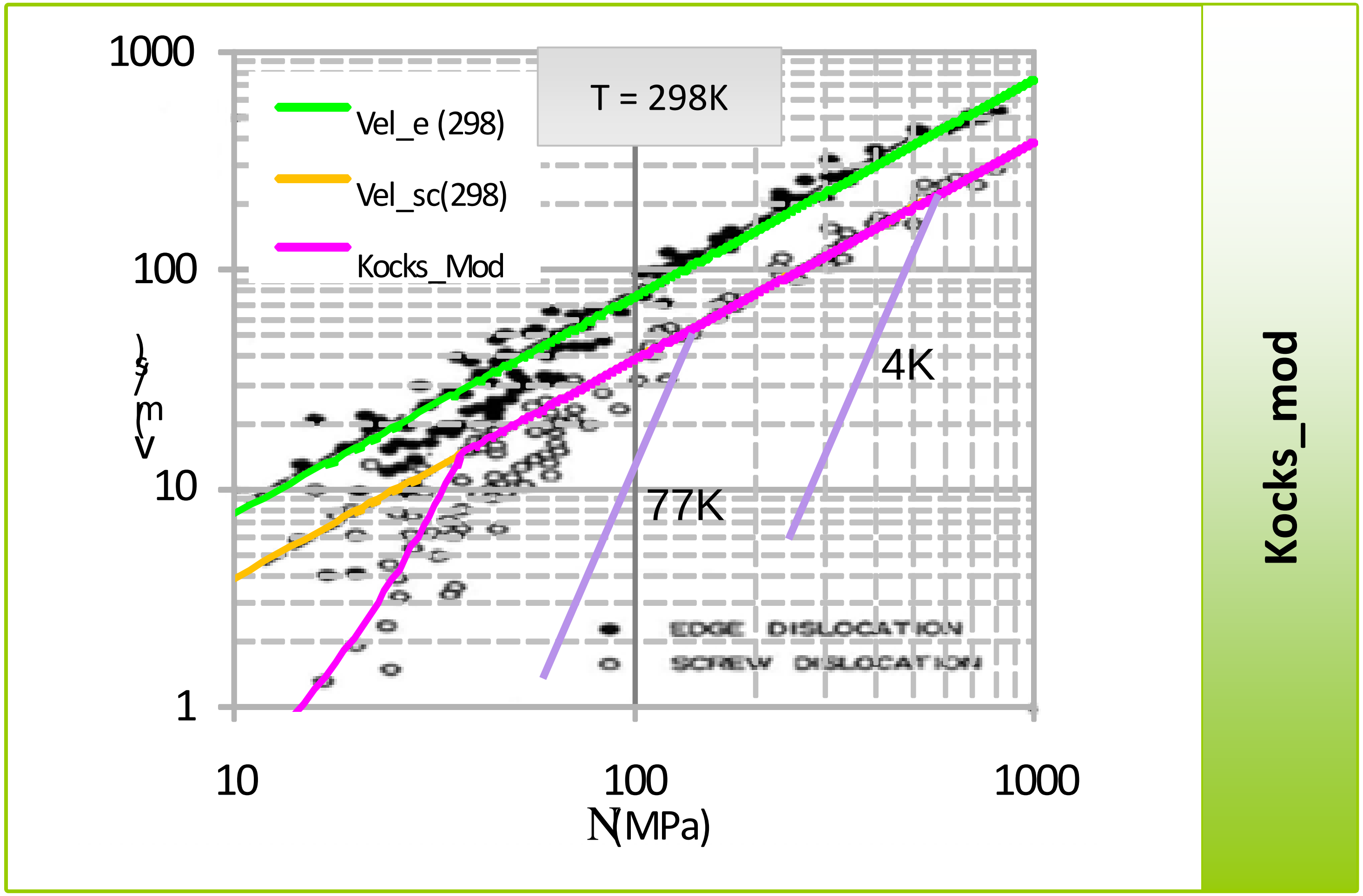
- ΔG : Activation energy
- $l_c(\tau^*)$: critical dk length

$$\Delta G(\tau^*) = \Delta H_0\left[1-\left(\frac{\tau^*}{\tau_p}\right)^p\right]^q$$

- ΔH_0 : barrier's height at zero stress
- τ_p : Peierls stress
- *p*, *q* : dimensionless fitting parameters

α_{corr}: fitting parameter ≈ 1 (to adjust athermal velocity in simulations)

Dislocation velocity RT: end of the DBTT transition

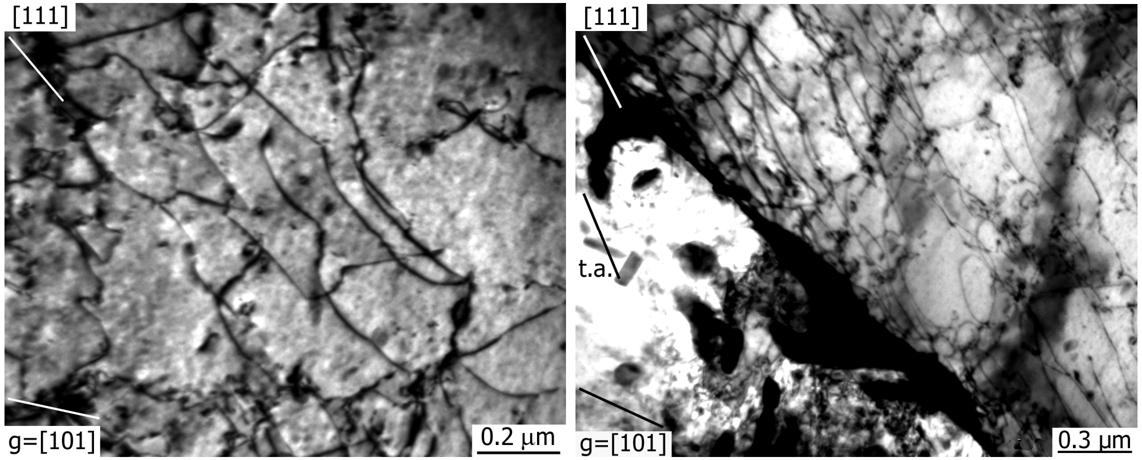


Linear dependence of velocity on SD length at low **τ***

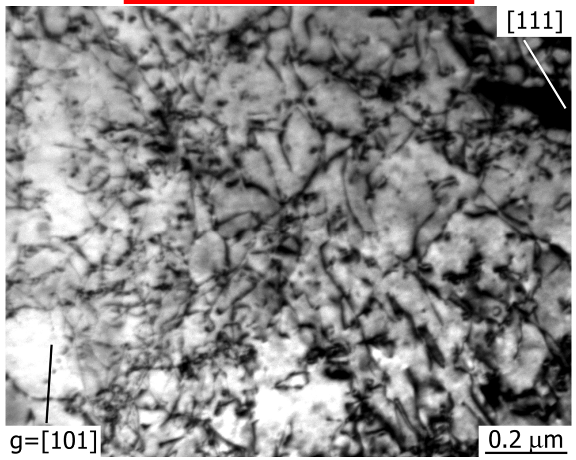
No SD length dependence at high **τ***

Cross-slip in ferritic RPV steel?

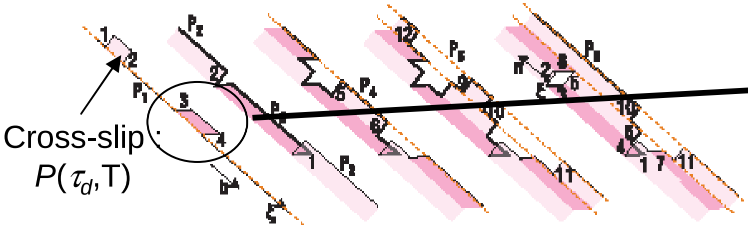
T = -196°C (ε_p = 2,5%)

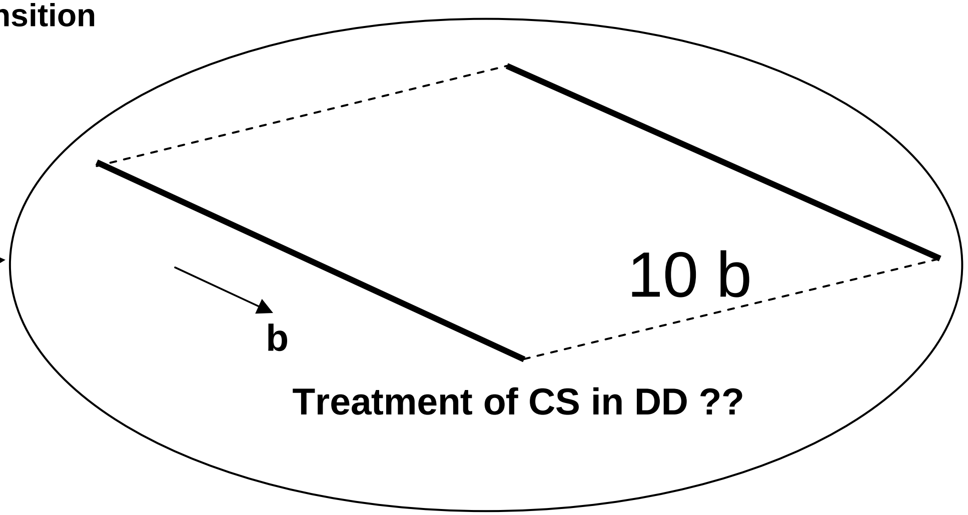


T = 0°C



TEM: unlike in pure Fe, CS is very active at all T° in the transition





Primary slip plane

Sketch: Marian et al 2005

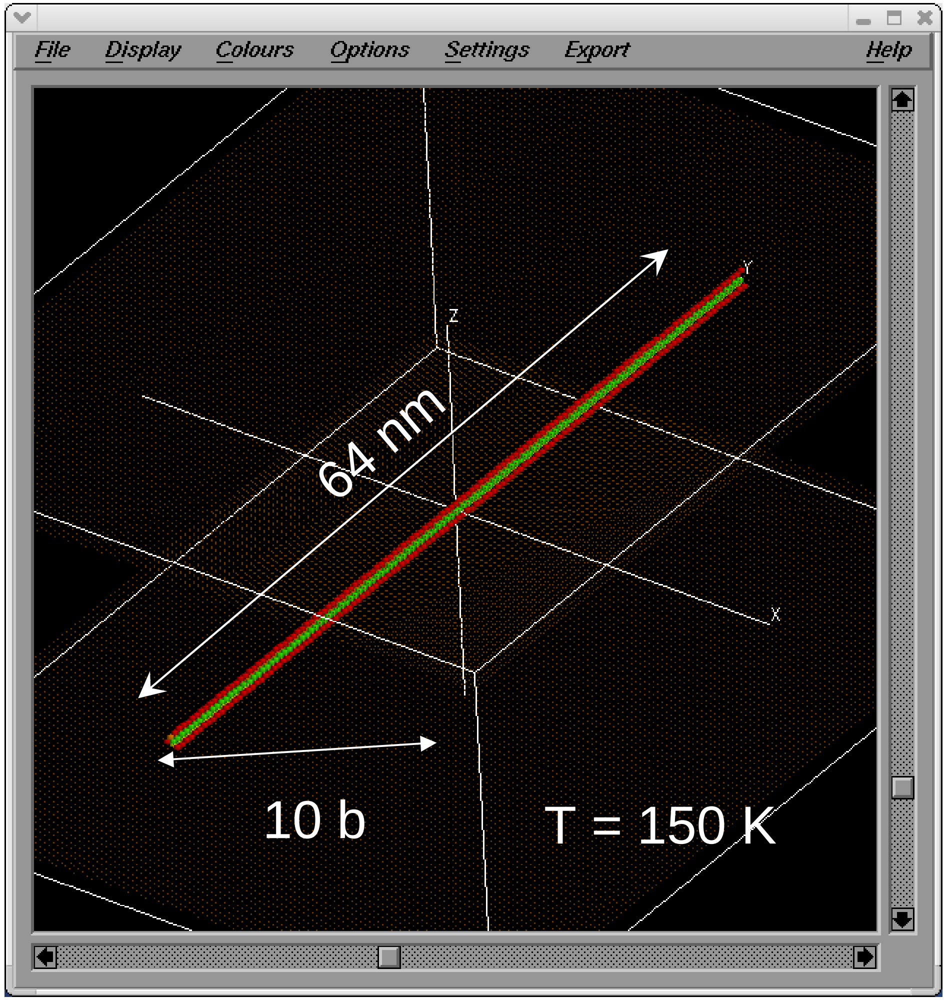
Information from MD simulations

Simulation duration 10^{-9} : 1 time step in DD

Simulated space: 10b lattice spacing in DD

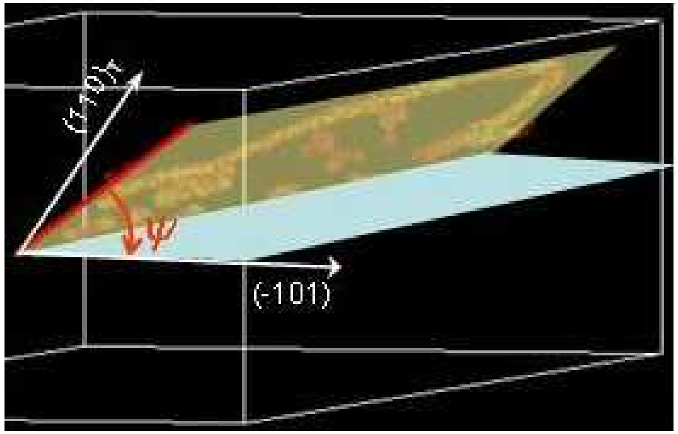
MD simulation conditions:

- **Constant T°= 50-150K**
- **Free surfaces (direction of slip)**
- Periodic along the line direction



J. Chaussidon (CEA/GPM2)

Cross-slip rules bcc: implementation in DD



MD: random CS at <u>high stress</u>

- |ψ| angle increases with ↑ T°

- |ψ| angle decreases with ↓ σ

MD results consistent with thermally activated CS

- Assume thermally activated CS
- Assume ΔG has the same dependence on (τ & T) in prim and CS planes

Rule-1: C-S probability

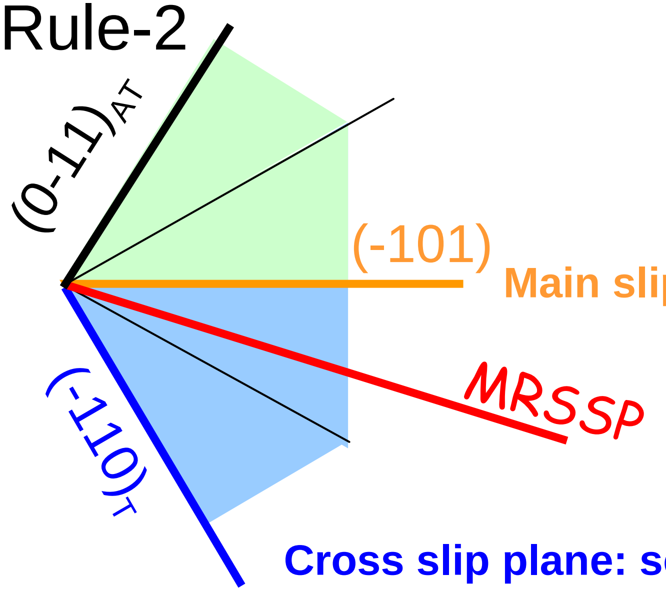
$$P_2 = 1 - P_1 = \frac{v_2}{v_1 + v_2}$$

With $v_1 = bX_1J_1$ and $v_2 = bX_2J_2$

Additionnal MD results: no kink pair nucleation in "twin planes"

Cross-slip rules bcc: implementation in DD

CS Rule-2



Main slip plane: closest {110} plane to the MRSSP

Cross slip plane: second closest {110} twin plane to the MRSSP

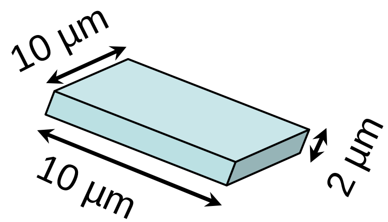
Twin zone: dislocation slip possible in 2 {110} slip planes

Anti twin zone: Cross-slip is inhibited

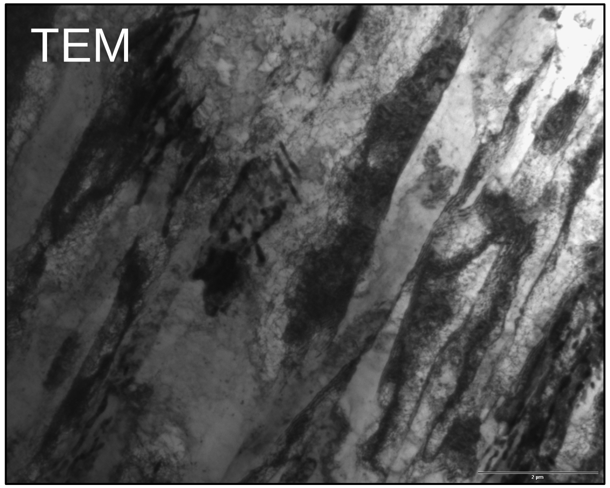
Simulation setup adapted to 16MND5 RPV steel?

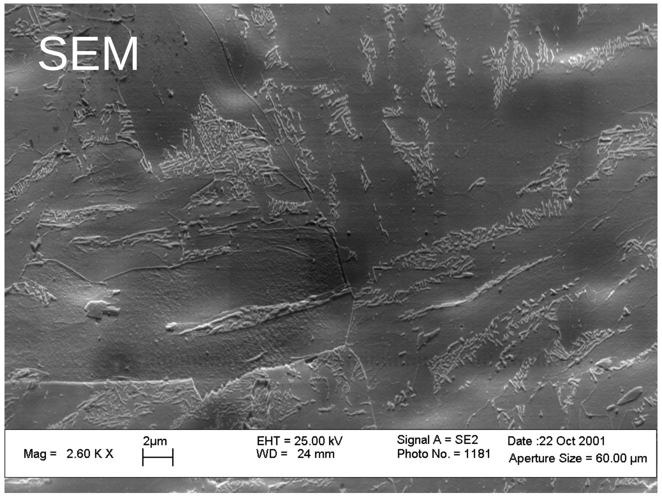
Initial configuration?

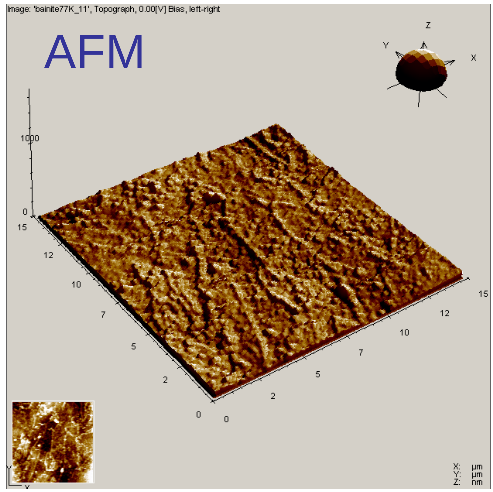
- 1- Simulation volume geometry?
- 2- Loading conditions at lath scale?
- 3- Initial dislocation sources?



Single lath

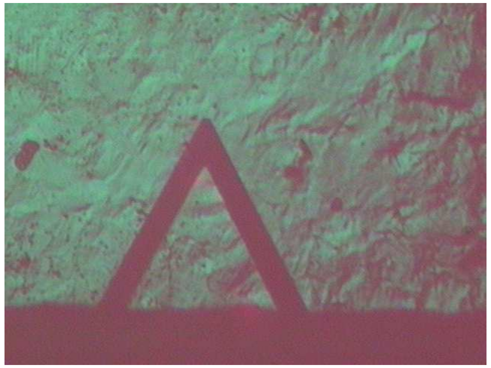


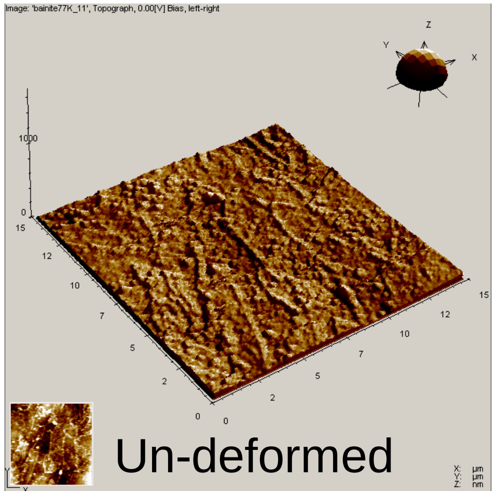


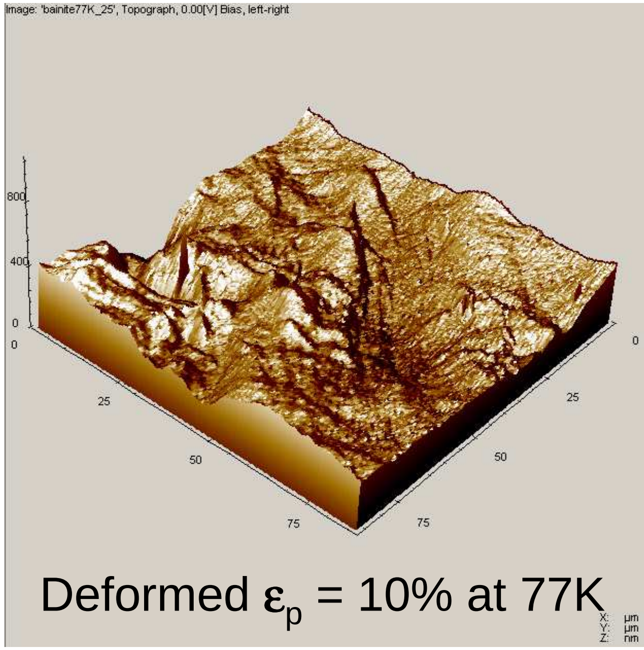


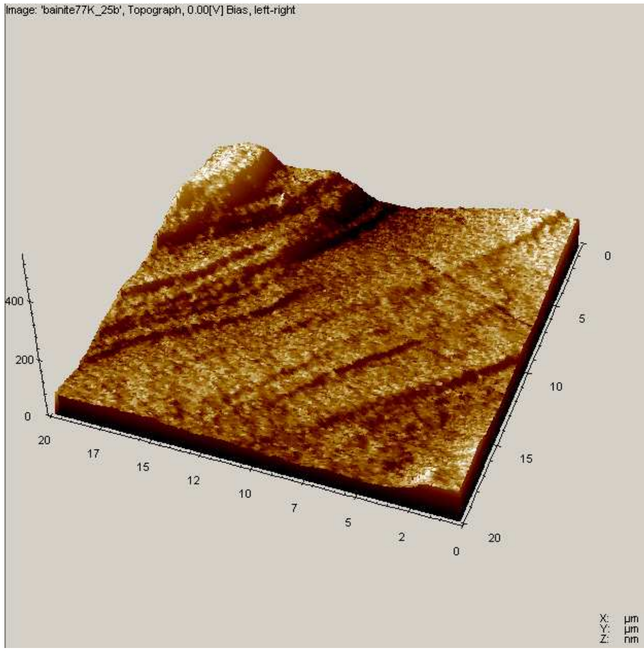
Undeformed RPV steel microstructure

2- Loading conditions at single lath scale?





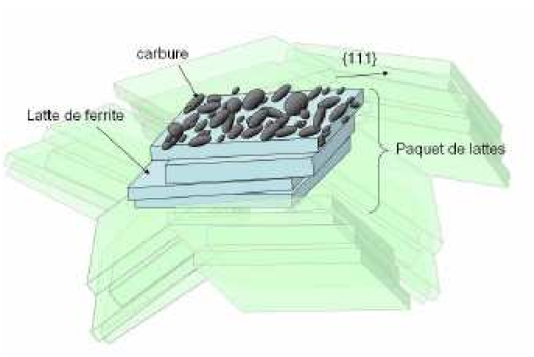


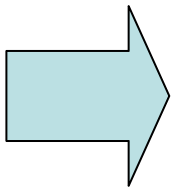


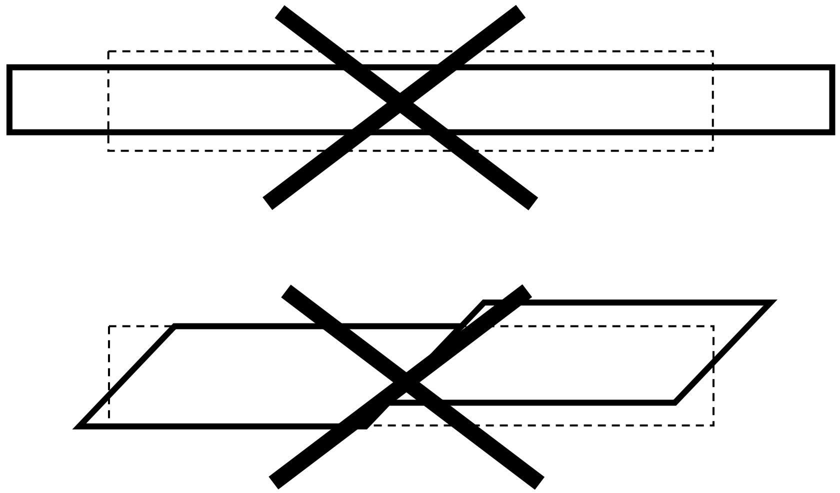
2- Loading conditions in single laths?

After tensile $\boldsymbol{\varepsilon}_p$:

Lath blocks are neither elongated nor sheared-off

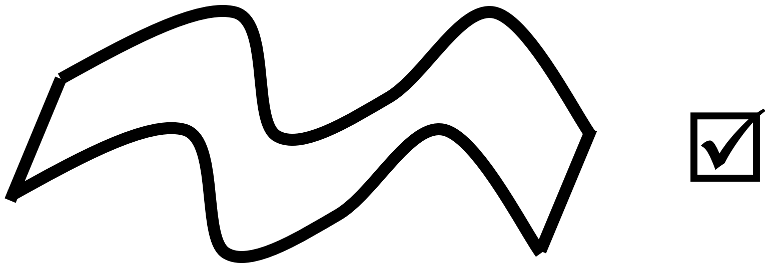






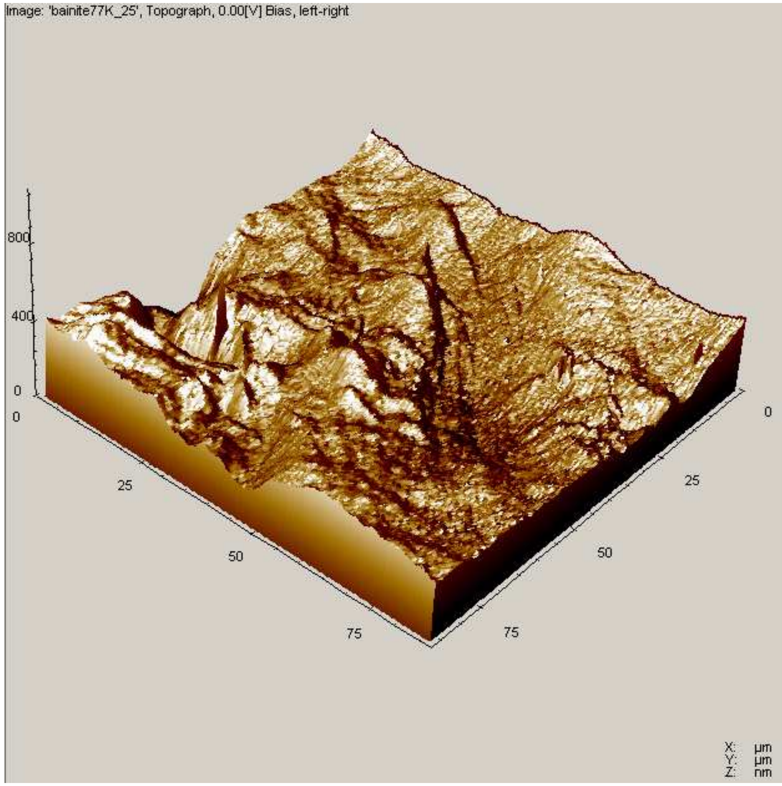
Lath blocks are folded-up (bending radius <u>smaller</u> than lath size)

Likely due to the inter-block boundary conditions (also observed in small austenitic grains)



TO SUMMARIZE…

RPV steel



≠

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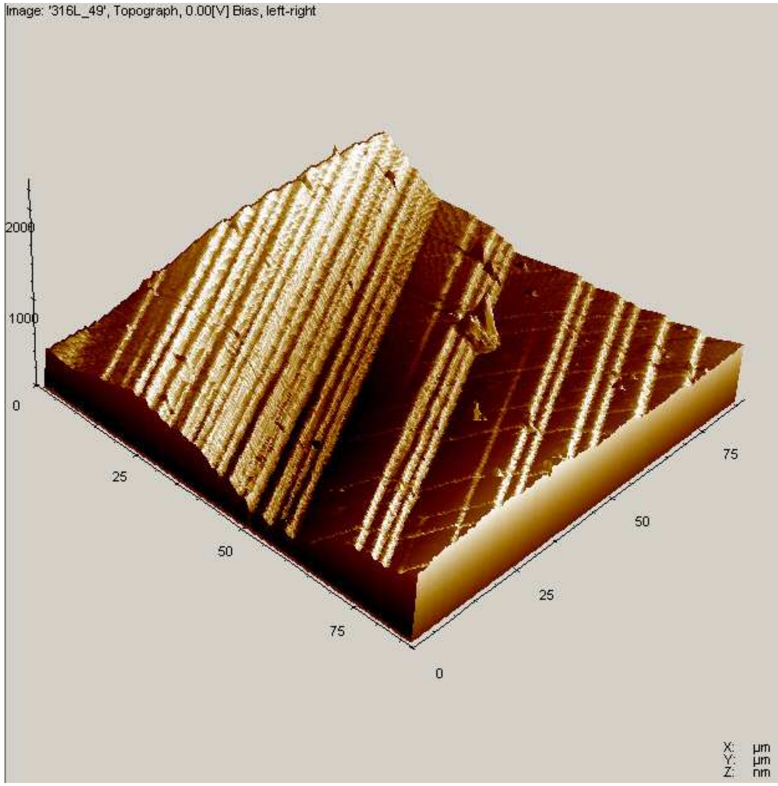
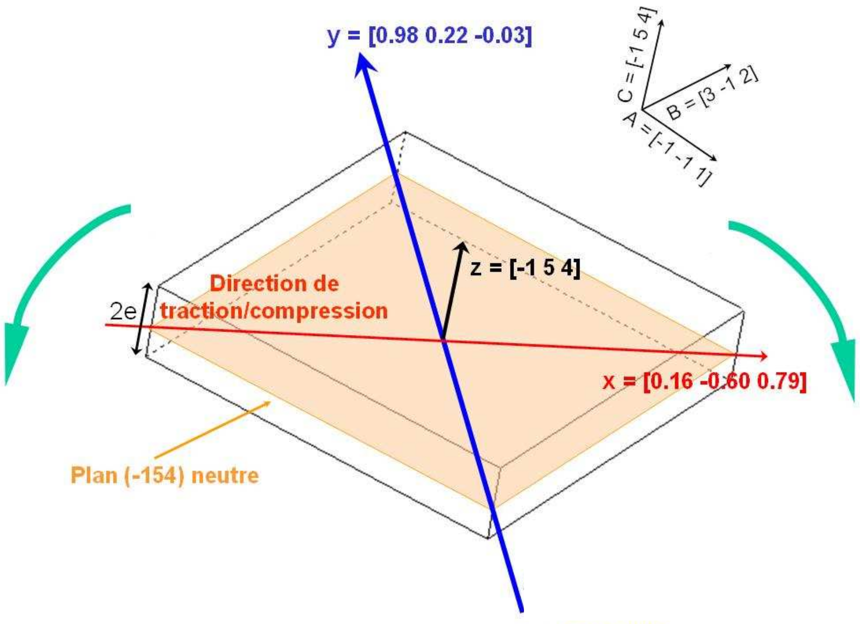
Austenite



2- Loading conditions in invidividual laths: bending

Single axis bending



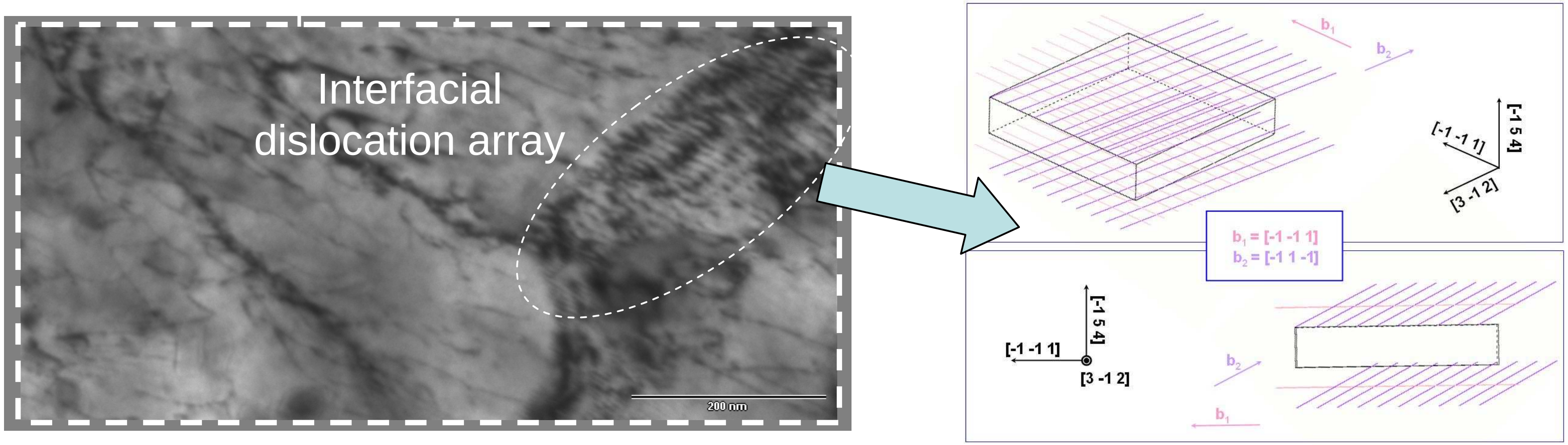
- Lath geometry → Homogeneous bending

$$\underline{\underline{\sigma}}_{app}(z) = \frac{z}{e}\begin{pmatrix} \sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- Stress vanishes in the neutral plane and becomes negative, further below

→ $\gamma = 0$

3- Initial dislocation structures



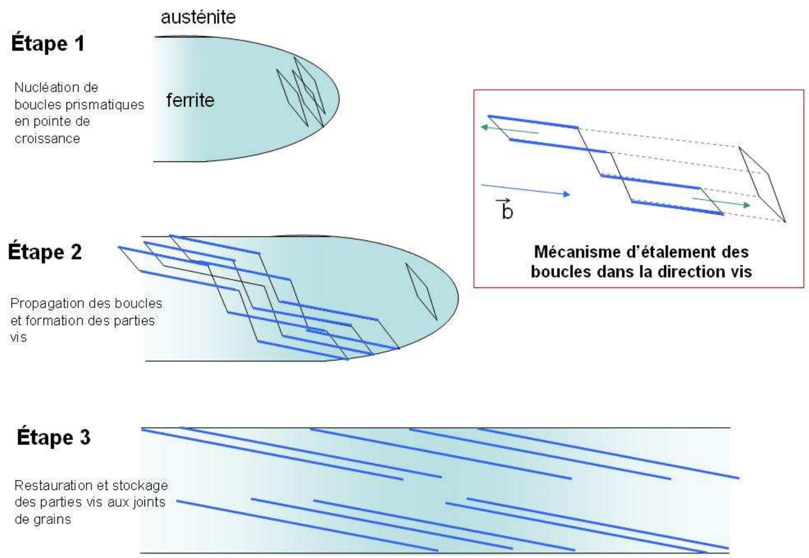
Why inter-lath sources?

- Intra-lath ρ ~ a few times 10^{14} m^{-2}
- Intra-lath L ~ 0.5-1.0 µm (lath thickness), µb/L↑↑ for FR mult.

- Inter-lath ρ > 10^{15}, with L ~ 10-20 µm

→ Very numerous SD, from one or two slip systems

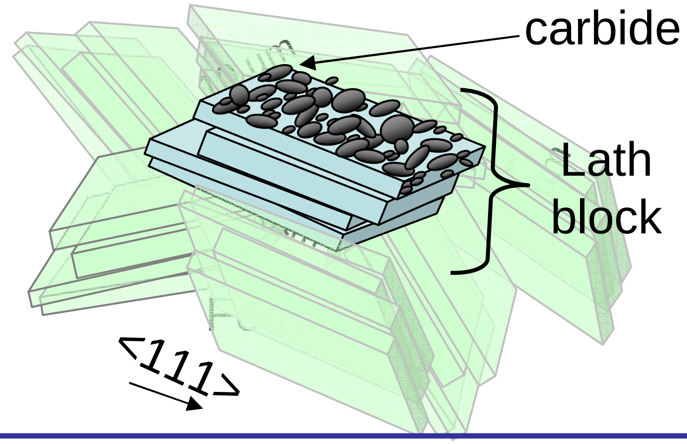
→ µb/L ↓↓



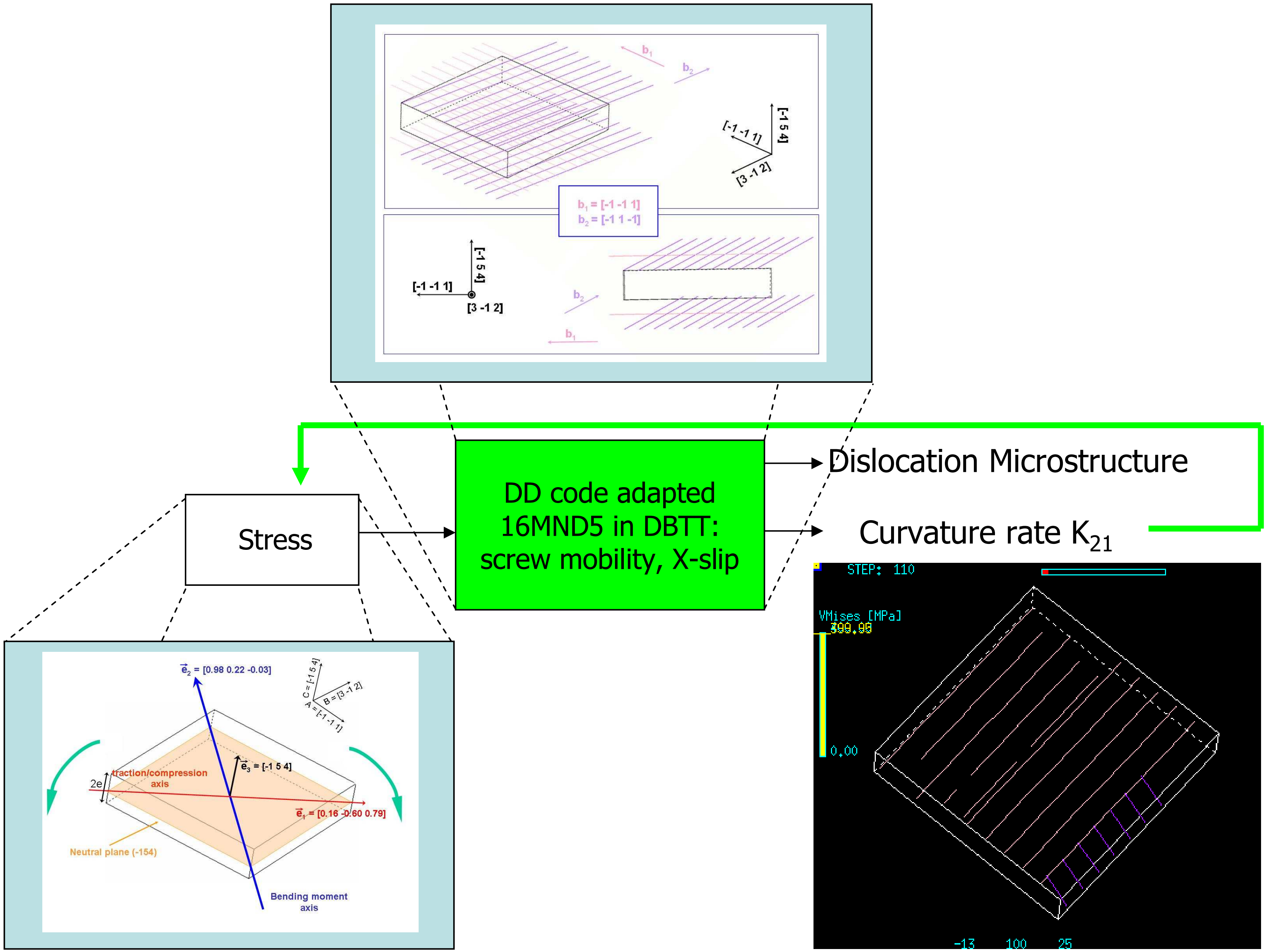
Simulation setup adapted to 16MND5 RPV steel

Initial configuration

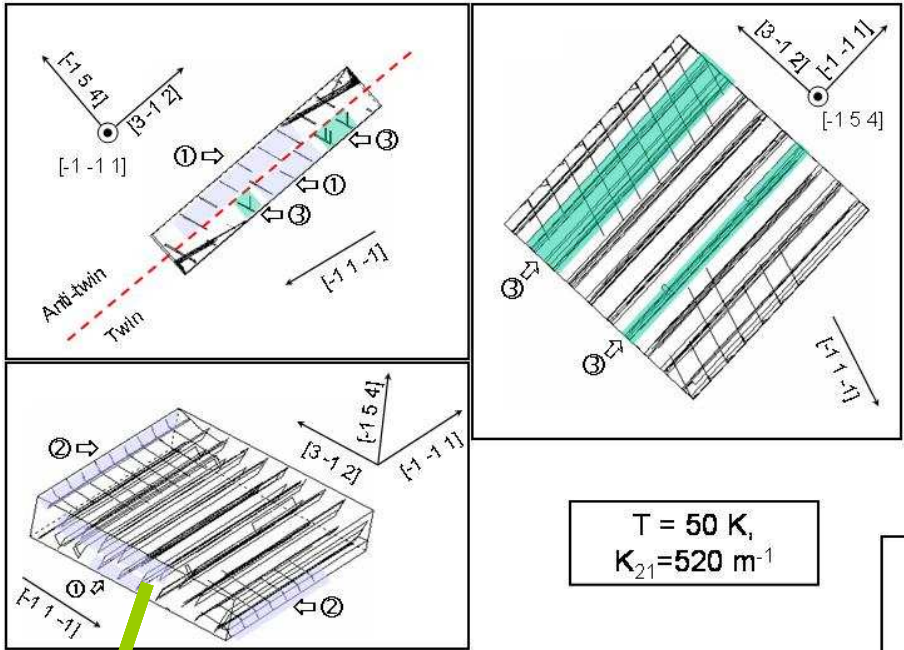
- Simulation volume geometry: single lath
- Loading conditions: single axis bending
- Initial dislocation sources: inter-lath screws



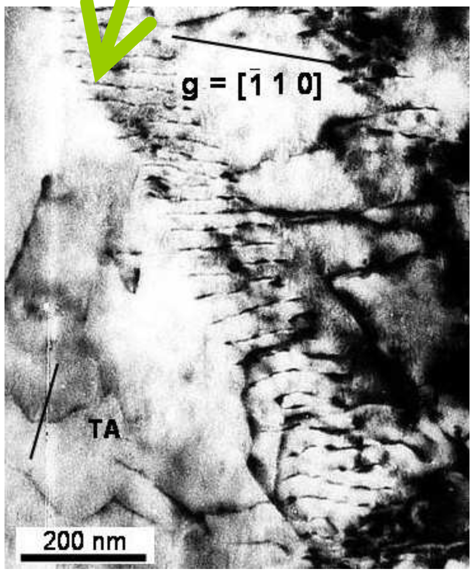
DD simulations adapted to 16MND5 RPV steel



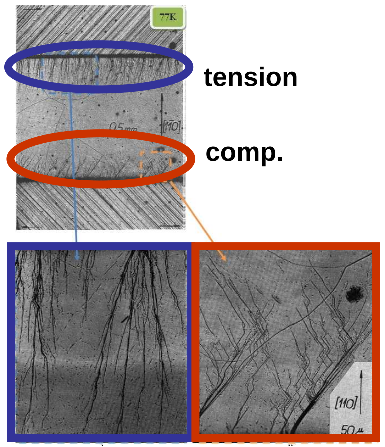
DD simulation results VS dislocation structures in deformed RPV steel



T = 50 K,
K_{21}=520 m^{-1}

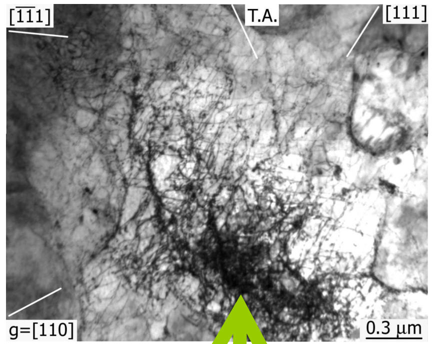


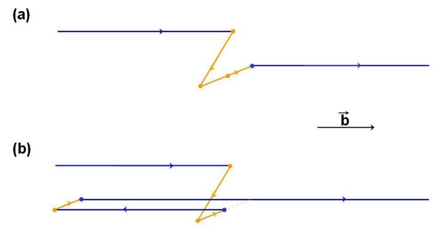
Signature of inter-lath SD sources



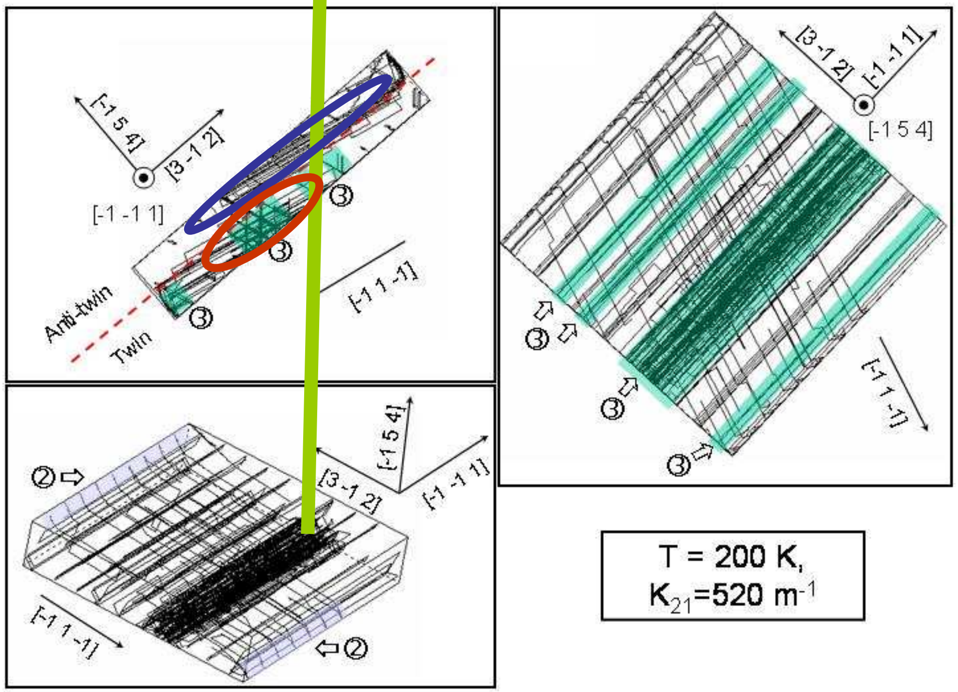
Signature of twin/anti-twin CS asymetry

Acta Materialia 56, 5466-5476, 2008





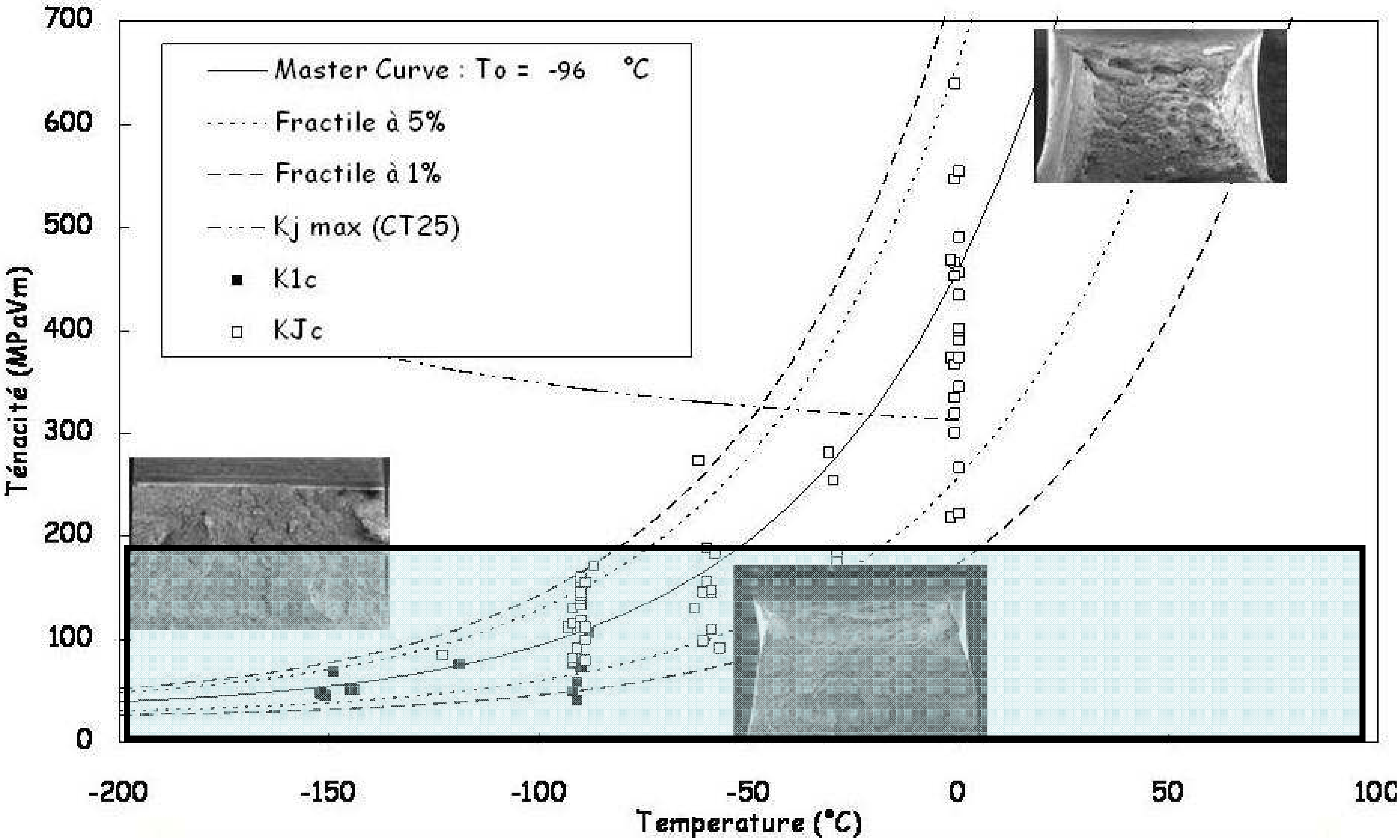
Signature of CS: wandering sources



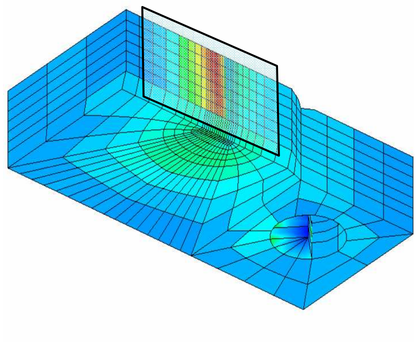
T = 200 K,
K_{21}=520 m^{-1}

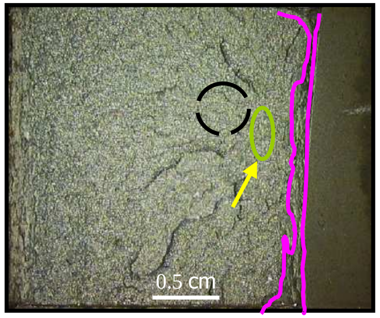
Acta Metallurgica, Vol. 11, 1963

Dislocation structures and cleavage initiation ??

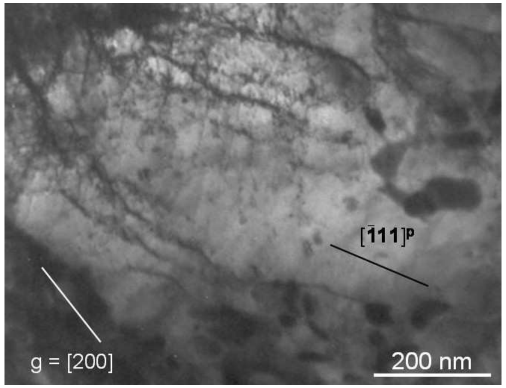


DD simulation results: internal stress evolutions

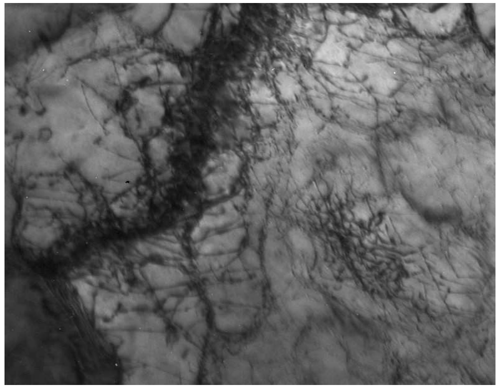




T = 50K

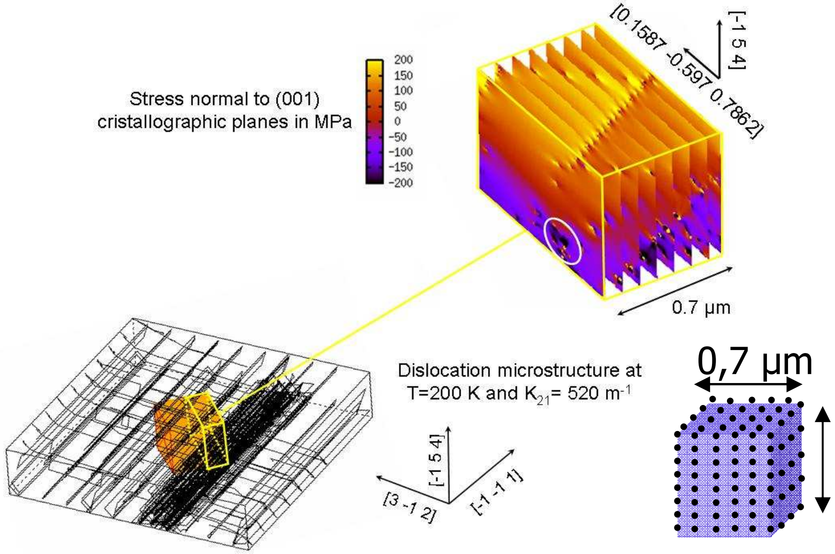


T = 200K



- **Dislocation structure: T° dependent**
- **Possible contribution of their long-range stress, on cleavage initiation?**

DD analysis of dislocation-induced internal stresses in RPV steel single lath:



Analysis volume:

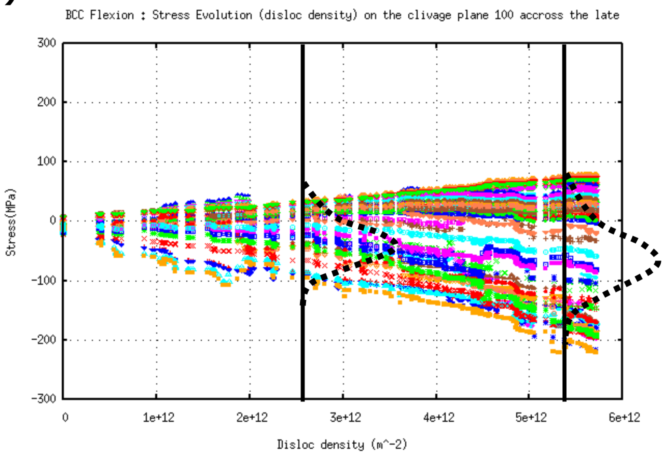
10^6 points

Evolution of intra-lath stress projectged in {100} cleavage planes

Total stress σ_{nn} (100) = $\sigma_d + \sigma_{app}$

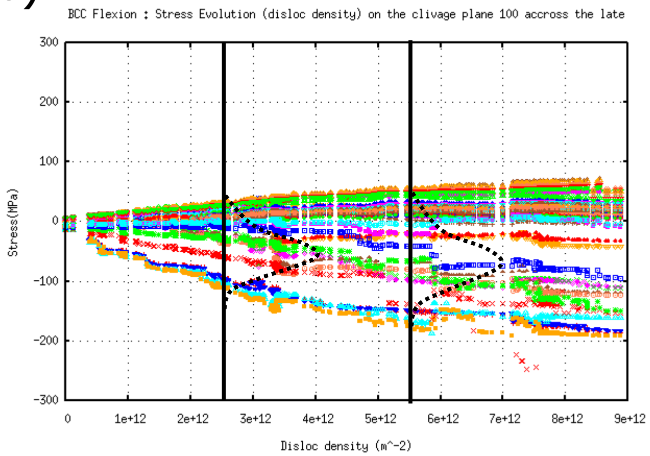
T = 50K

(100)



T = 200K

(100)

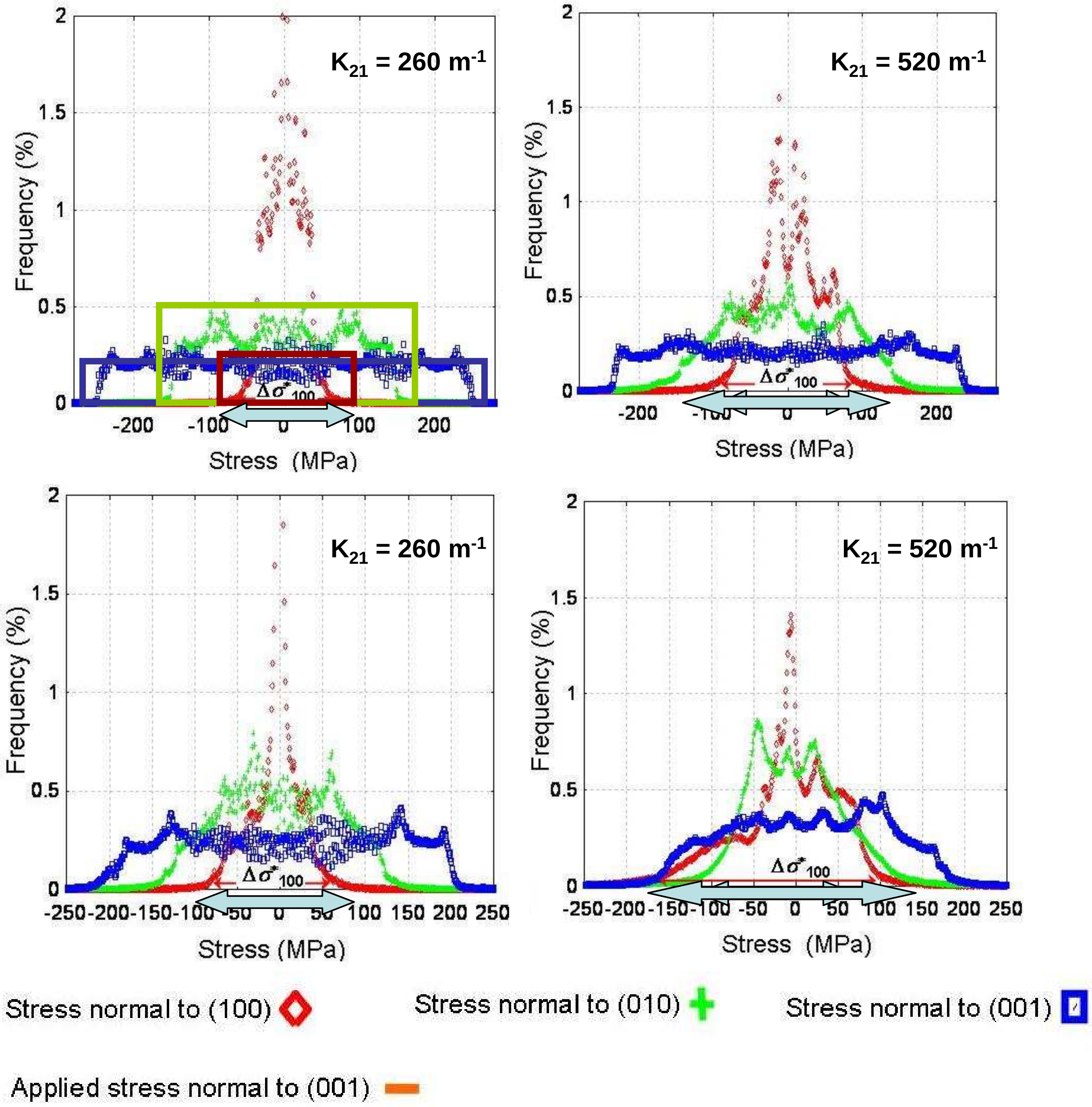


- ☞ **T° dependent evolutions of the [100] cleavage stress di stributions**
- ☞ **Max stress increases with decreasing T° (compatible evo lution of macro critical ceavage stress σ_u(T))**

T = 200K

$\sigma_{nn} = \sigma_d + \sigma_{app}$

T = 50K



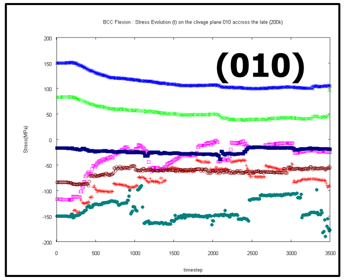
DD simulations of plastic deformation of RPV steel: internal stress evolutions

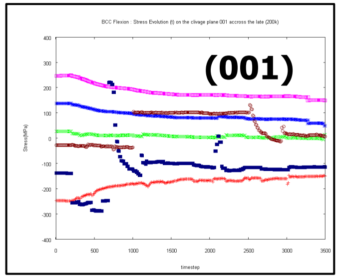
- In (010) & (001) cleavage planes

Maximum stress decrease with K_{21} ↑

➢ Efficient plastic relaxation

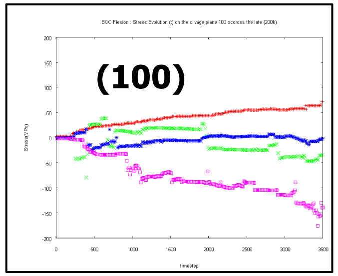
➢ Planes NOT prone to cleavage





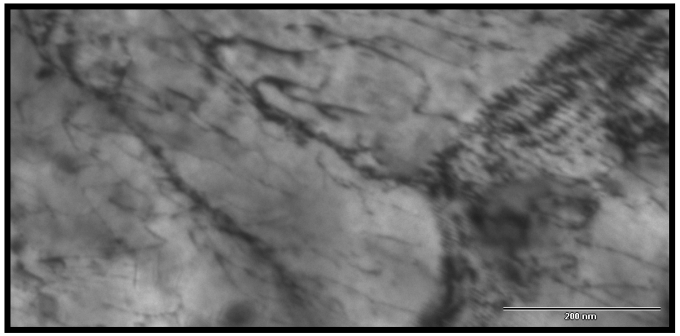
- Maximum stress in (100) planes, increase with K_{21} ↑

- Prone to cleavage



Selective loading of (100) plane → limited set of slip systems w/r loading direction

→ Limitation associated with lath growth during the initial bainitic transformation

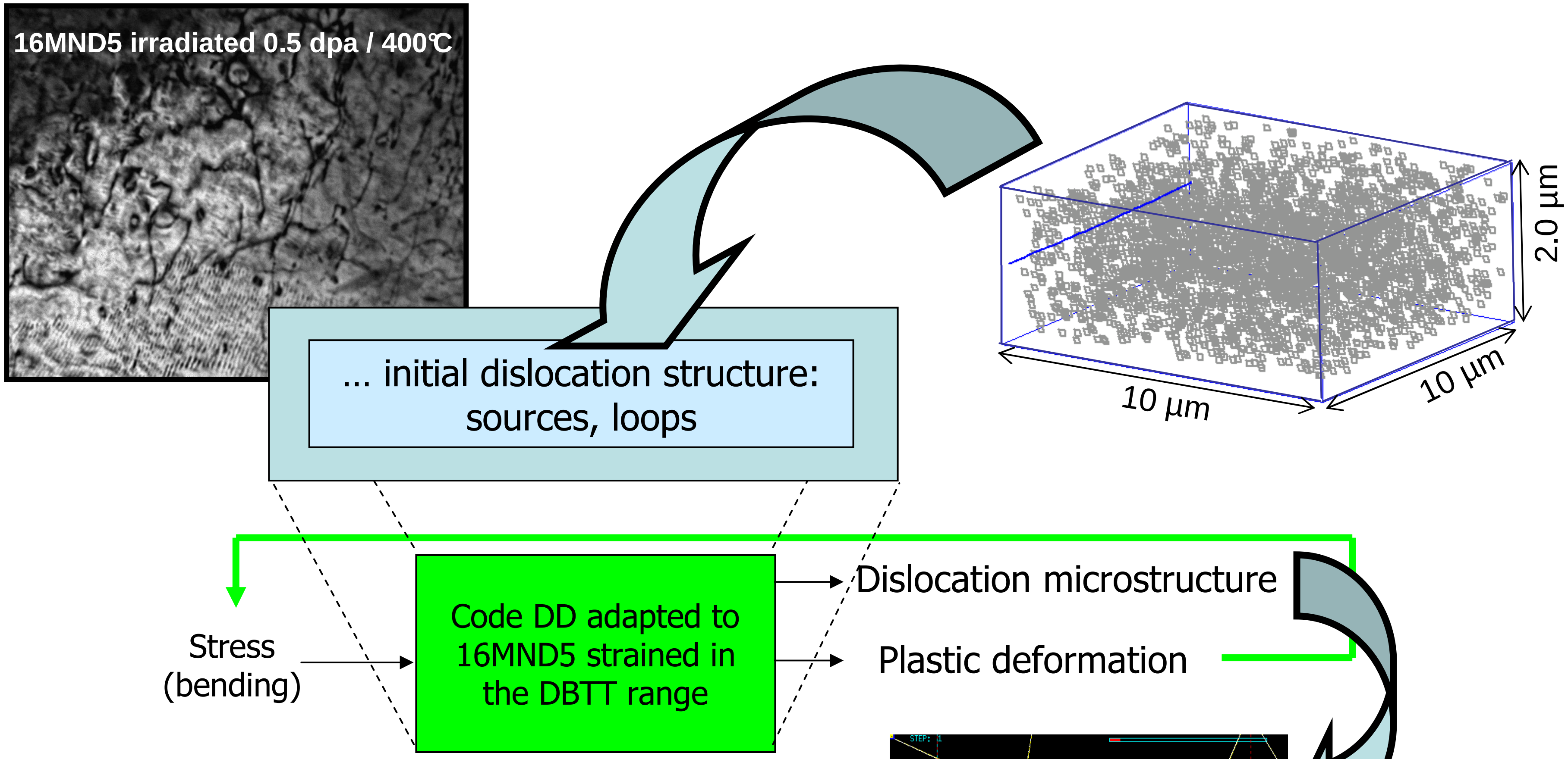


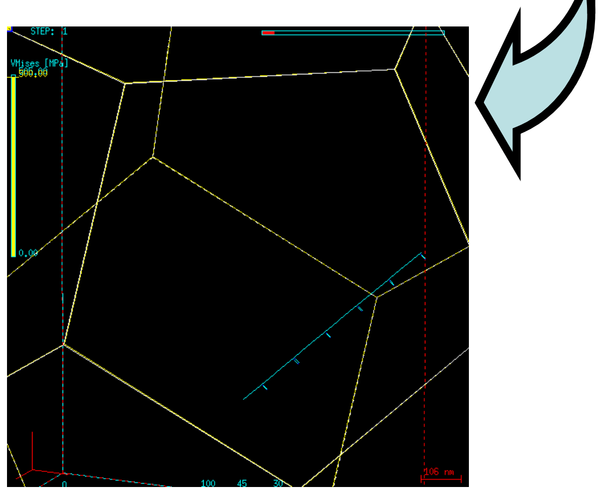
Selective loading effect (on (100) planes) more pronounced at decreasing T°

↓

Possible contribution to T°dependance of material thoughness

Perspective: PERFORM60 WP1-2 project





Expected model predictions: hardening and strain localisation

THE END