The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
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IAEA
International Atomic Energy Agency

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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

Dislocation dynamics simulations of post-irradiation plastic deformation in austenitic stainless steels

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12 – 23 April 2010
Miramare – Trieste, Italy

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DEN/DMN/SRMA

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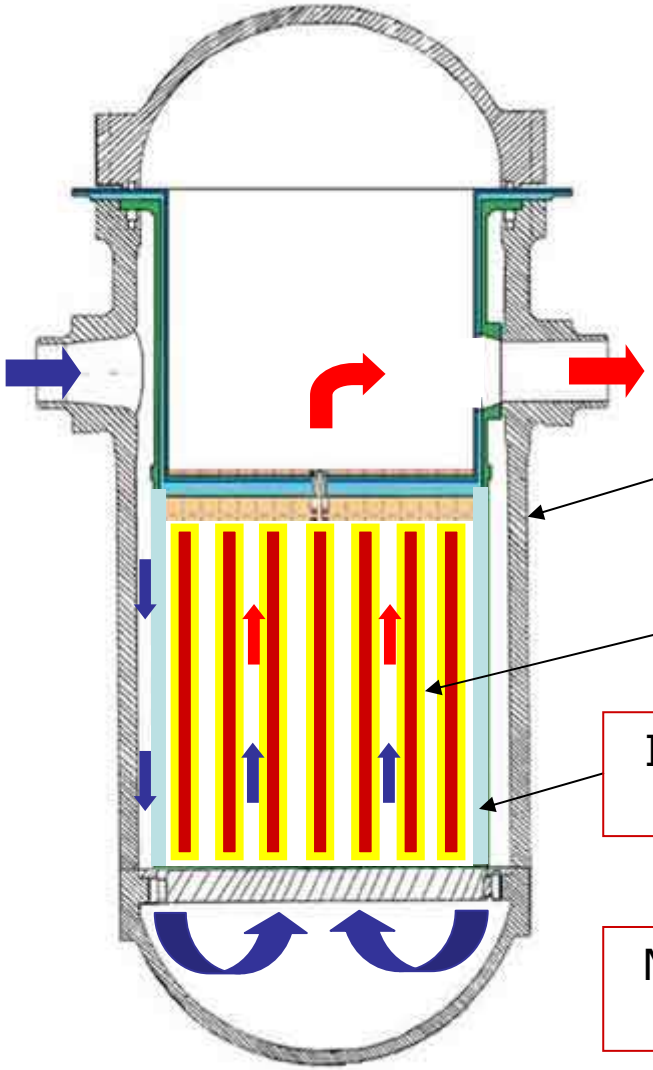
DD simulations of post-irradiation plastic deformation in austenitic steels

Irradiation-induced modifications in different metallic alloys

RPV in Pressurized Water Reators



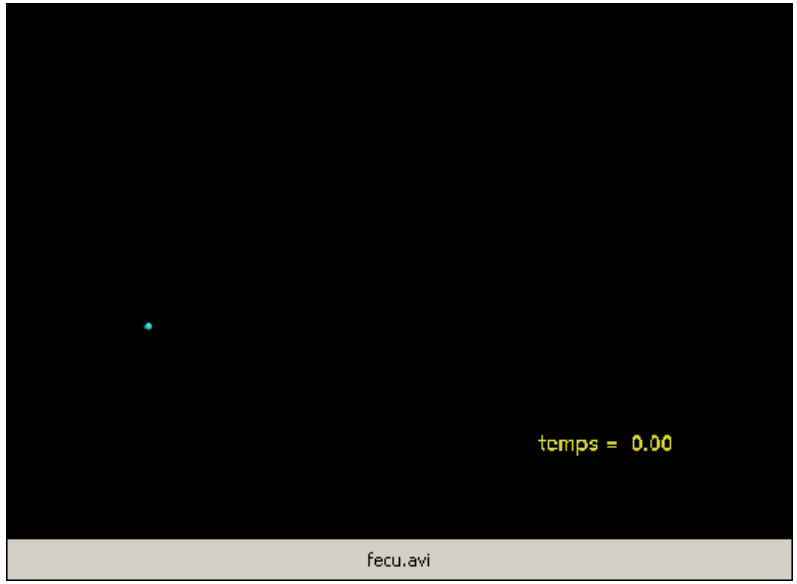
Ferritic RPV steel walls

Zircalloy cladding
Uranium fuel

Internal Structures in austenitic steels

Neutrons irradiations
300-350°C

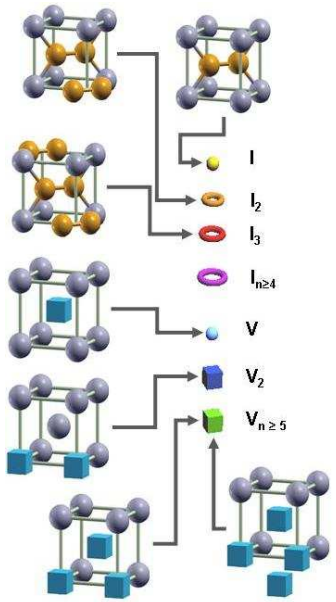
What happen, during irradiation of metals?

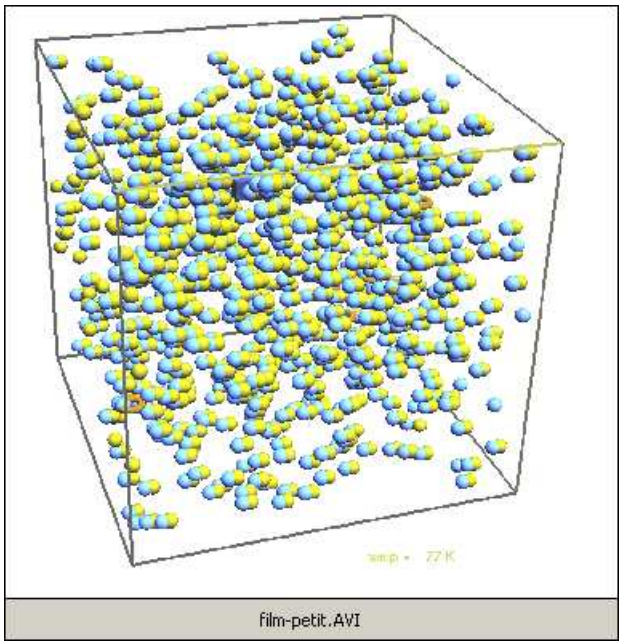


Short term evolutions:
collision cascades (MD)

Courtesy CEA/SRMP

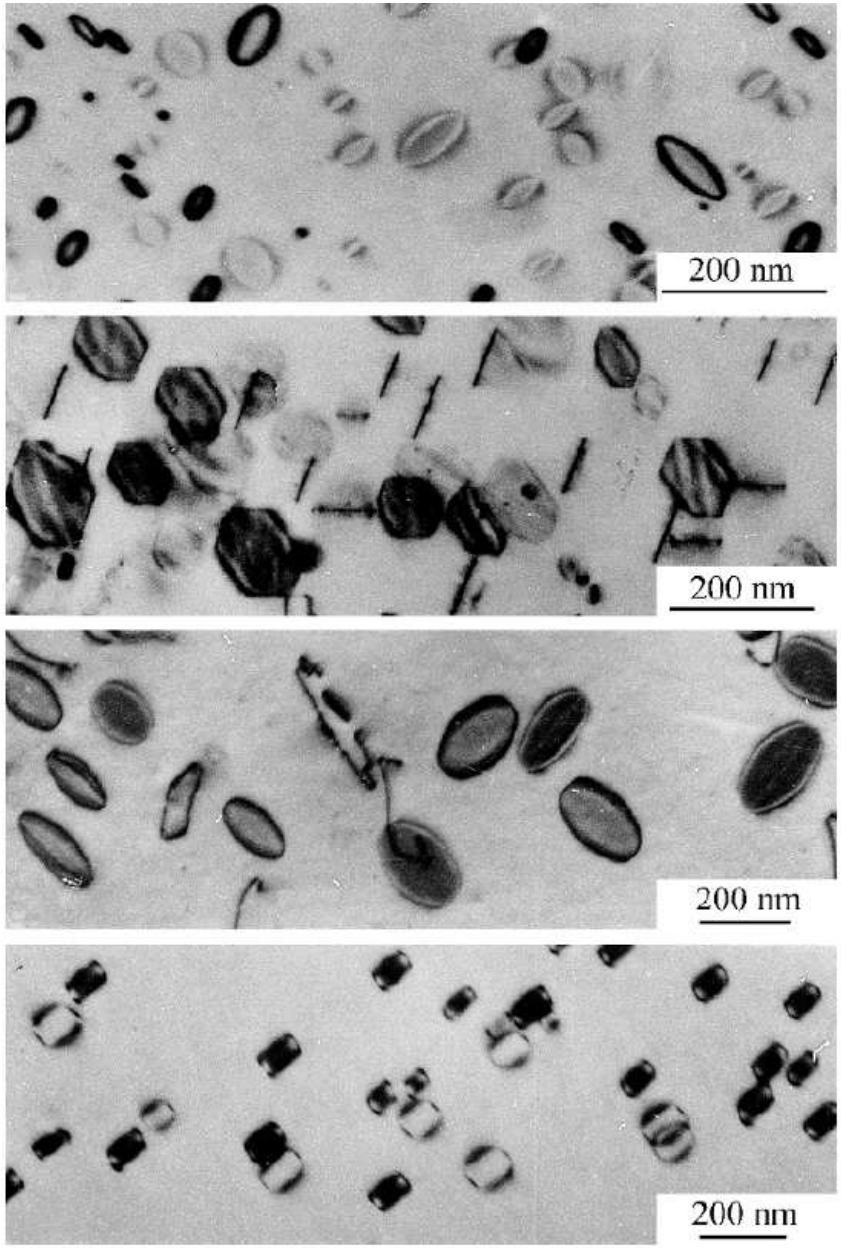
Long term evolutions: diffusion, germination, growth of point defect cluster (KMC)





Courtesy CEA/SRMP

Irradiation defect loops in various metals



Al

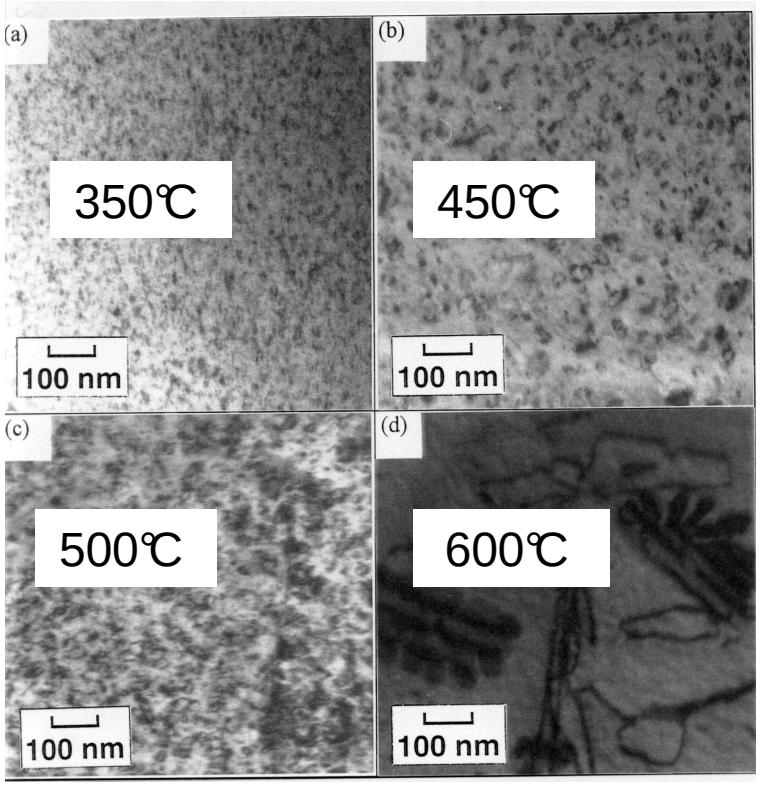
Cu

Ni

Fe

Irradiation 10 dpa
(Kiritani 1994)

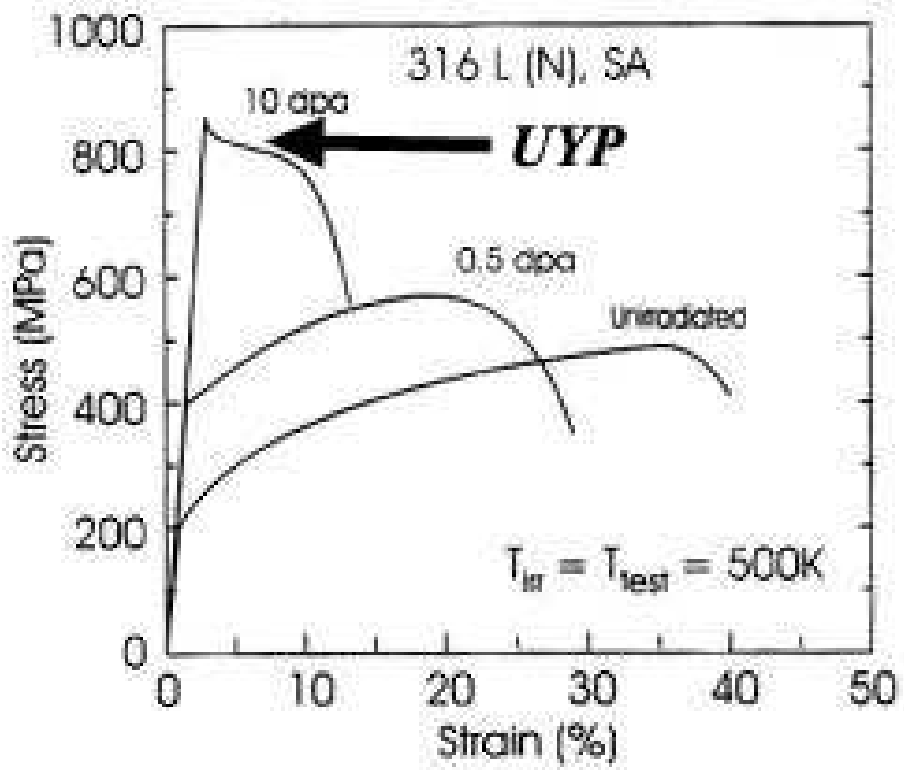
Austenitic steel, 3 dpa



Consequence of loops in tensile properties of metals

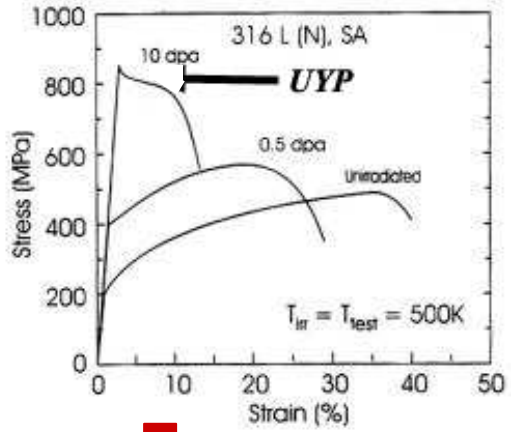
Irradiated Austenitic Stainless Steels

Dose dependent reduction of ductility
Hardening (< 3 dpa)
Hardening/Softening instability(> 3 dpa)



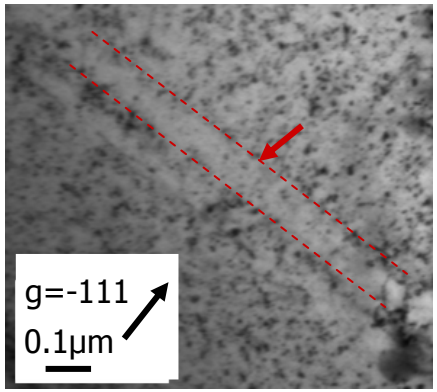
Post irradiation plasticity: a multi-scale phenomena

Irradiated Austenitic Stainless Steels



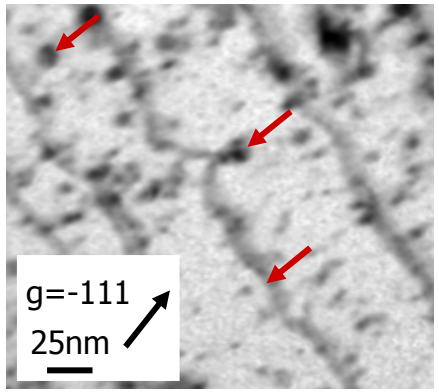
- Millimeter

Dose dependent reduction of ductility
Hardening
Hardening/Softening (> 3 dpa)



- Micrometer

Strain localisation into clear bands



- Nanometer

Interstitial Frank loops
Dislocation/loop interactions

- Q1

How works the observed strain localisation mechanisms?

- Q2

The reason of the hardening/softening observed at high dose (> 3 dpa) ?

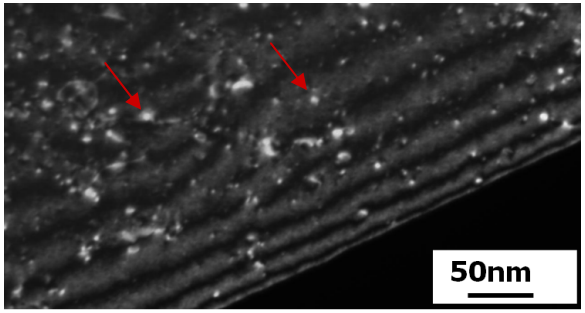
- Approach

Step1: Observation
Step2: Analysis with the help of simulations

Step1- Plastic deformation after irradiation: observations

Goal: Accurate information on dislocation/defect cluster interactions

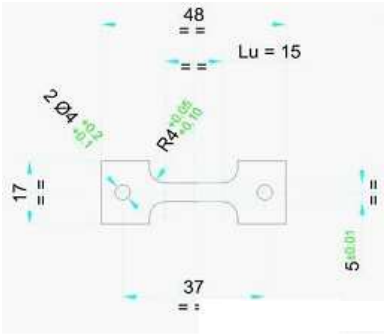
Irradiations:
T_{irr} = 350°C
Ions Xe 95 MeV
2-5 dpa - 7 µm thick

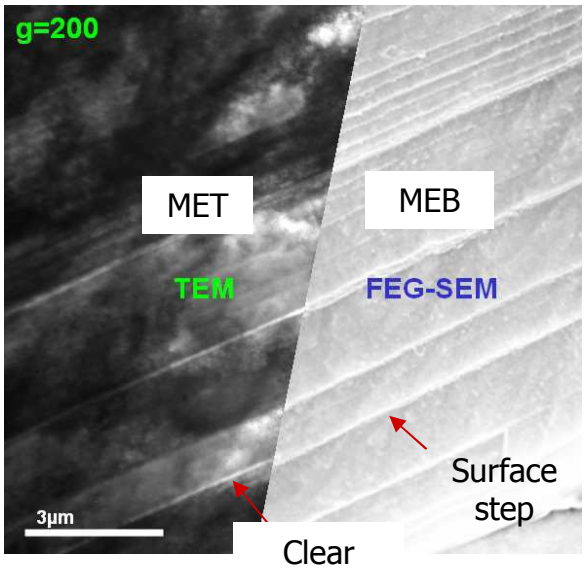


Frank loops
Mean diameter ~ 6-10 nm
Density ~ 10^{22} m^{-3}
Representative of saturation density

Foil preparation: back-side eletrocpolishing

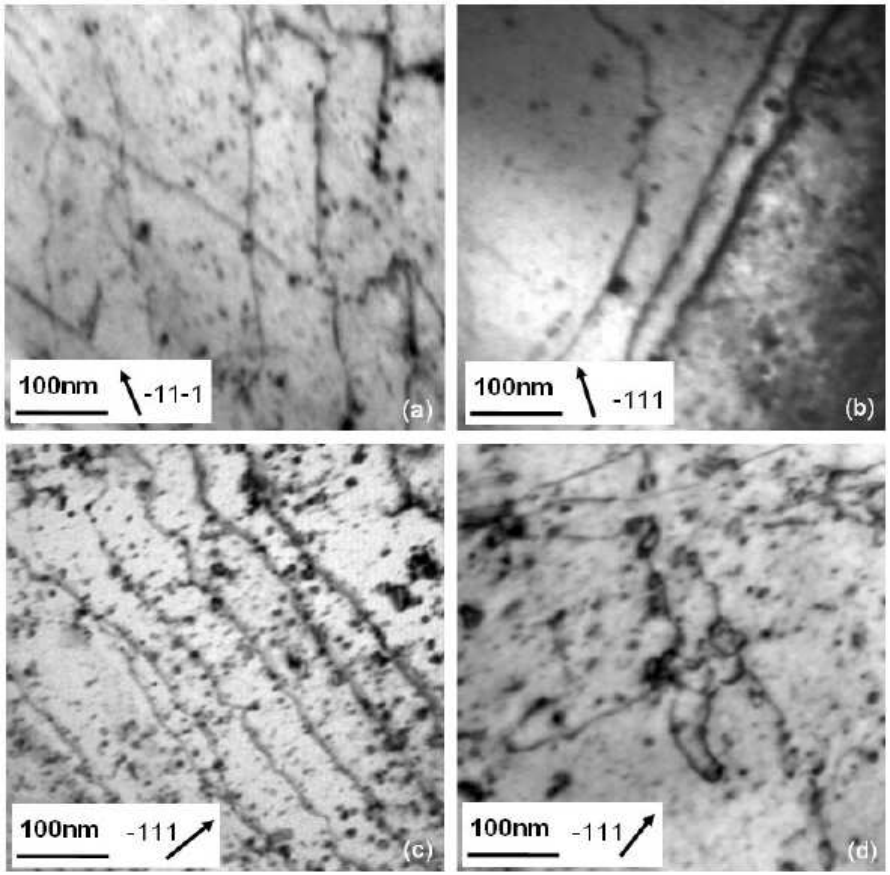
Deformation:
Uni-axial Tension
T_{def} =350°C
ε = 8%
ε = 10^{-4} s^{-1}





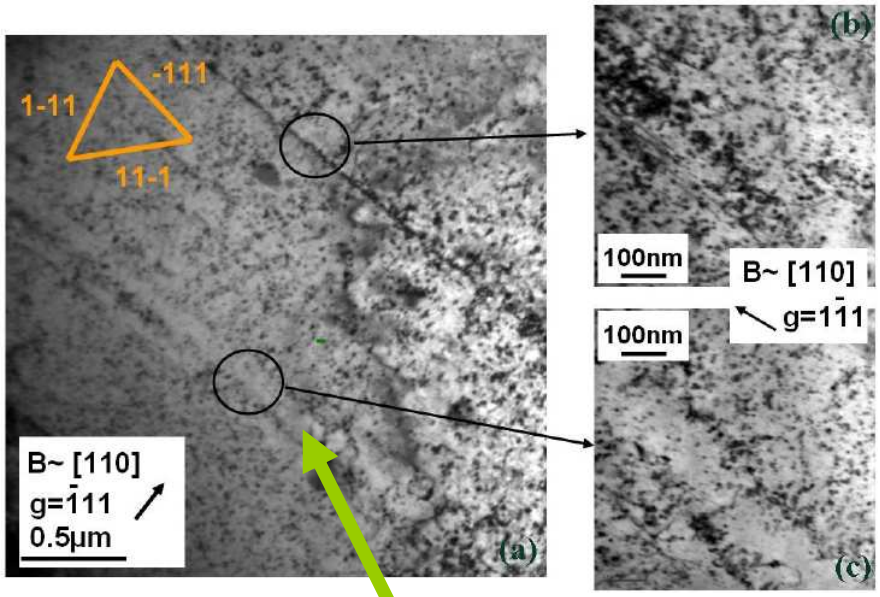
Strain localisation

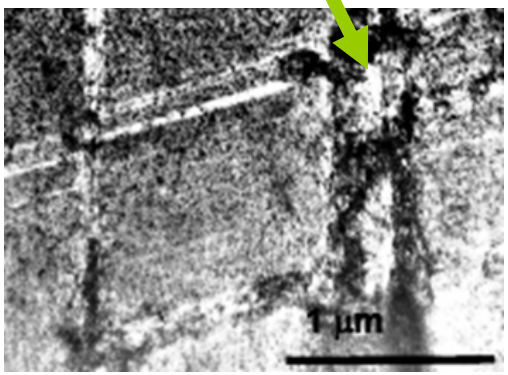
Plastic deformation after irradiation: observations



Mostly screw type pile-ups

Jog size ~ Irradiation loop size





(K. Farrell ORNL)

Neutrons Irradiations (~ cm)

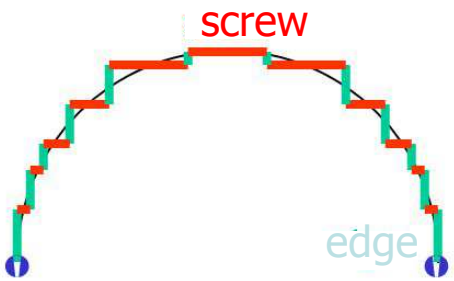
Dislocation dynamics

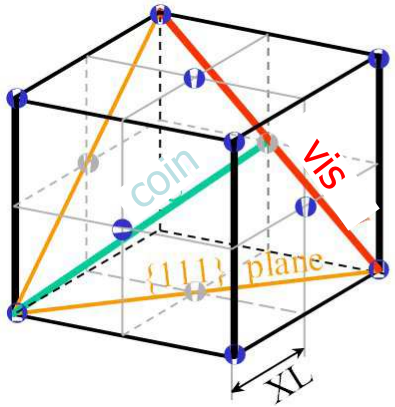
Dislocation model

12 slip systems for fcc crystals

Edge and screw segments

Discrete lattice





Lattice spacing and time step

Nanometric loops

DD	« micro »	« nano »
XL	10 b	0.08 b
dt	5. 10^{-10} s	5. 10^{-14} s

Interaction rules

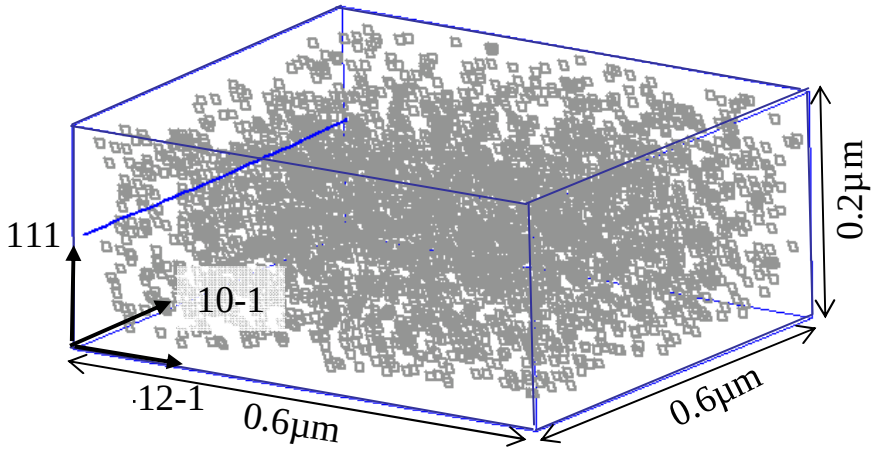
~~Cross slip~~ - Climb - ~~Obstacle~~ - Recombinaison - Jonction

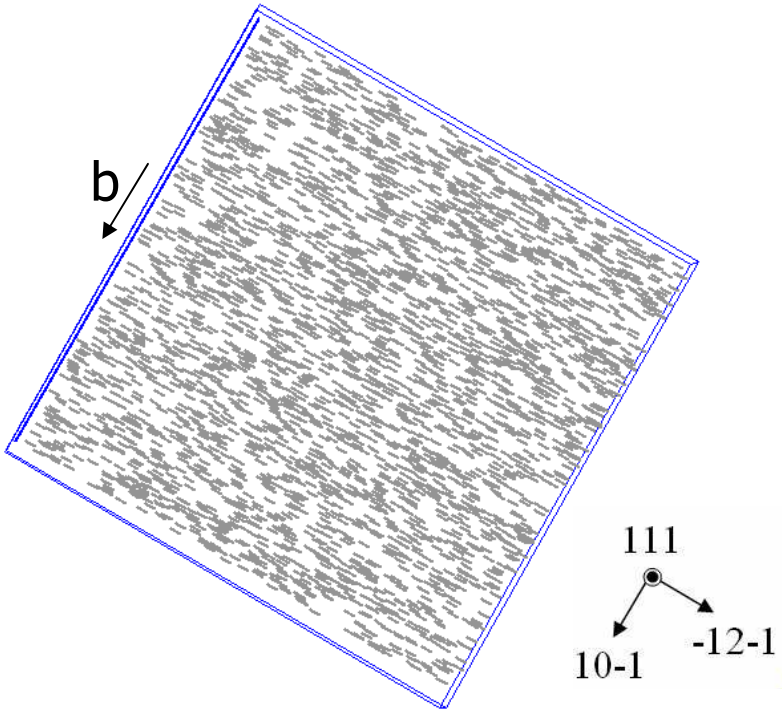
Model fcc crystal: Cu elastic parameters

Examined configuration

Frank loop population

- Random position
- D=10nm, L=50nm



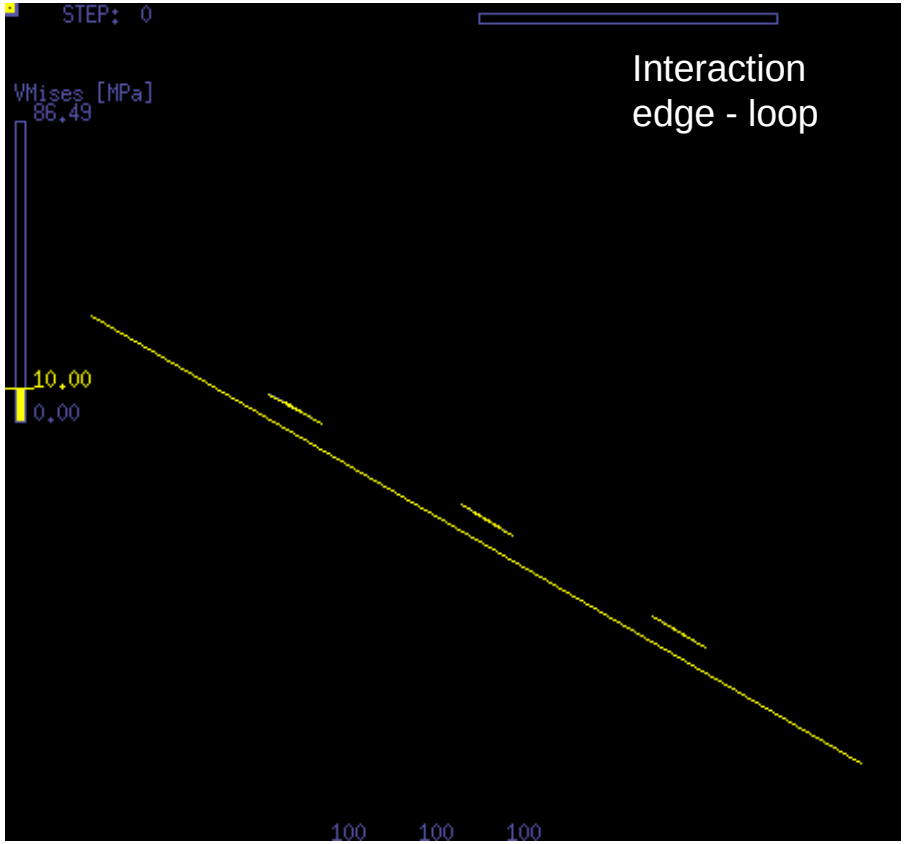


Loading conditions

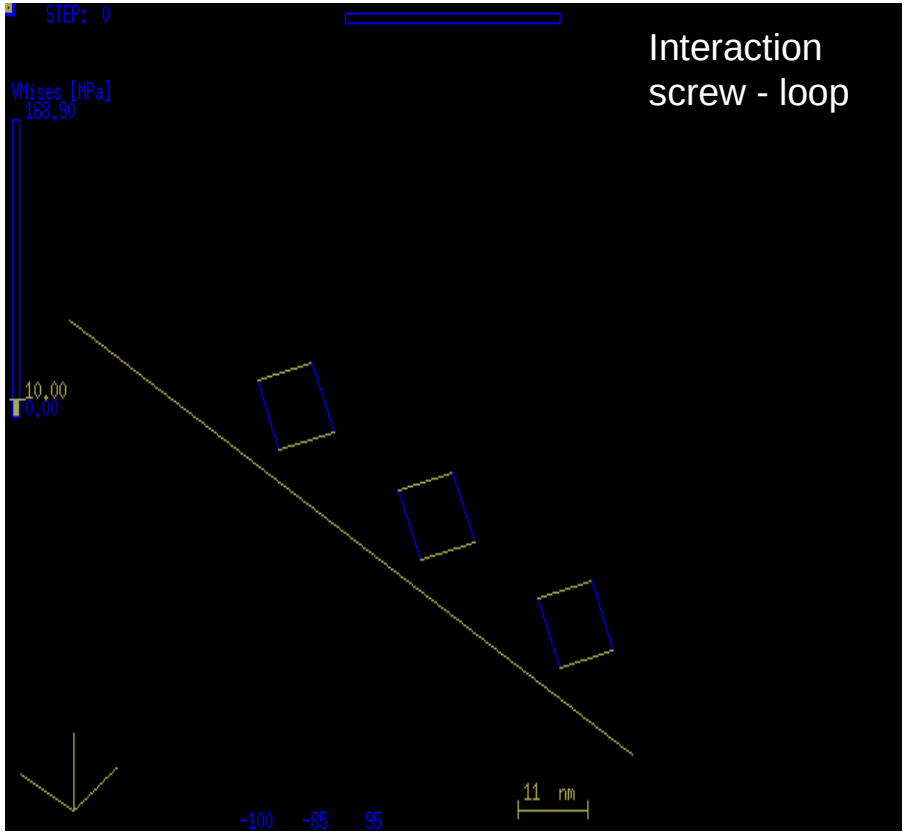
- Single slip
- $\dot{\varepsilon}$ =1.2 $10^{5}s^{-1}$

Dislocation/loop interactions

Rules come from MD simulation results



Interaction
edge - loop



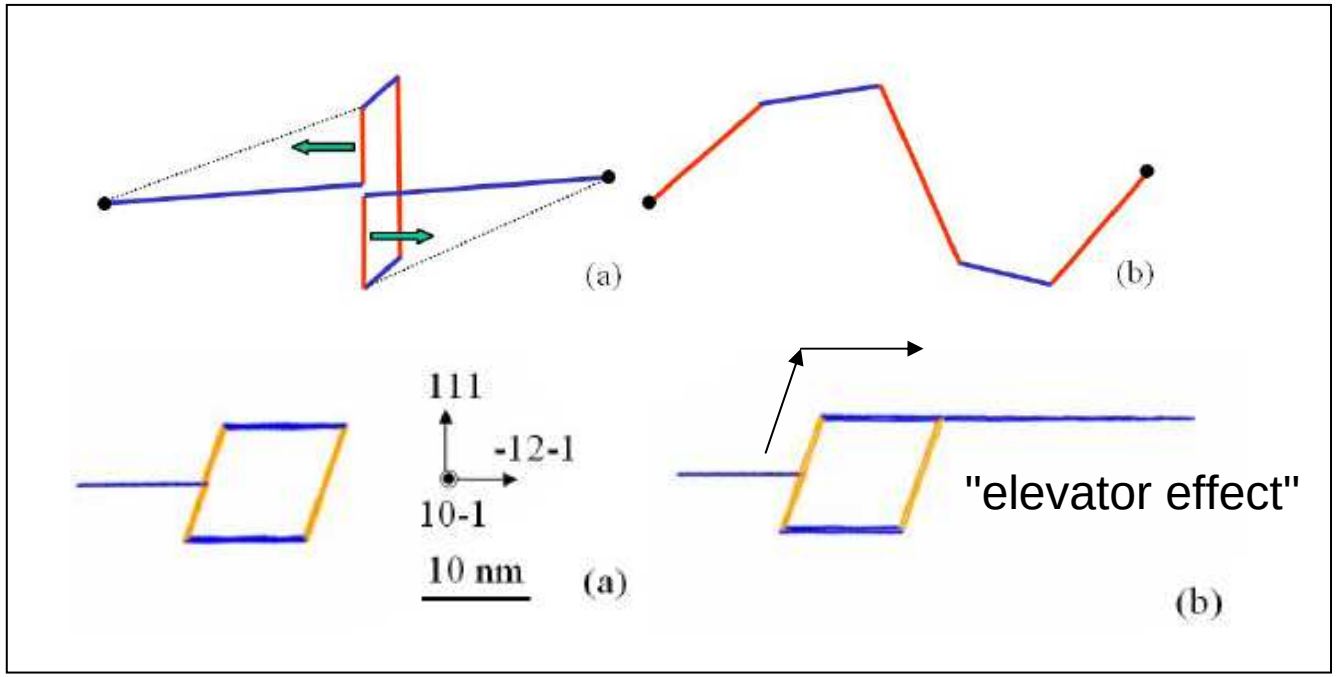
Interaction
screw - loop

Elementary dislocation/loop Interactions

Local interaction rules implemented in DD → MD simulations

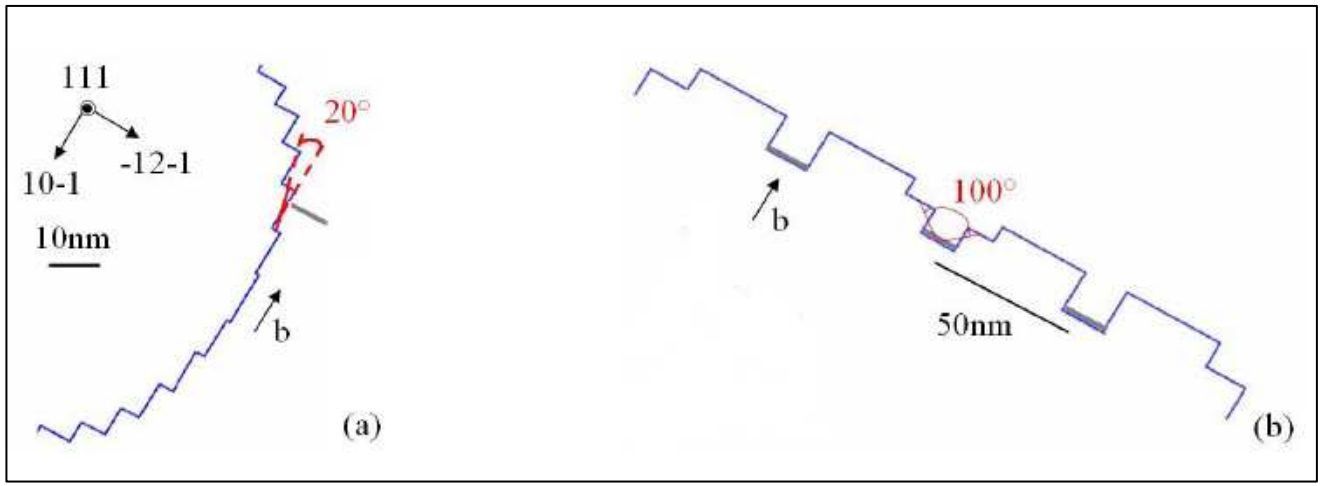
Screw/loop

σ_{crit} = 340 MPa



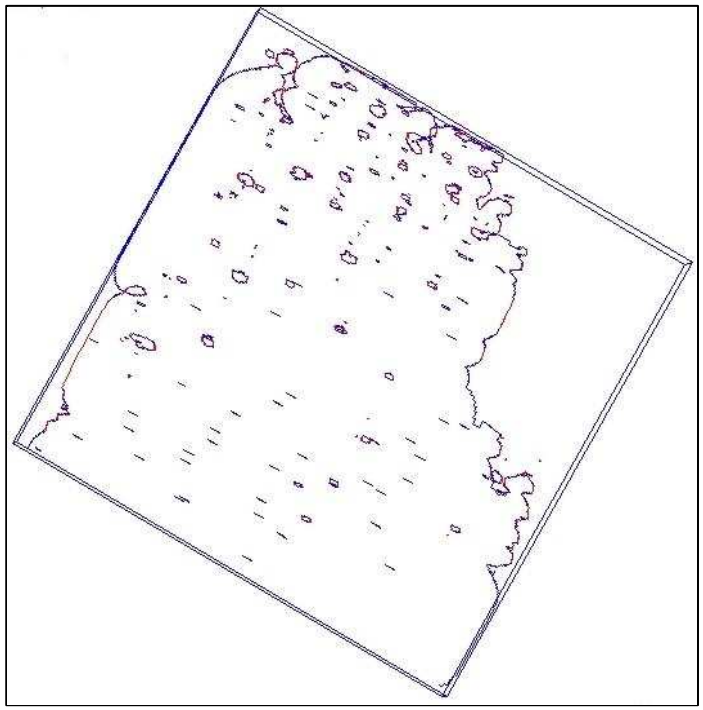
Edge/loop

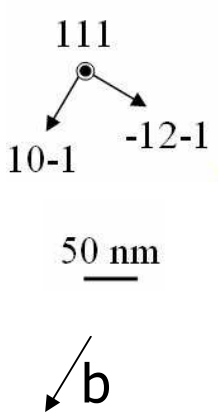
σ_{crit} = 130 MPa



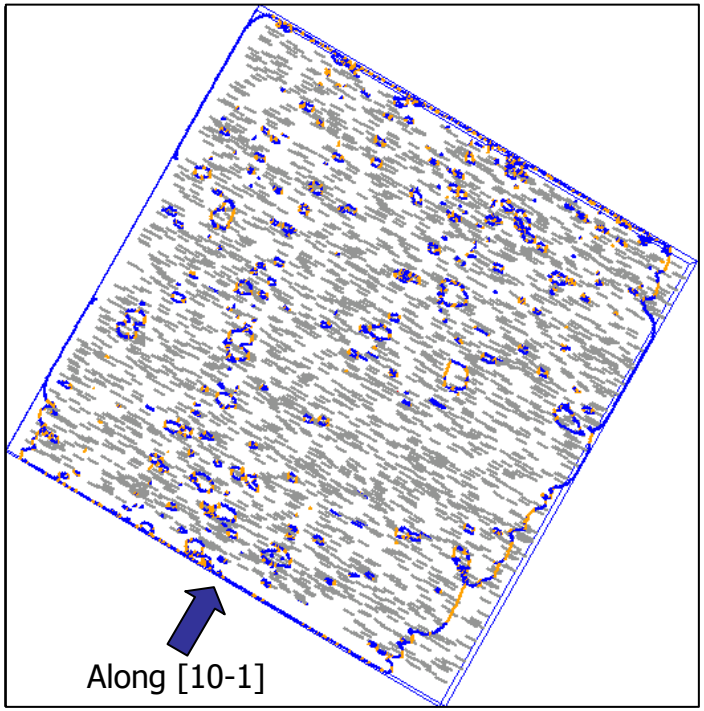
Case 1: Glide of an isolated dislocation $\tau_{nuc} >> \tau_{obst}$

Edge-type source





Screw-type source



Max. stress applied ~ 120-160MPa

Max. stress applied ~ 200-260MPa

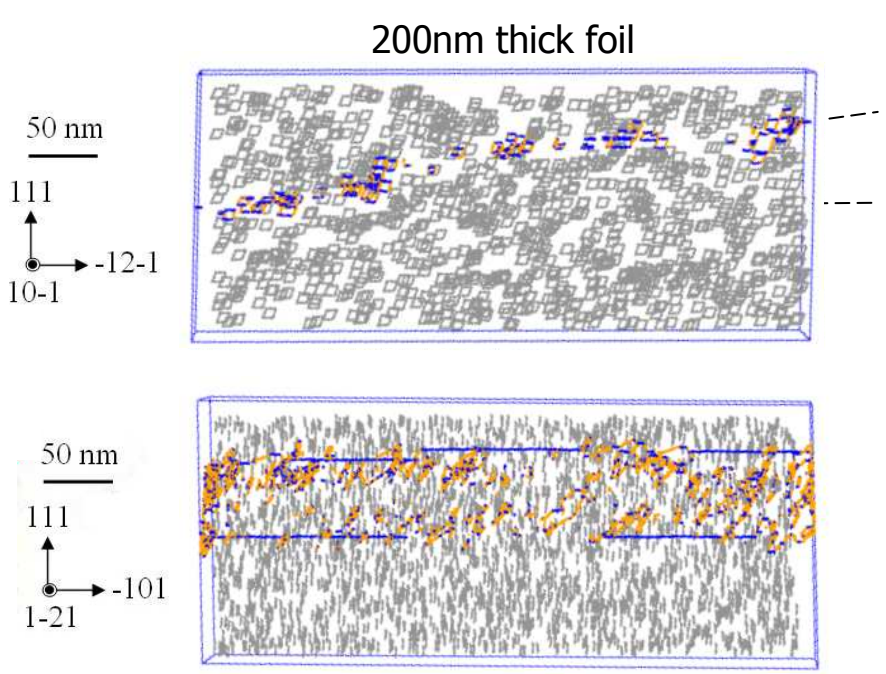
Easy shear propagation
Generation of long screw segments
Planar slip

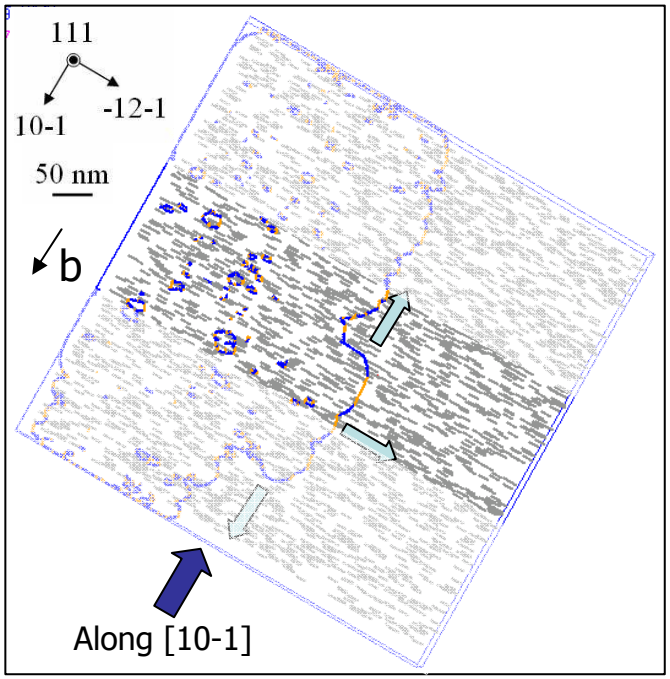
Loop unfaulting
Helix
Strong pinning

⇨ **Plasticity is controled by screw dislocations**

Case 1: Glide of an isolated dislocation $\tau_{nuc} >> \tau_{obst}$

Screw-type source





Helix unpinning → Glide plane change

⇨ **Average glide plane is tilted away from initial plane**

Activation of a screw line → Edge portions → Transport of the helix

⇨ **Partial loop cleaning**

⇨ **No clear band of finite thickness**

Case 2: Collective glide of dislocations $\tau_{nuc} < \tau_{obst}$

Screw-type source

τ_{nuc} =120MPa

τ_{obst}
- edge = 120-160MPa
- screw = 200-260MPa

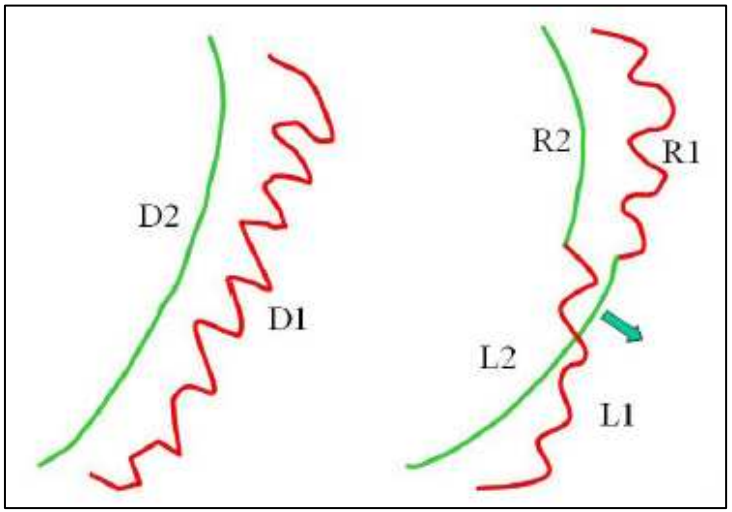
Dislocation glide with the help of *collective* effects

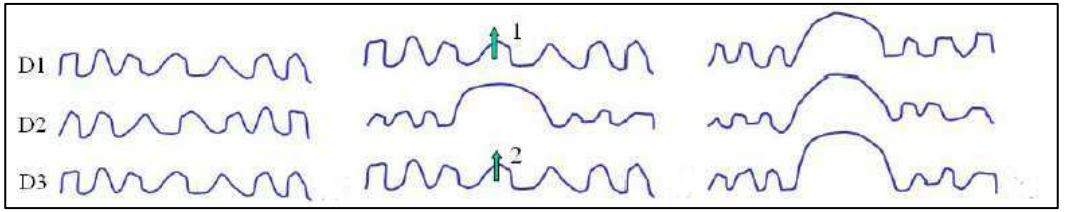
Collective effects

Dislocation pile-ups

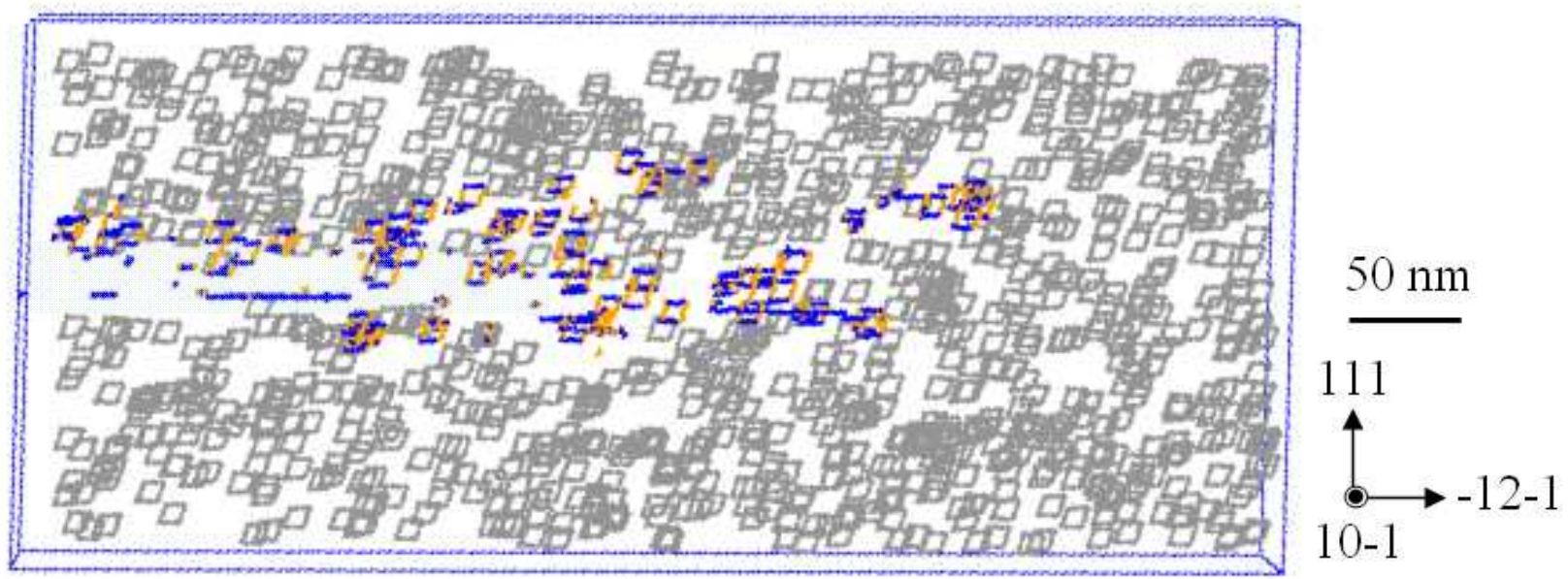
Arm exchanges

Dislocation avalanches



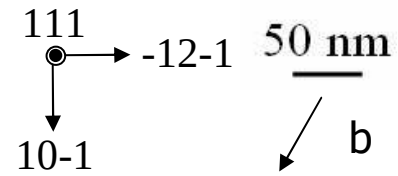


Case 2: Collective glide of dislocations $\tau_{nuc} < \tau_{obst}$

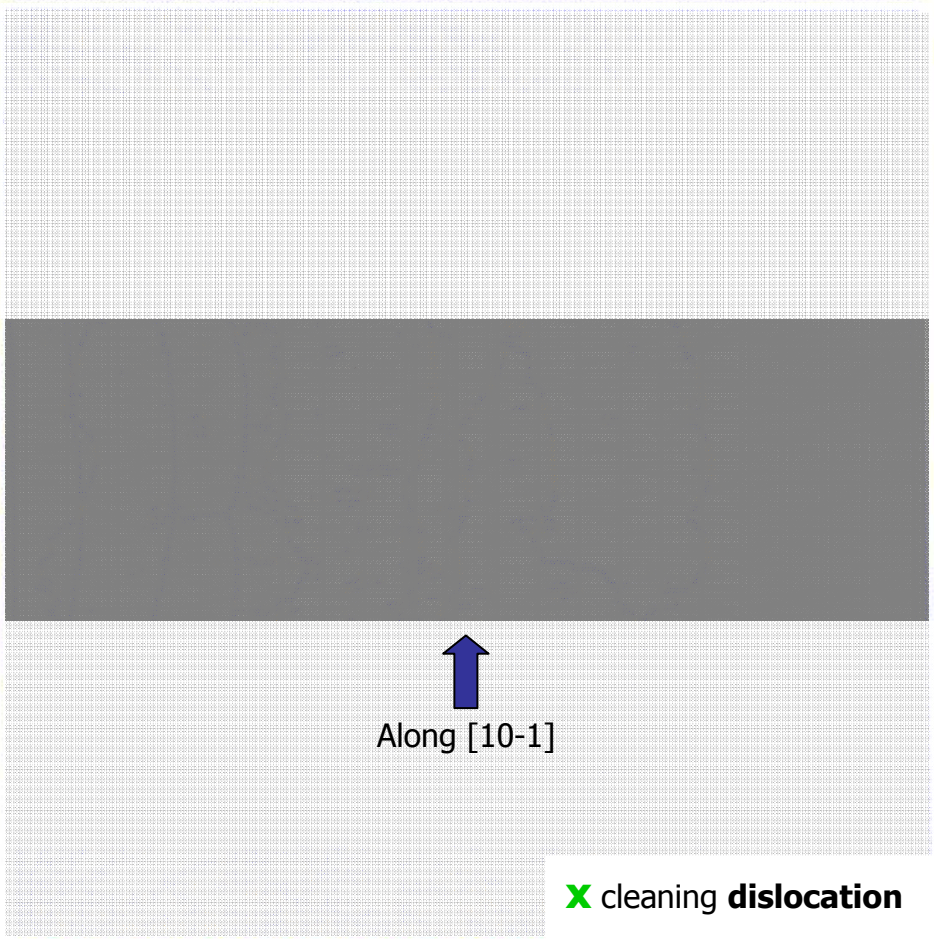


Formation of a clear band // (111) of finite thickness

Case 2: Collective glide of dislocations $\tau_{nuc} < \tau_{obst}$



Microstructure of a clear band



Leading dislocations

Dislocations with helix jogs

Clear and broaden the band

Following dislocations

Straigth dislocations

"Push" the leading dislocations

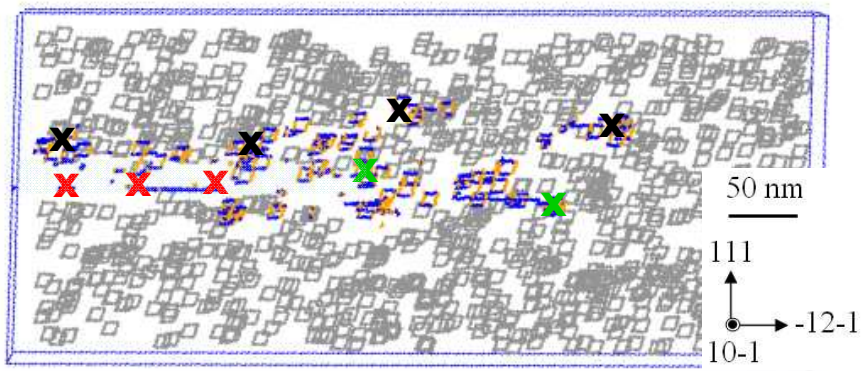
At band periphery

Accumulation of debris

X cleaning **dislocation**

X pushing **dislocation**

X arrested **dislocation**



Case 2: Collective glide of dislocations $\tau_{nuc} < \tau_{obst}$

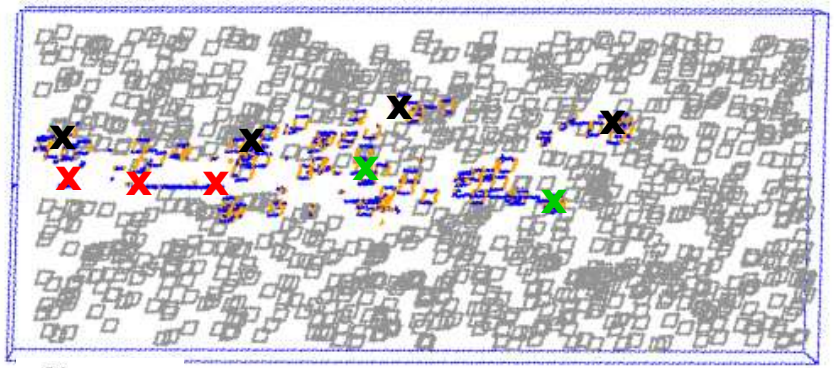
Broadening

Helix ⇨ Re-emission of screw dislocations in new slip planes

⇩

Dislocation pile-ups ⇨ Activation of dislocation glide oin the new slip planes

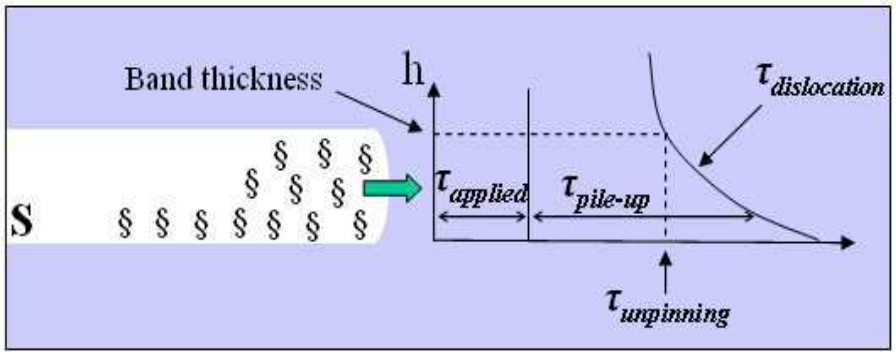
$\tau_{dislocation} = \tau_{applied} + \tau_{pile\text{-}up}$ *(number of dislocations)* $> \tau_{unpinning}$ *(defect strength, defect density)*



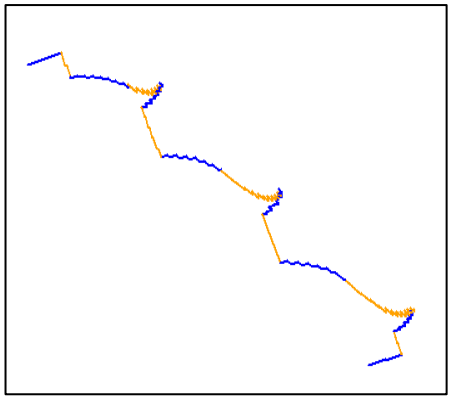
X leading **dislocations**

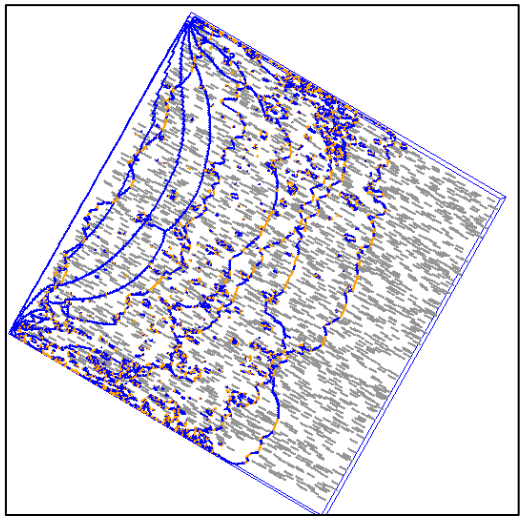
X pushing **dislocations**

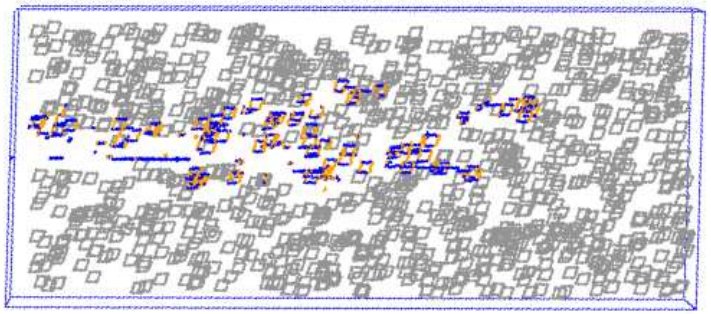
X arrested **dislocations**



Conclusion Dislocation Dynamics analysis







Clear band formation scenario

→ Helix clear the initial defect loops

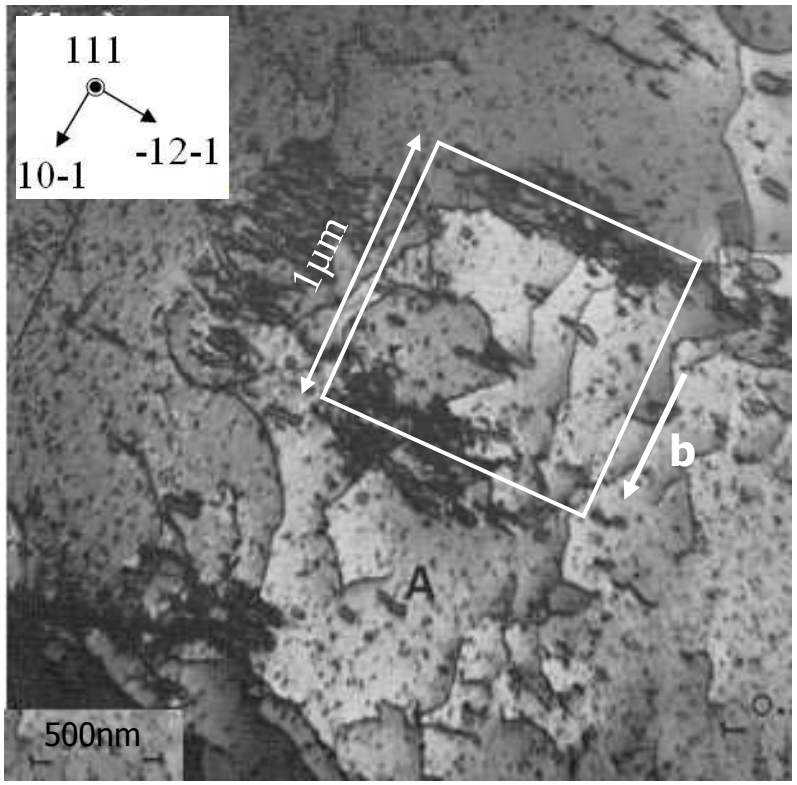
→ Clear band broaden by slip plane change

→ Collective effects necessary

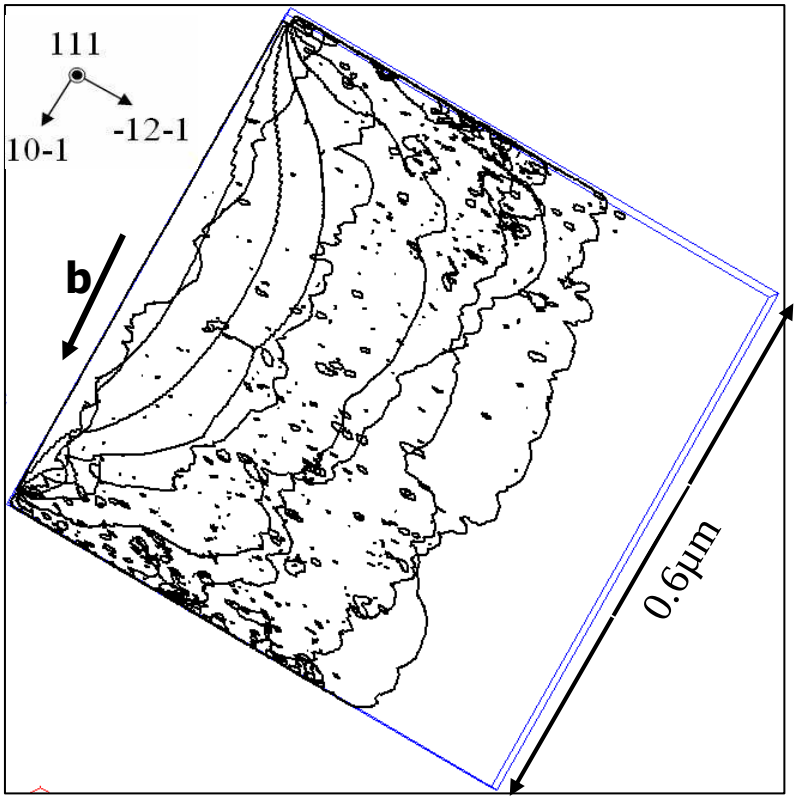
IV Comparaison simulation / experiment

Comparison simulation / experiment

Microstructure of clear bands



Cu irradiated and deformed:
foil parallel to the clear band [Sharp, 67]



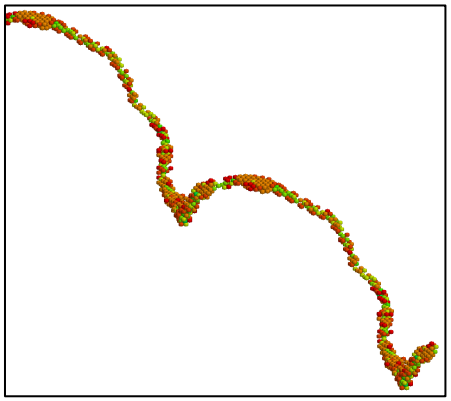
Dislocation Dynamics

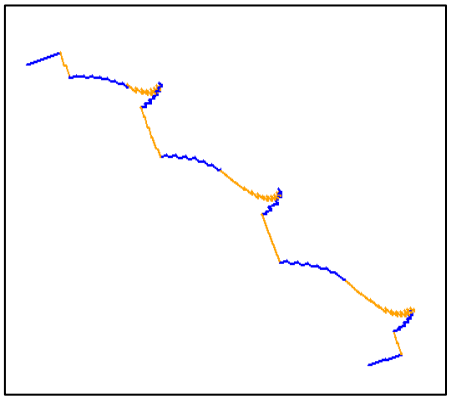
⇨ Longs screw segments

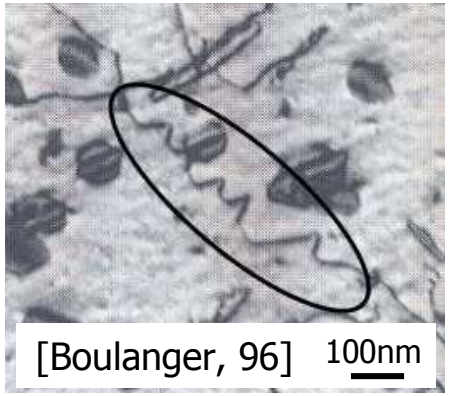
⇨ Accumulation of jogs and debris in small zones

Comparison simulations / experiments

Elementary dislocation/loop interactions

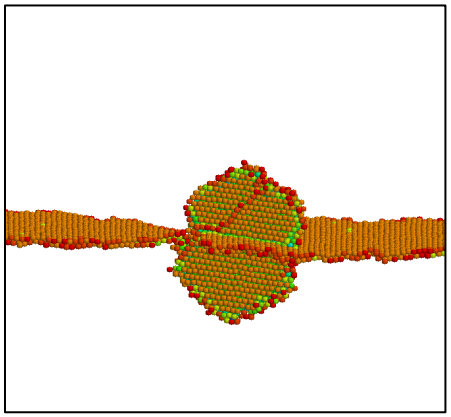


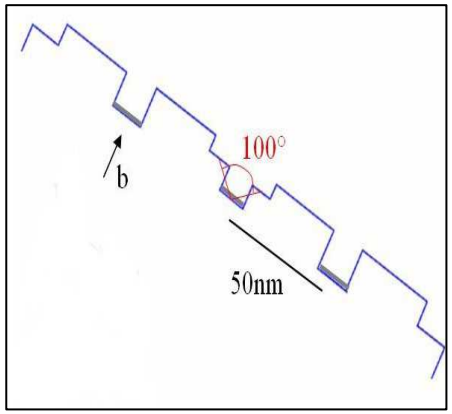


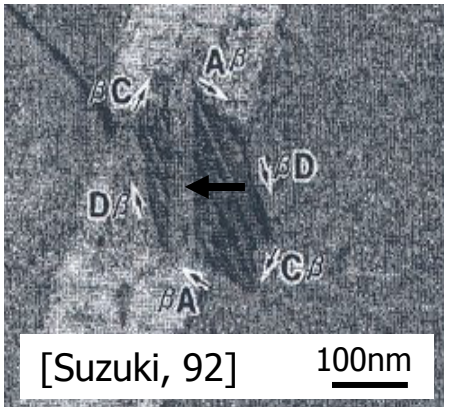


⇨ Absorption in the form of helix

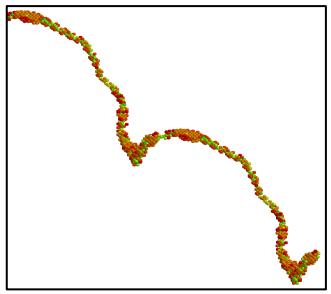
⇨ Loop shear





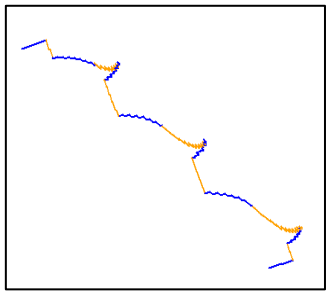


Conclusions



New clear band formation scenario

Multi-scale modelling

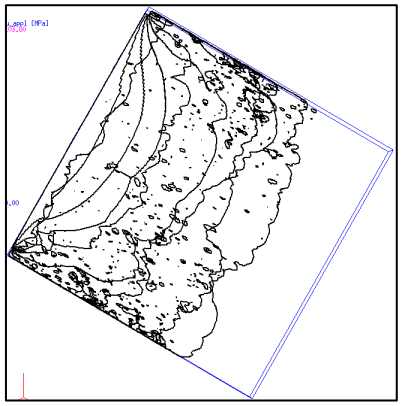


<u>Molecular Dynamics</u>
Dislocation/loop interaction mechanisms

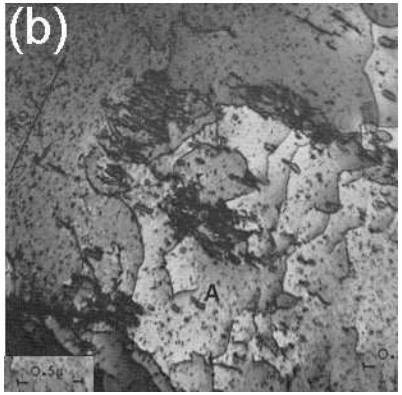
→ Difference screw / edge
→ Screw = Unfaulting - Absorption - Helix – Change of glide plane

<u>Dislocation Dynamics</u>
Collective interaction dynamics (leading to finite thickness clear band)

→ Realistic description of elementary dislocation/loop interactions
→ Cleaning + Broadening = helix + dislocation pile-ups



<u>Experimental validation</u>



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