PHYSICALLY-BASED CONSTITUTIVE EQUATIONS FOR IRRADIATED RPV AND INTERNALS

- Ghiath Monnet, EDF R&D, MMC
- Ludovic Vincent, CEA DEN, SRMA
- Chu Mai, EDF R&D, MMC
- Lionel Gélébart, CEA DEN, SRMA

This project received funding under the Euratom research and training programme 2014-2018 under grant agreement N° 661913

Summary

- What is a crystalline law ?
- The rate equation
- Stress components
- Microstructure evolution during deformation

What is a crystalline law ?

The stress-strain curve is needed in many mechanical applications

Non-crystallographic Laws

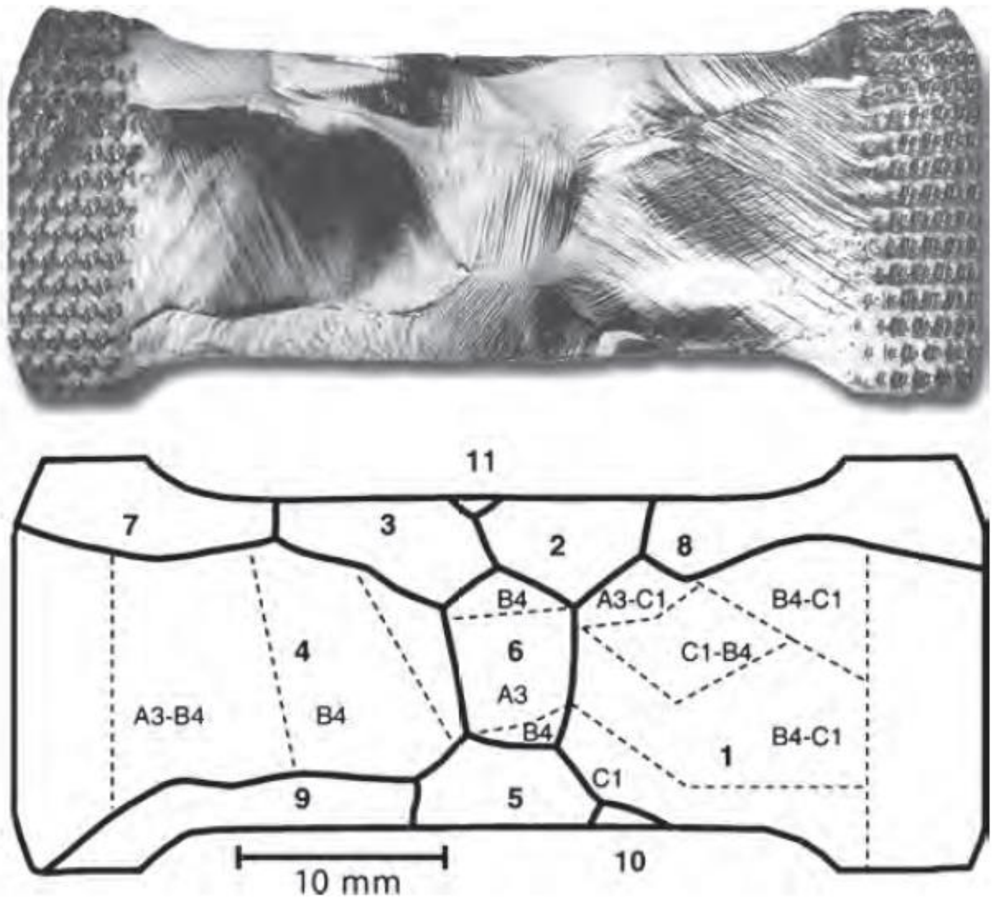
$$\sigma = \sigma_o + k\,\varepsilon^n$$ [Hollomon, Ludwig]

$$\frac{\varepsilon}{\varepsilon_o} = \frac{\sigma}{\sigma_o} + \alpha\left(\frac{\sigma}{\sigma_o}\right)^n \qquad \sigma_o = E\varepsilon_o$$ Ramberg-Osgood

- ❑ Not predictive
- ❑ Uniform homogeneous local/macroscopic behavior
- ❑ No explicit grain representation, nor physical properties

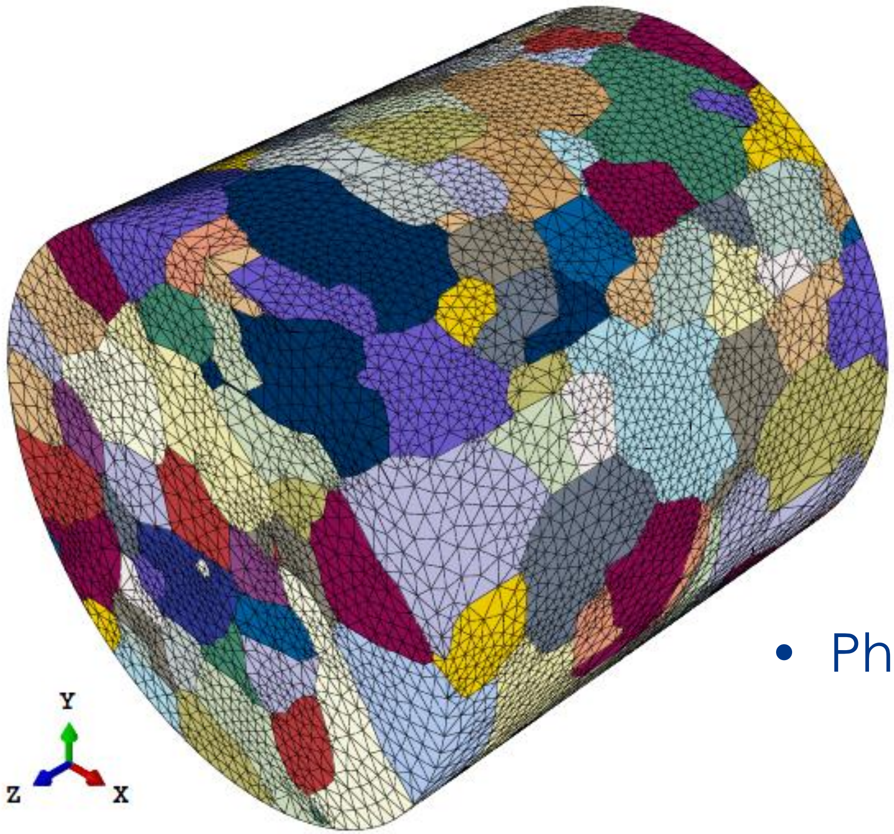
F. Roters et al. Crystal Plasticity Finite Element Methods:
in Materials Science and Engineering, Wiley VCH, Weinheim, 2010.

What is a crystalline law ?



In metallic alloys, plasticity is accommodated by slip on specific planes along specific directions

What is a crystalline law ?



Homogenization calculations

+ Boundary conditions

➔ Local stress field

Need mechanical local response

- Phenomenological crystalline Laws

$$\tau_c^s = f(T, \gamma_{cum}^i)$$

No microstructure explicit variables

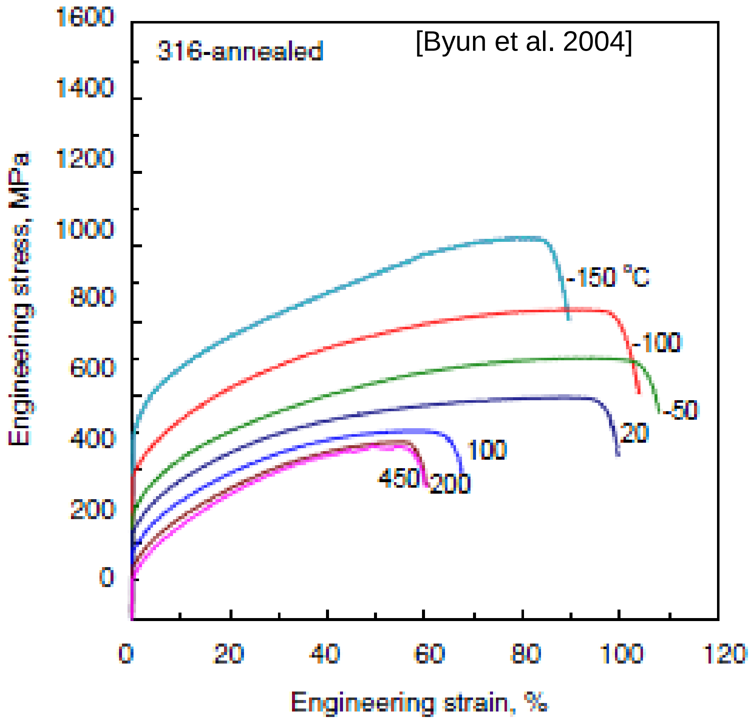
What is a crystalline law ?

- Physically-based Crystalline Laws
- Mechanical properties are determined by **physical properties** P_i (elastic constants, grain size, dislocation density, obstacles size/density, etc.) AND **test parameters** T_i (temperature, strain rate, applied load, etc.)

  - The rate equation $\dot{\gamma}^s = f(P_i, \tau^s_{eff})$ τ^s_{eff} ?
  - Stress decomposition $\tau^s_{app} = f(\tau^s_f, \tau^s_{HP}, \tau^s_{forest}, \tau^s_{sc}, \tau^s_{eff} ..)$
  - Microstructure evolution $\partial Q^s_i = f(T_i, P_i, \gamma^s, \Delta\gamma)$

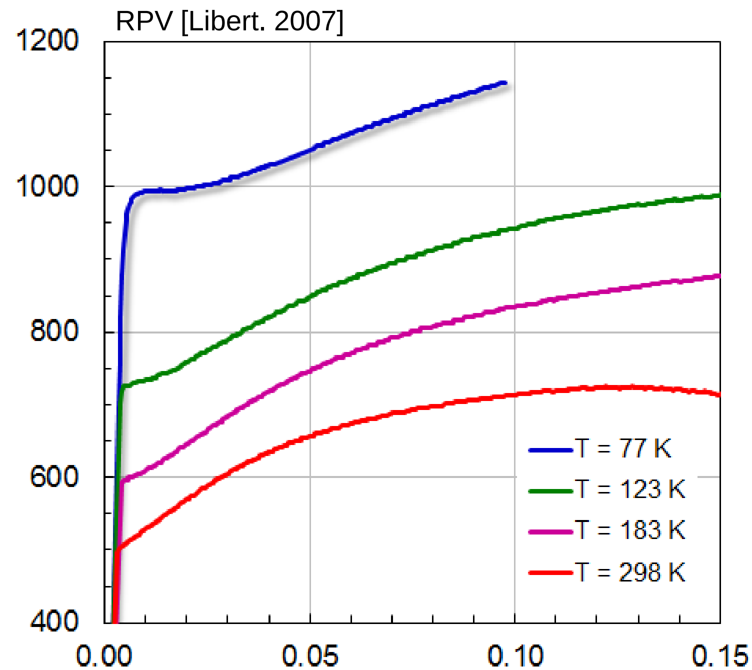
What is a crystalline law ?

FCC – type behavior



- unambiguous slip planes
- no fragile regime
- temperature-dependent parameters

BCC – type behavior



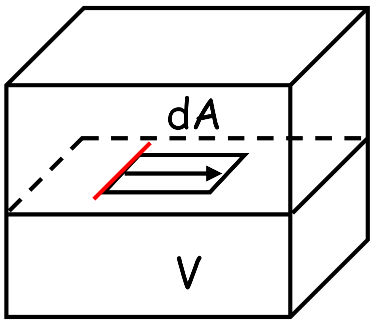
- many slip planes/non-crystallographic
- ductile-fragile transition
- Temperature-dependent mechanisms

Summary

- What is a crystalline law ?
- The rate equation
- Stress components
- Microstructure evolution during deformation

Rate equation: the Orowan relation

If a dislocation of length L and Burgers vector b moves by dx in a volume V:



$$d\gamma = \frac{bdA}{V} = \frac{bLdx}{V} = b\rho dx$$

$$\dot{\gamma} = \frac{d\gamma}{dt} = \frac{b\rho dx}{dt} = b\rho v$$

$$\dot{\gamma}^s = b\rho_m^s v^s$$

Orowan relation

$$\tau_{app}^s = \tau_c^s + \tau_{eff}^s$$

Dislocation velocity and strain rate = f(τ_{eff})

Rate equation

$$\dot{\gamma}^s = b\rho_m^s v_o \exp\left(-\frac{\Delta G(\tau_{eff}^s)}{kT}\right)$$

Rate equation: a thermal regime

$$\dot{\gamma}^s = b\rho_m^s v_o \exp\left(-\frac{\Delta G(\tau_{eff}^s)}{kT}\right) \qquad V^* = -\frac{\partial \Delta G}{\partial \tau_{eff}^s}, \quad \beta = \frac{1}{kT}$$

Stress components $\tau_c^s = \lim_{\dot{\gamma}^s \to 0}(\tau_{app}^s) \qquad \tau_{app}^s = \tau_{eff}^s + \tau_c^s$

When $\tau_{eff}^s \langle\langle \tau_c^s$ (FCC – type behavior)

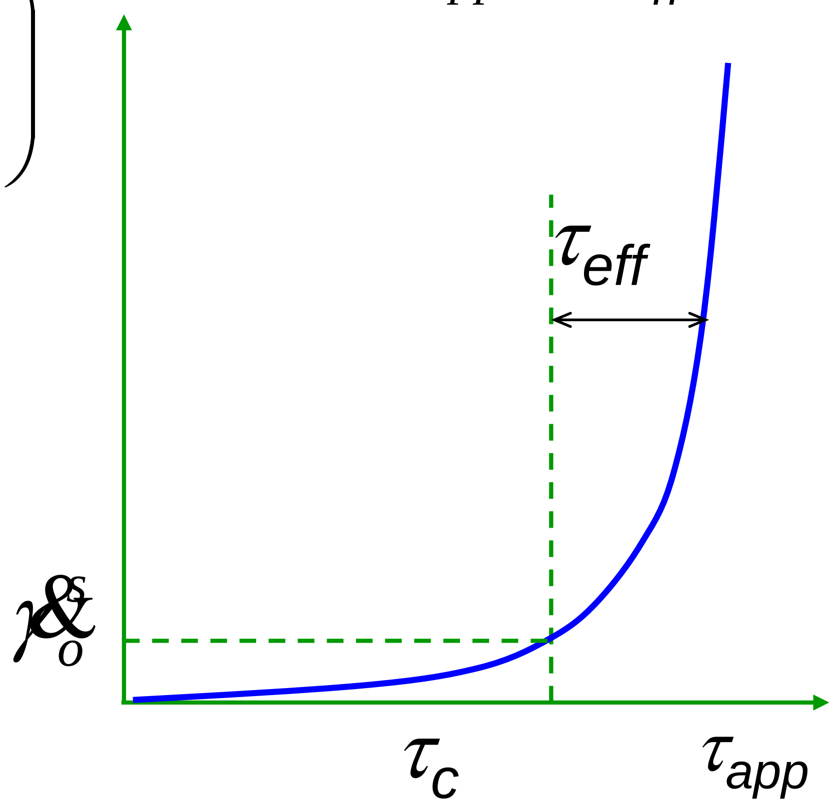
$$\dot{\gamma}^s = b\rho_m^s v_o \exp - \beta(A - V\tau_{eff}^s) = \dot{\gamma}_o^s \exp(\beta V\tau_{eff}^s) = \dot{\gamma}_o^s \left[\exp\left(\frac{\tau_{app}^s}{\tau_c^s} - 1\right)\right]^{\beta V \tau_c^s}$$

$$\dot{\gamma}^s = \dot{\gamma}_o^s \left(\frac{\tau_{app}^s}{\tau_c^s}\right)^{\beta V \tau_c^s} = \dot{\gamma}_o^s \left(\frac{\tau_{app}^s}{\tau_c^s}\right)^n$$

Rate equation: a thermal regime

$$\dot{\gamma}^s = \dot{\gamma}_o^s \left(\frac{\tau_{app}^s}{\tau_c^s} \right)^{\beta V \tau_c^s} = \dot{\gamma}_o^s \left(\frac{\tau_{app}^s}{\tau_c^s} \right)^{n}$$

$$\tau_{app}^s = \tau_{eff}^s + \tau_c^s$$



k = 1.4E-24

T = 300 K

V = 100 b^3

τ_c = 50 MPa

n = 190

τ_c plays the role of threshold of the flow stress

Summary

- What is a crystalline law ?
- The rate equation
- Stress components
- Microstructure evolution during deformation

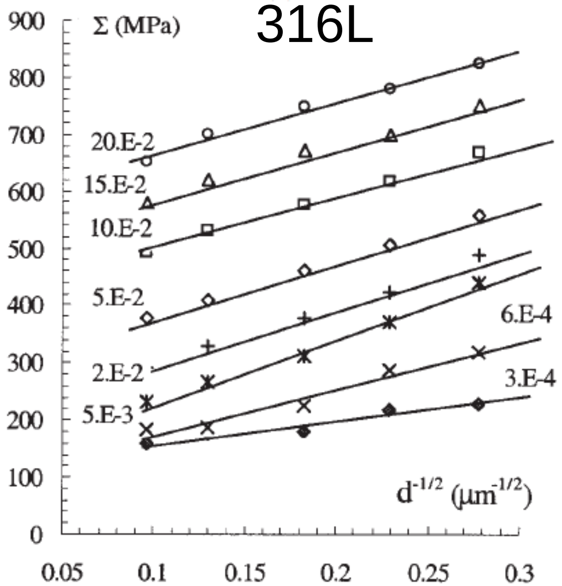
Stress components

- The applied stress must exceed:
  - Solid solution: τ_f
  - Hall-Petch (grain size) effect: τ_{HP}
  - Local obstacles (dislocations, precipitates, loops..): τ_{obs}
- To overcome lattice and phonon dynamical fiction : the effective stress τ_{eff}

Stress components: friction stress τ_f

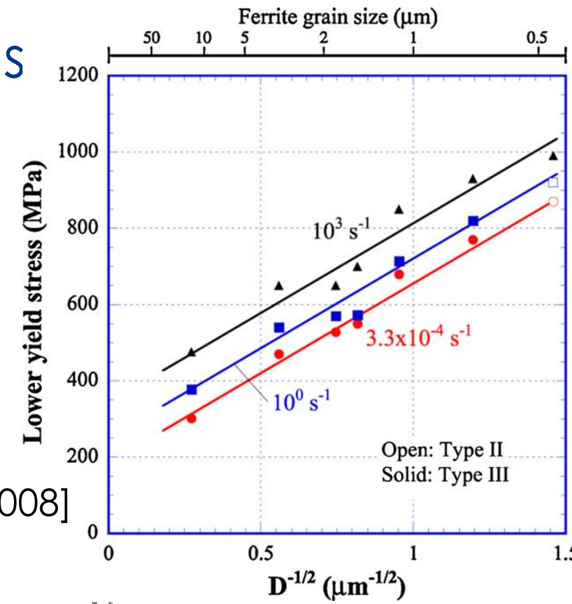
- Stress necessary to start moving dislocations
- Results from:
  - interstitial solute atoms (solid solution of C, N , H, etc.)
  - substitutional solute atoms: Ni in Al, Cu in Al, (Cr, Mn, Ni, S, Mo, etc.) in Fe
- Depends on temperature and strain rate
- Cannot be predicted (no reliable model)
- Material property

Stress components: Hall-Petch effect τ_{HP}



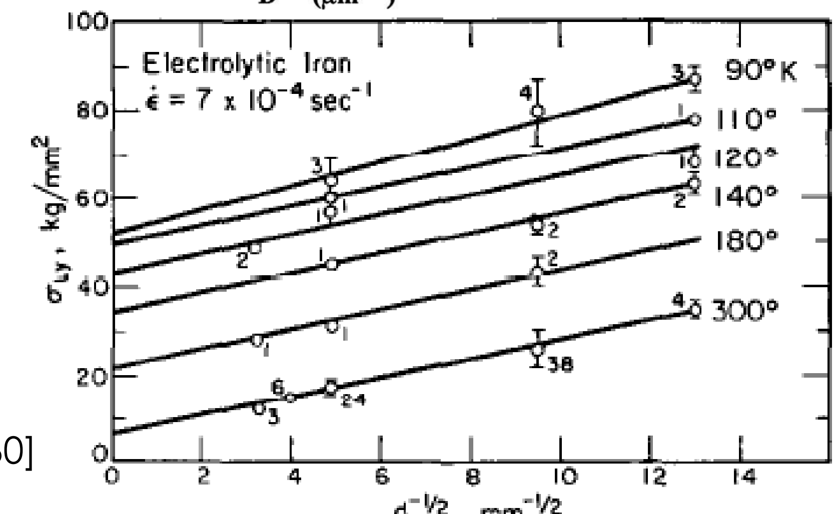
[Feaugas et al. 2003]

Ferritic steels



[Tsushida et al 2008]

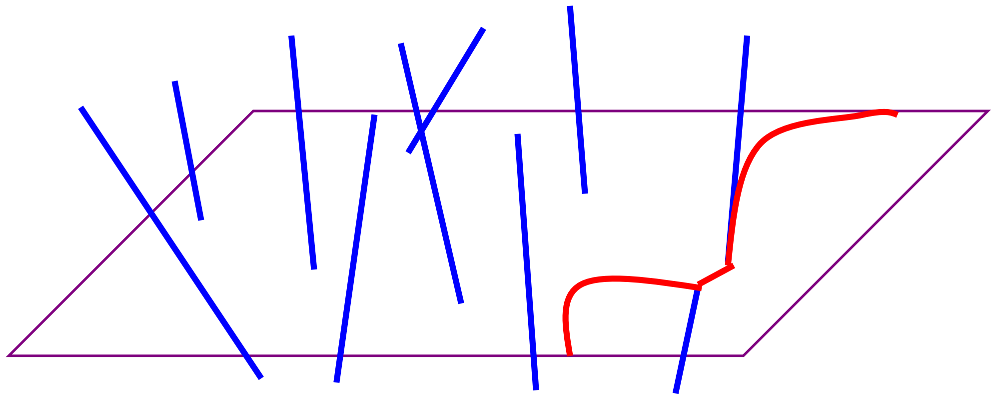
$$\tau_{HP} = \frac{\mu}{\mu(300\ K)} \frac{K}{\sqrt{d_{grain}}}$$



[Conrad et al. 1960]

Local obstacles: forest dislocations

- Principal obstacles in all materials
- Resulting from dislocation - dislocation interactions (junctions, annihilation, jogs)
- Density increases with deformation (strain hardening)



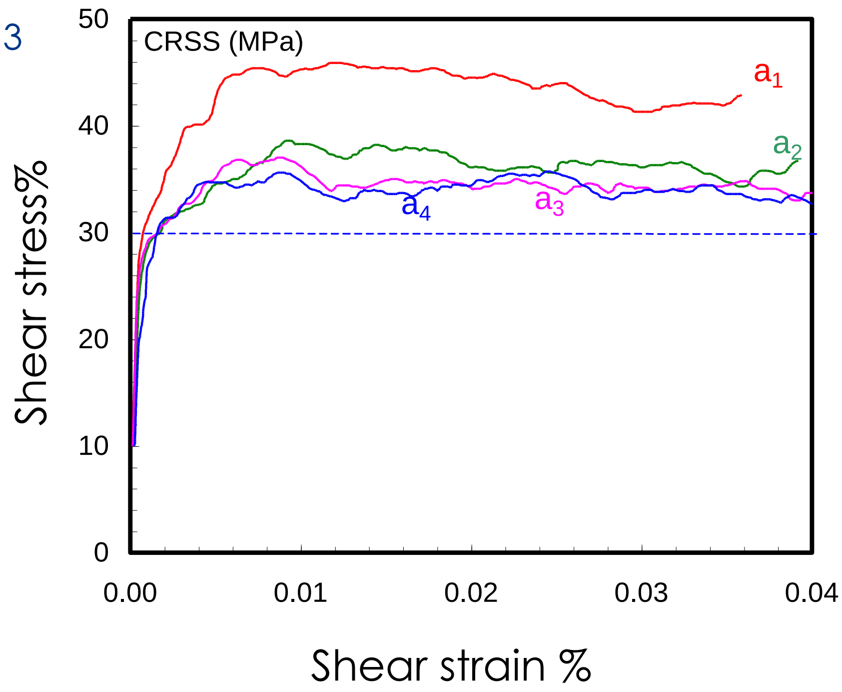
Average forest dislocation spacing

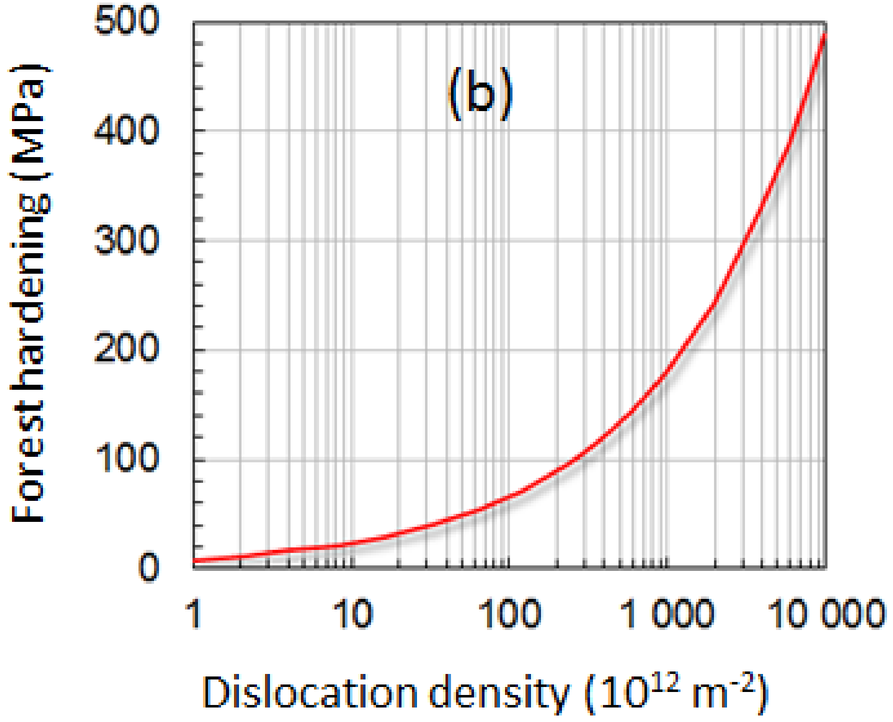
$$l = \frac{1}{\sqrt{\rho_{forêt}}}$$

Strengthening is given by : $\Delta\tau_{forêt} = \alpha\frac{\mu b}{l} = \alpha\mu b\sqrt{\rho_{forêt}}$

Local obstacles: forest strengthening

- Simulation volume : 10 × 10 × 10 μm^3
- Forest density : 10^{12} m^{-2}
- DD simulations at constant strain rate





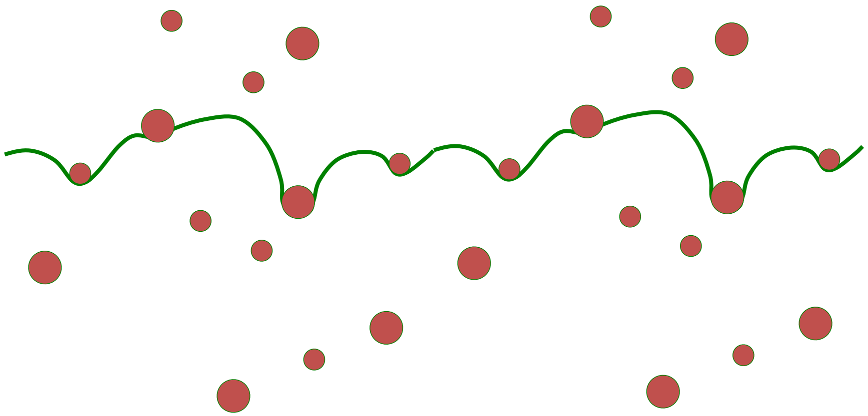
$$\Delta\tau_{forest} = \mu b\sqrt{a_{forest}\rho_{forest}}$$

Local obstacles: forest hardening in FCC

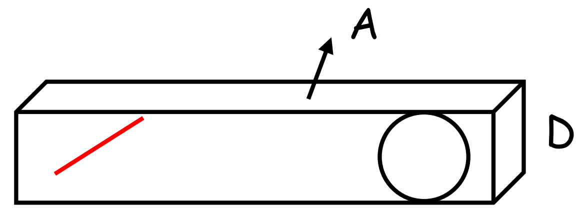
	A2	A3	A6	B2	B4	B5	C1	C3	C5	D1	D4	D6
A2	a^*	a^*	a^*	a_{col}	$a_{glissile}$	$a_{glissile}$	a_{Hirth}	$a_{glissile}$	a_{Lomer}	a_{Hirth}	a_{Lomer}	$a_{glissile}$
A3		a^*	a^*	$a_{glissile}$	a_{Hirth}	a_{Lomer}	$a_{glissile}$	a_{col}	$a_{glissile}$	a_{Lomer}	a_{Hirth}	$a_{glissile}$
A6			a^*	$a_{glissile}$	a_{Lomer}	a_{Hirth}	a_{Lomer}	$a_{glissile}$	a_{Hirth}	$a_{glissile}$	$a_{glissile}$	a_{col}
B2				a^*	a^*	a^*	a_{Hirth}	a_{Lomer}	$a_{glissile}$	a_{Hirth}	$a_{glissile}$	a_{Lomer}
B4					a^*	a^*	a_{Lomer}	a_{Hirth}	$a_{glissile}$	$a_{glissile}$	a_{col}	$a_{glissile}$
B5						a^*	$a_{glissile}$	$a_{glissile}$	a_{col}	a_{Lomer}	$a_{glissile}$	a_{Hirth}
C1							a^*	a^*	a^*	a_{col}	$a_{glissile}$	$a_{glissile}$
C3								a^*	a^*	$a_{glissile}$	a_{Hirth}	a_{Lomer}
C5									a^*	$a_{glissile}$	a_{Lomer}	a_{Hirth}
D1										a^*	a^*	a^*
D4											a^*	a^*
D6												a^*

Example: CFC crystallographic structure

Local obstacles: precipitation hardening



Precipitates of size D and density C



Number of encountered precipitates

$$n = DAC$$

For Orowan precipitates
(impenetrable precipitates)

$$\Delta\tau^{s}_{Orowan} = \left(\frac{\ln 2D/b}{\ln l/b}\right)^{\frac{3}{2}} \frac{\mu b}{2\pi l} \ln\left(\frac{l}{b}\right)$$

Free planner spacing

$$l = \frac{1}{\sqrt{DC}}$$

For shearble precipitates

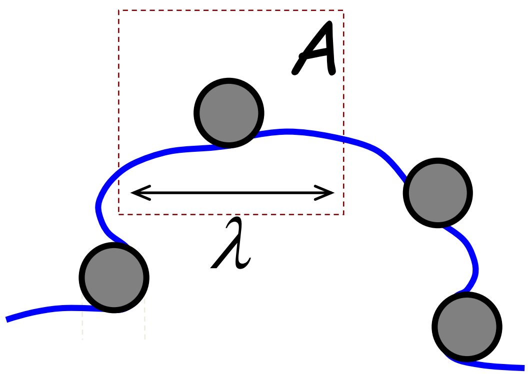
$$\Delta\tau^{s}_{prc} = \left(\frac{\Omega_{prc}}{\Omega_{\infty}} \frac{\ln 2D/b}{\ln l/b}\right)^{\frac{3}{2}} \frac{\mu b}{2\pi l} \ln\left(\frac{l}{b}\right)$$

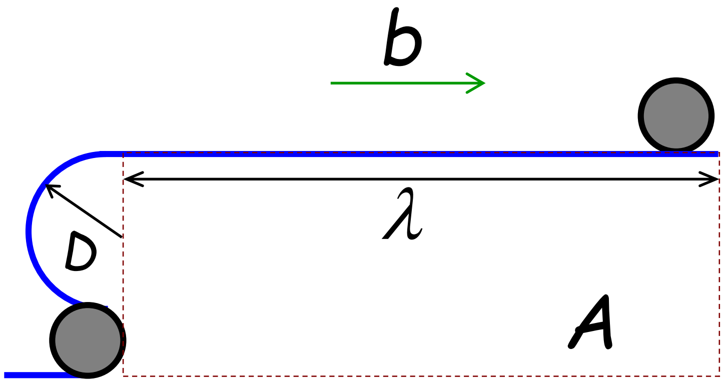
$$\Delta\tau^{s}_{prc} = \mu b \sqrt{a_{prc} D_{prc} C_{prc}}$$

[Monnet, Acta materialia, 2015]

Local obstacles: precipitation hardening

Random distribution of obstacles with planner density ρ





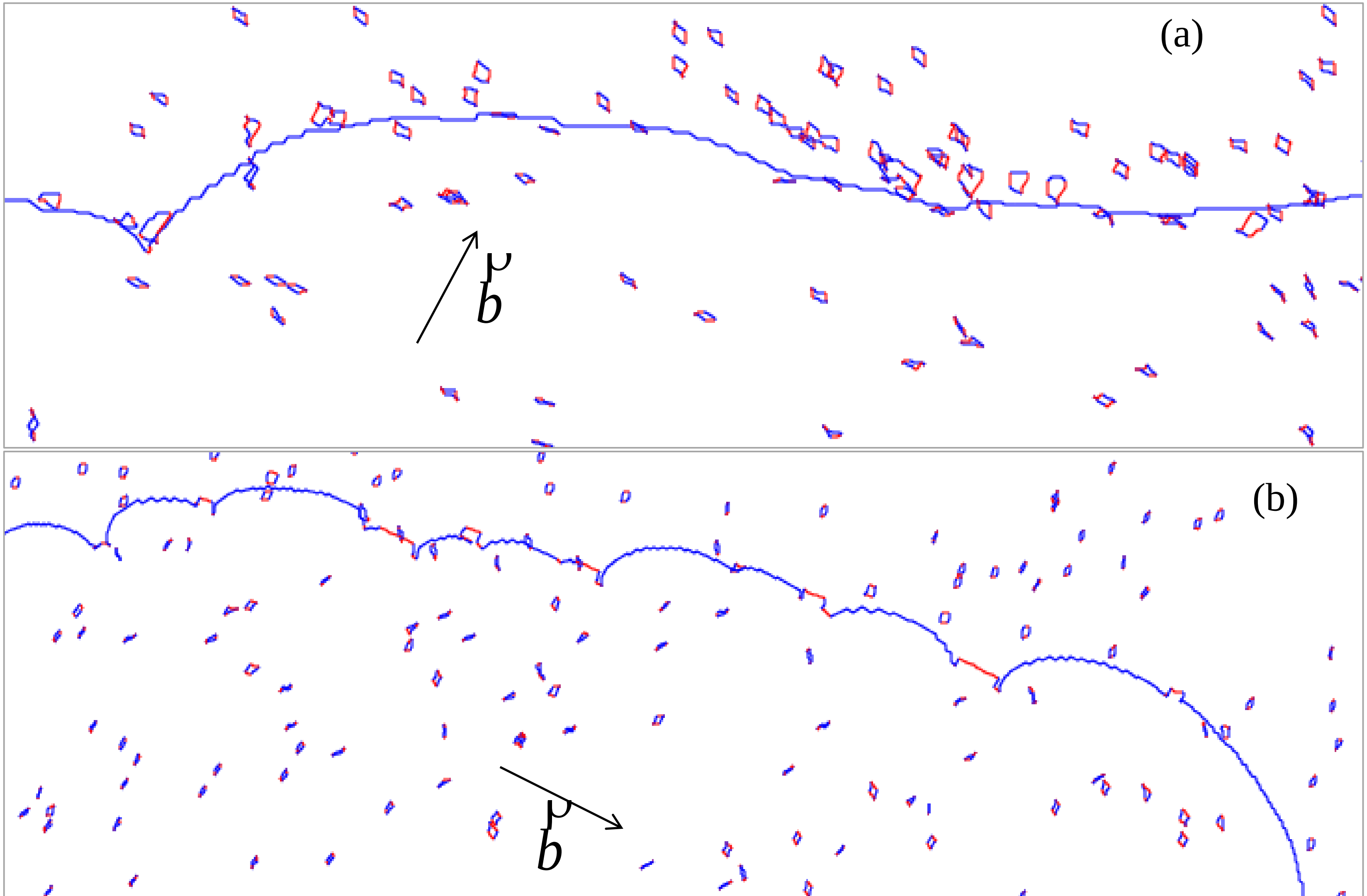
$$l = \frac{1}{\sqrt{DC}}$$

$$l = \frac{1}{(D+2R)\rho}$$

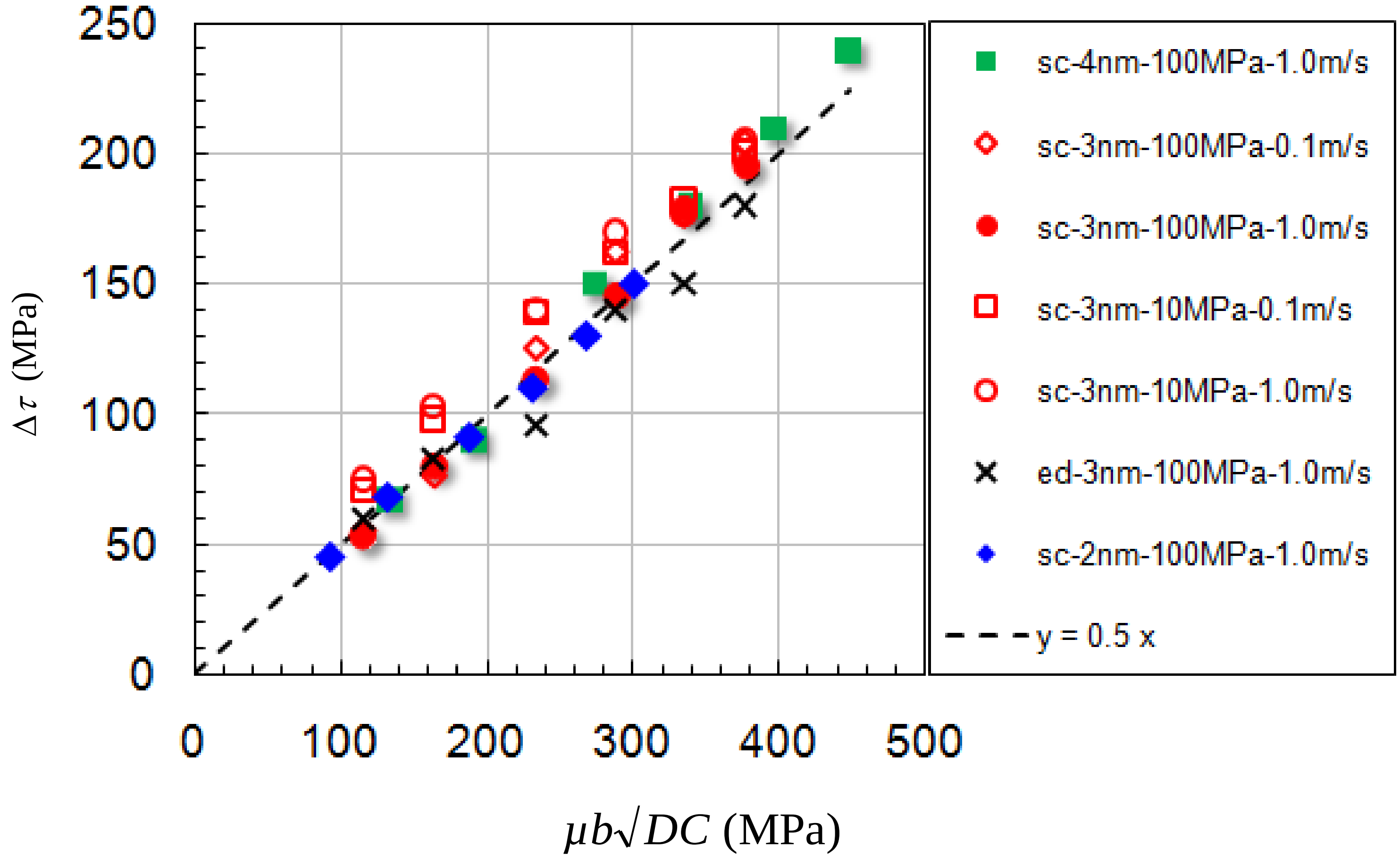
$$\tau^{s}_{obs} = \alpha^{s}\mu b\sqrt{DC}$$

$$\tau^{s}_{obs} = \begin{cases} 0 \\ \alpha^{s}\mu b\sqrt{DC} - \tau^{s}_{eff} \end{cases}$$

Local obstacles: dislocation loops



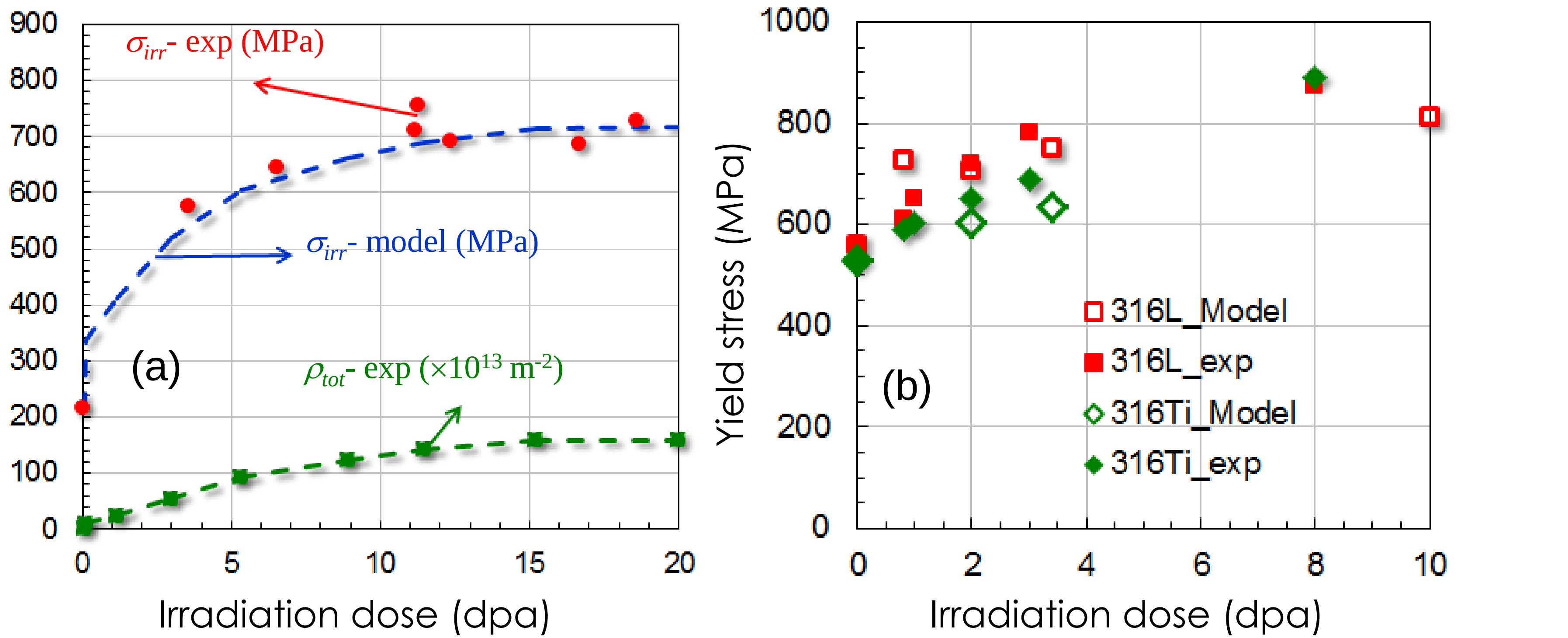
Local obstacles: dislocation loops



$$\tau_{DL} = \alpha_{forest}\mu b\sqrt{\rho_{DL}}$$

[Monnet, Scripta materialia, 2015]

Local obstacles: dislocation loops



$$Rp = M\tau_c = M(\tau_{ss} + \alpha\mu b\sqrt{\rho_{tot}} + \tau_{HP} = \tau_{ss} + \alpha\mu b\sqrt{\rho_{forest} + \rho_{DL}} + \tau_{HP})$$

G. Monnet, Multiscale modeling of irradiation hardening: Application to important nuclear materials, JNM 2018

Summary

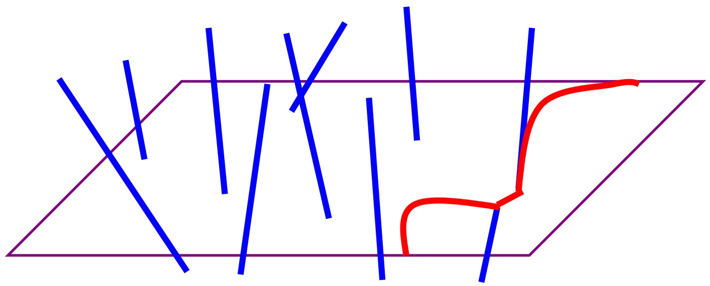
- What is a crystalline law ?
- The rate equation
- Stress components
- Microstructure evolution during deformation

Microstructure evolution: storage rate

$$d\rho^s = f(\gamma^i, T,, etc.)$$

- Density on system s varies with slip on system s $\quad d\rho^s = f(\gamma^s)$

- A fraction of mobile dislocations stops at the forest which leads to a generation of new dislocation



- Assuming a dislocation of length L to stop after displacement over l, the accommodated shear strain:

- The corresponding stored density:

$$d\gamma^s = \frac{\lambda L b}{V}$$

$$d\rho^s = \frac{L}{V}$$

$$d\rho^s = \frac{d\gamma^s}{b\lambda}$$

Microstructure evolution: storage rate

- λ is called free mean path of dislocations
- λ scales with average spacing of the forest density

$$\lambda \propto \frac{1}{\sqrt{\rho^{s}_{forest}}}$$

- λ must decrease with the forest strength

$$\lambda \propto \frac{1}{\alpha\sqrt{\rho^{s}_{forest}}}$$

- λ can be given as:

$$\lambda \propto \frac{K}{\alpha\sqrt{\rho^{s}_{forest}}}$$

- l obeys the harmonic sum for superposition

$$\frac{1}{\lambda} = \frac{1}{\lambda_1} + \frac{1}{\lambda_2} \propto \frac{\alpha_1\sqrt{\rho^1}}{K_1} + \frac{\alpha_2\sqrt{\rho^2}}{K_2}$$

Microstructure evolution: storage rate

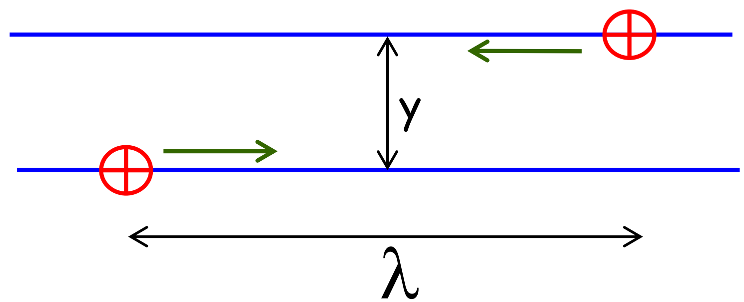
- the total storage rate

$$d\rho^s = \frac{d\gamma^s}{b\lambda} = \frac{d\gamma^s}{b}\left(\sum_{i=1}^{N} \frac{\alpha_i \sqrt{\rho^i}}{K_i}\right)$$

$$\dot{\rho}^s = \frac{1}{b}\left(\sum_{i=1}^{N} \frac{\sqrt{a^{is}\rho^i}}{K_i}\right)\dot{\gamma}^s$$

Microstructure evolution: recovery rate

- Dislocation multiplication ⇒ closer dislocations ⇒ strong attraction between dipoles
- Annihilation by: cross-slip (screw) and climb (edge) dislocations ⇒ recovery rate



- All dislocations gliding on slip planes closer than "y" annihilate when they get close to each other
- Dislocations of length L within a distance λ can annihilate
- Annihilated density $$d\rho^s = -\frac{Ly\lambda\rho^s}{V}$$
- Accommodated strain $$d\gamma^s = \frac{bL\lambda}{V}$$

$$d\rho^s = -\frac{y\rho^s d\gamma^s}{b}$$

Microstructure evolution: total rate

$$d\rho_{+}^{s} = \frac{d\gamma^{s}}{b}\left(\sum_{i=1}^{N}\frac{\alpha_i\sqrt{\rho_i^{s}}}{K_i}\right)$$

$$d\rho_{-}^{s} = -\frac{1}{b}\left(y\rho^{s}\right)d\gamma^{s}$$

$$\dot{\rho}_{total}^{s} = \frac{\dot{\gamma}^{s}}{b}\left(\sum_{i=1}^{N}\frac{\alpha_i\sqrt{\rho^{i}}}{K_i} - y\rho^{s}\right)$$

Summary of the crystalline law: FCC

- Rate equation

$$\dot{\gamma}^s = \dot{\gamma}_o^s \left(\frac{\tau_{app}^s}{\tau_c^s} \right)^n$$

- Stress decomposition

$$\tau_c^s = \tau_f^s + \sqrt{\mu^2 b^2 \sum_{i=1}^{N} a^{si} \rho^i + \Delta\tau_i^2} + \tau_{HP}$$

- Microstructure evolution

$$\frac{\dot{\rho}^s}{b\dot{\gamma}^s} = \frac{1}{d_{grain}} + \left(\frac{\sqrt{a^{self}\rho^s}}{K_{self}} + \frac{\alpha^s \sqrt{\rho_{obs}^s}}{K_{obs}} - y\rho^s \right)$$

$$\dot{C}_{DL}^s = -\lambda_{DL} \frac{D_{DL}^s}{b} C_{DL}^s \left| \dot{\gamma}^s \right|$$

$$\dot{C}_{DL}^s = -\lambda_{DL} \frac{D_{DL}^s}{b} C_{DL}^s \left| \dot{\gamma}^s \right|$$

Summary of the crystalline law

- rate equation

$$\frac{1}{\dot{\gamma}^s} = \frac{1}{\dot{\gamma}^s_{drag}} + \frac{1}{\dot{\gamma}^s_{friction}}$$

$$\dot{\gamma}^s_{drag} = \dot{\gamma}^s_o \left(\frac{\tau^s_{app}}{\tau^s_c} \right)^n$$

$$\dot{\gamma}^s_{friction} = \rho^s_m b \, H \, l^s_{sc} \exp\left(-\frac{\Delta G_o}{kT} \left(1 - \sqrt{\frac{\tau^s_{eff}}{\tau^s_o}} \right) \right)$$

- stress decomposition $\tau^s_{app} = \tau^s_{eff} + \tau^s_f + \sqrt{{\tau^s_{self}}^2 + {\tau^s_{LT}}^2} + \tau^g_{HP}$

$$\rho^s_{obs} = \sum_{j \neq s} \rho^j_{dis} + \rho_{carbide} + \rho_{SC} + \rho_{DL}$$

$$\tau^s_{TL} = \frac{\alpha^s \mu b}{\lambda^s - l_c} - \tau^s_{eff}$$

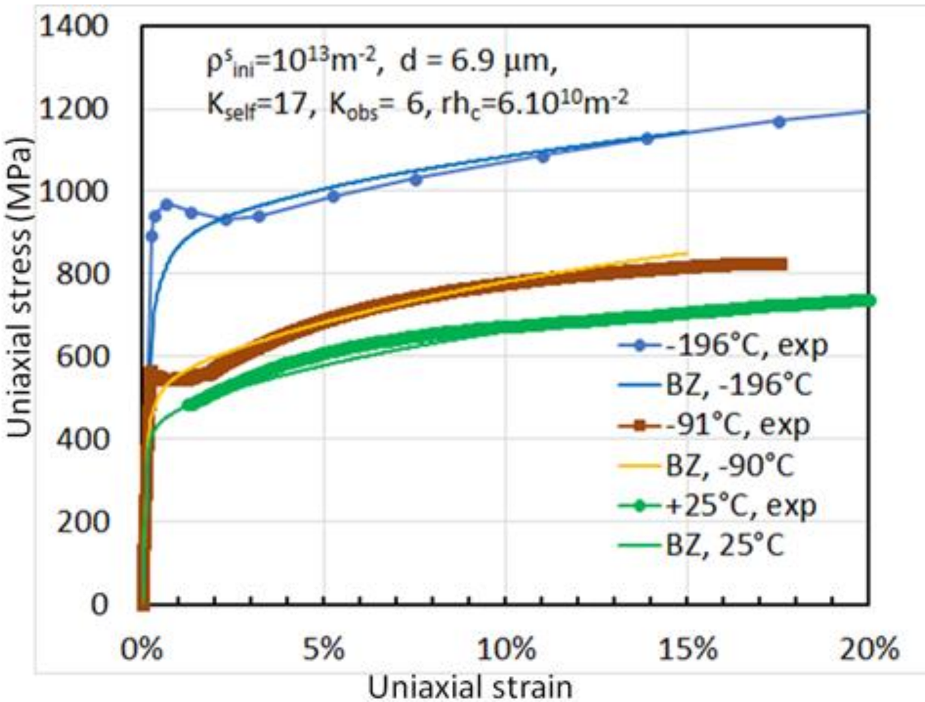
- Microstructure evolution

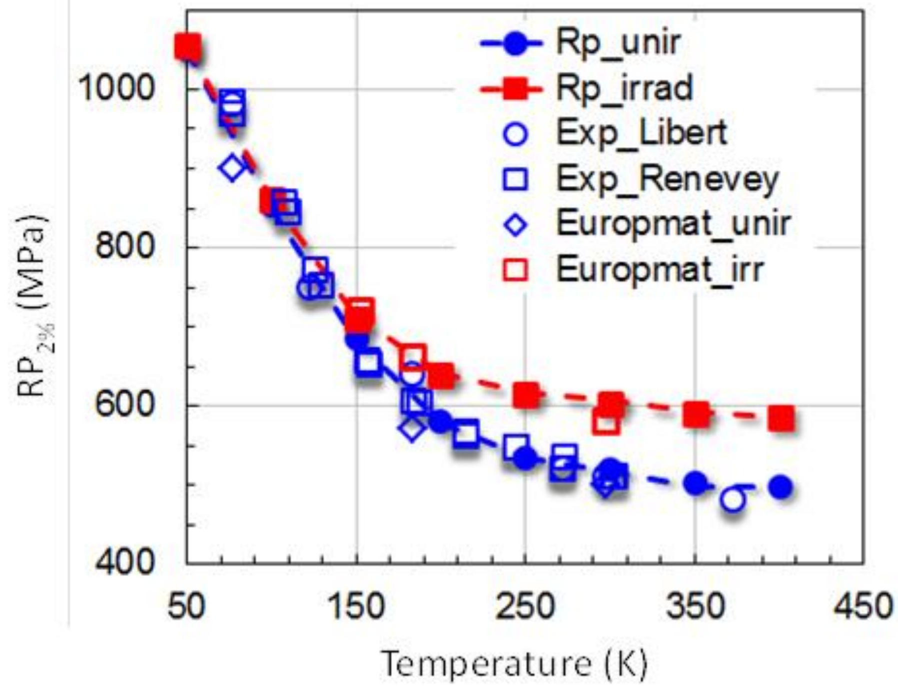
$$\frac{\dot{\rho}^s}{b \dot{\gamma}^s} = \frac{1}{d_{grain}} + \left(1 - \frac{\tau^s_{eff}}{\tau_o} \right) \left(\frac{\sqrt{a^{self} \rho^s}}{K_{self}} + \frac{\alpha^s \lambda^s \rho^s_{obs}}{K_{obs}} - y \rho^s \right)$$

$$\dot{C}^s_{DL} = -\lambda_{DL} \frac{D^s_{DL}}{b} C^s_{DL} \left| \dot{\gamma}^s \right|$$

$$\dot{C}^s_{DL} = -\lambda_{DL} \frac{D^s_{DL}}{b} C^s_{DL} \left| \dot{\gamma}^s \right|$$

Validation : RPV steels





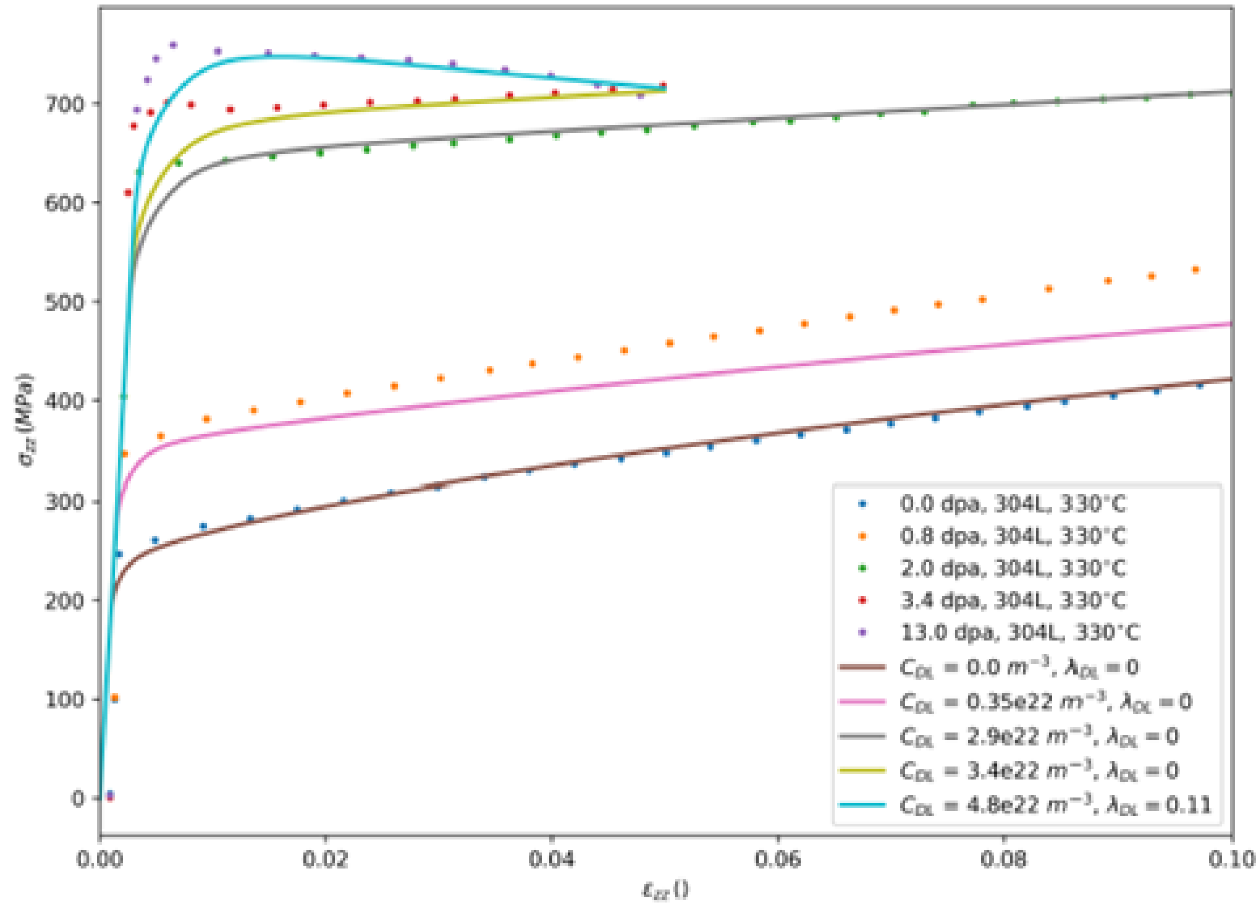
Comparison with experiment

RPV Euromaterial A

Effect of irradiation in RPV

Euromaterial A

Validation : Internals



Comparison with experiment irradiated 304L

Conclusions

- It is possible to model plastic deformation at physical basis
- Fundamental mechanisms can be treated separately
- Hardening sources cannot be added linearly