MatISSE

Multiscale Modeling of Radiation Hardening in RPV and Austenitic Stainless Steels: from the Atomic to the Continuum Scale

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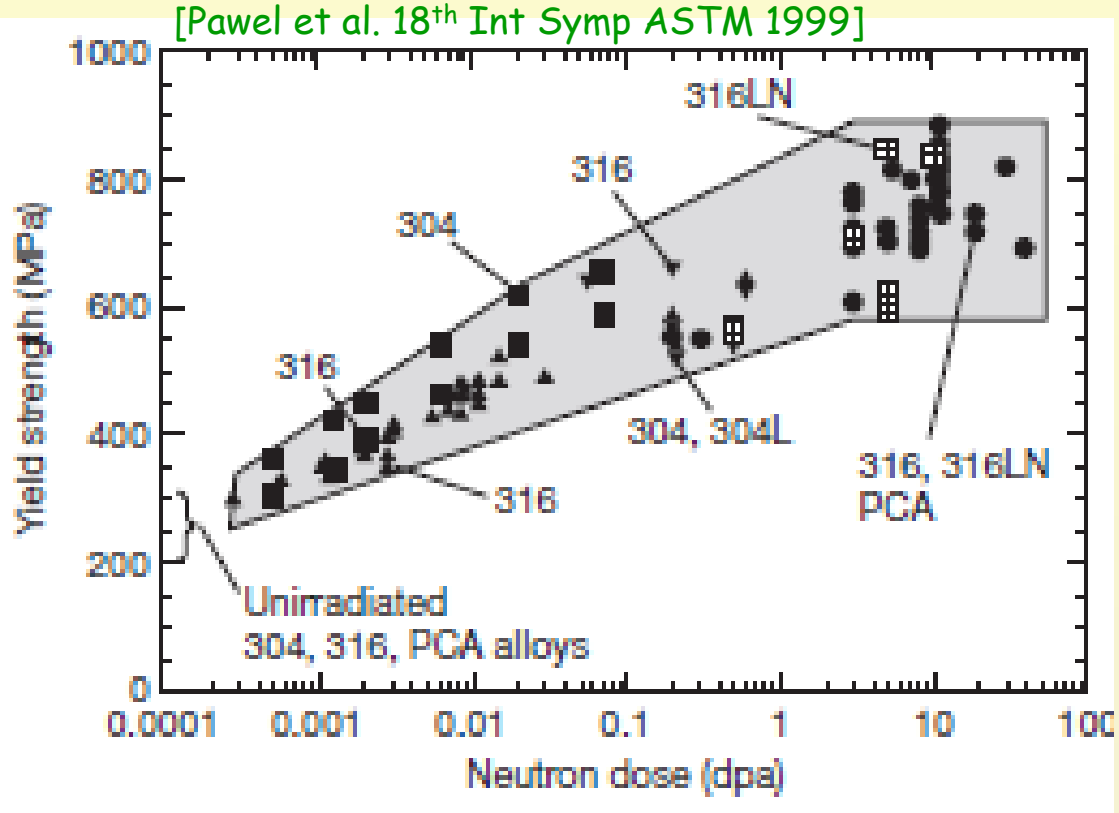
Irradiation induced hardening

Material
+ Dose

Mechanical properties

[Pawel et al. 18th Int Symp ASTM 1999]

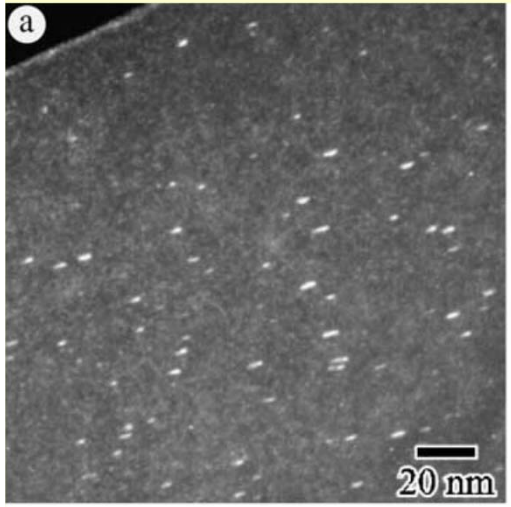


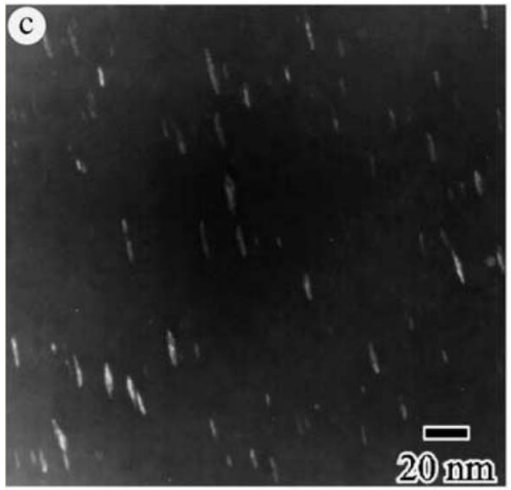
Radiation hardening of internal steels

Empirical approach in predicting radiation hardening

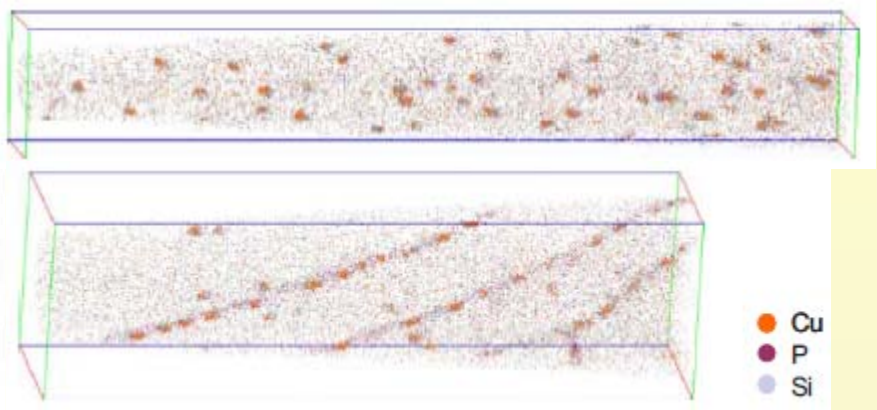
Irradiation microstructures

316SS, 1&5 dpa



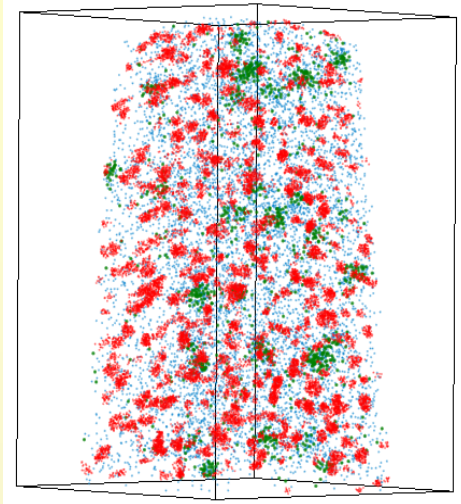


Solute clusters in RPV steels

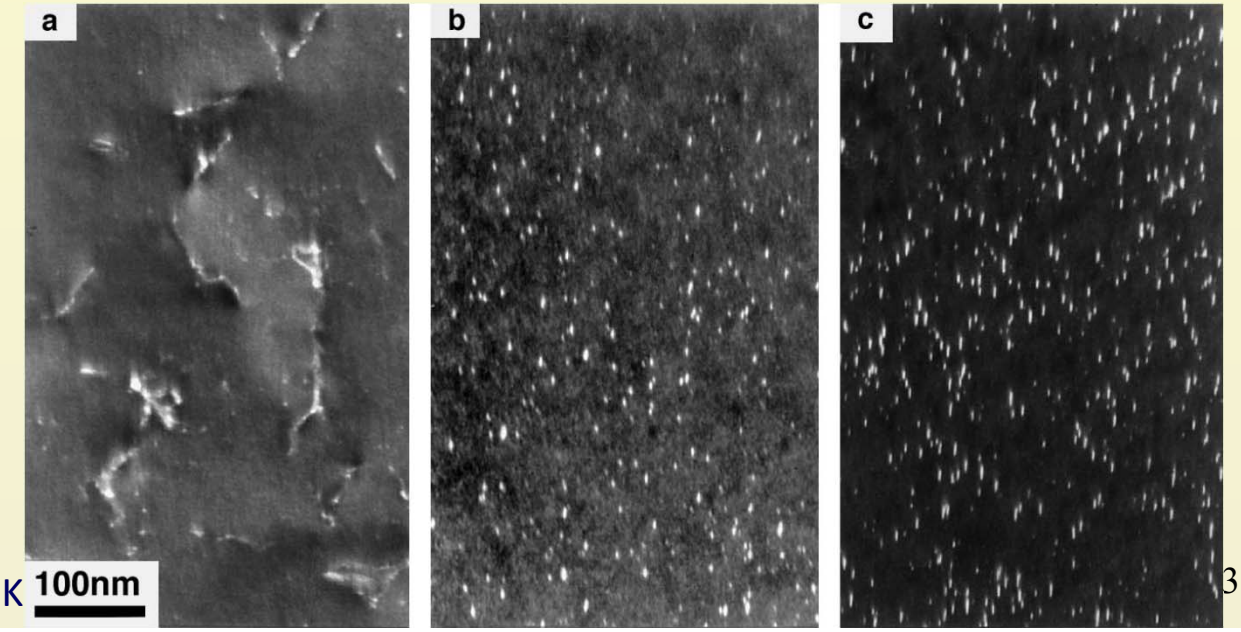


3nm

0.6 dpa neutron, Fe-12%Cr alloys



Cr- and NiSiPCr- clusters



316LN, 3dpa,
T = 363 K, 523 K

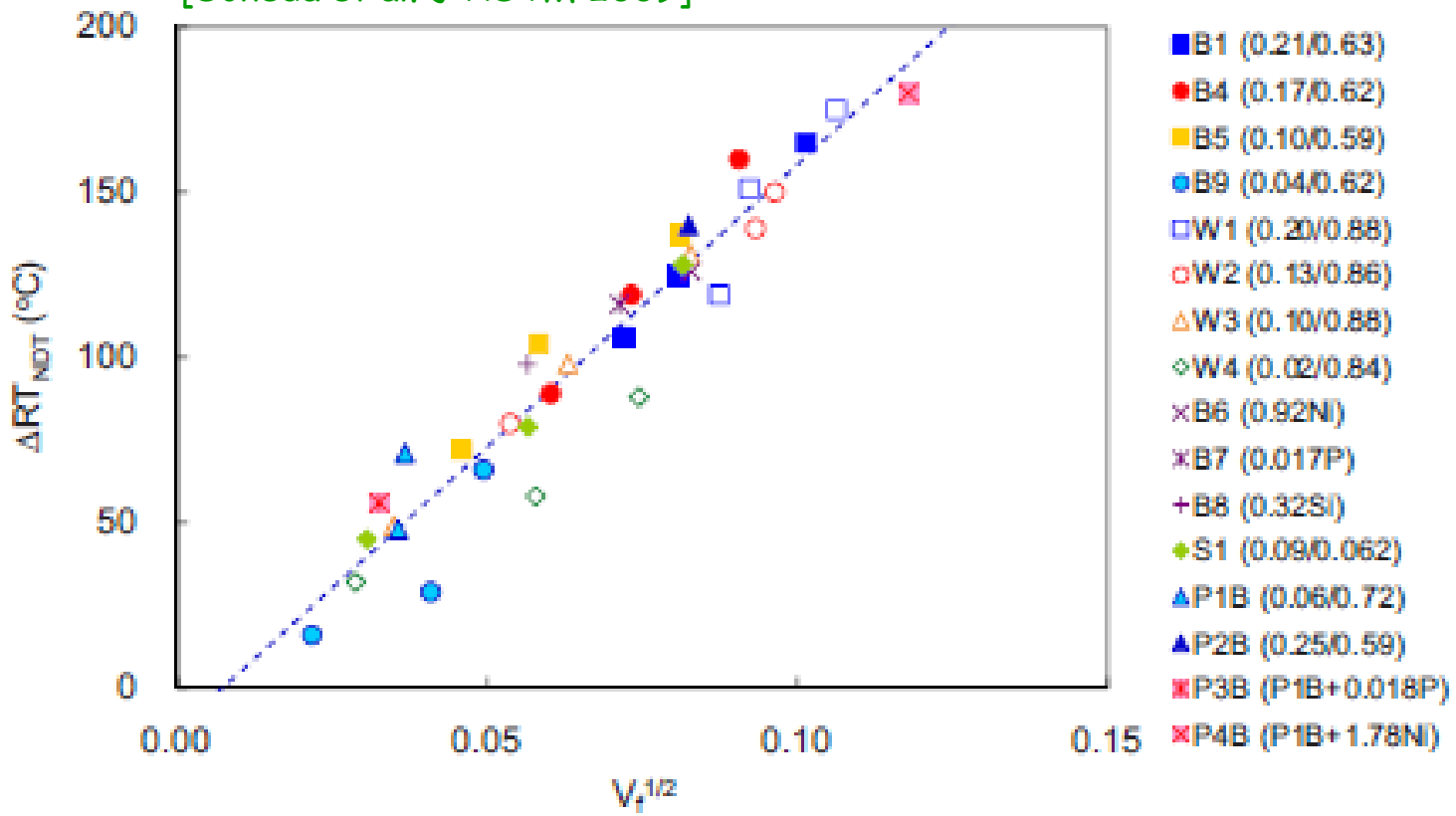
Irradiation induced hardening

Dose
Composition

Radiation
microstructure

Mechanical
properties

[Soneda et al. J ASTM 2009]



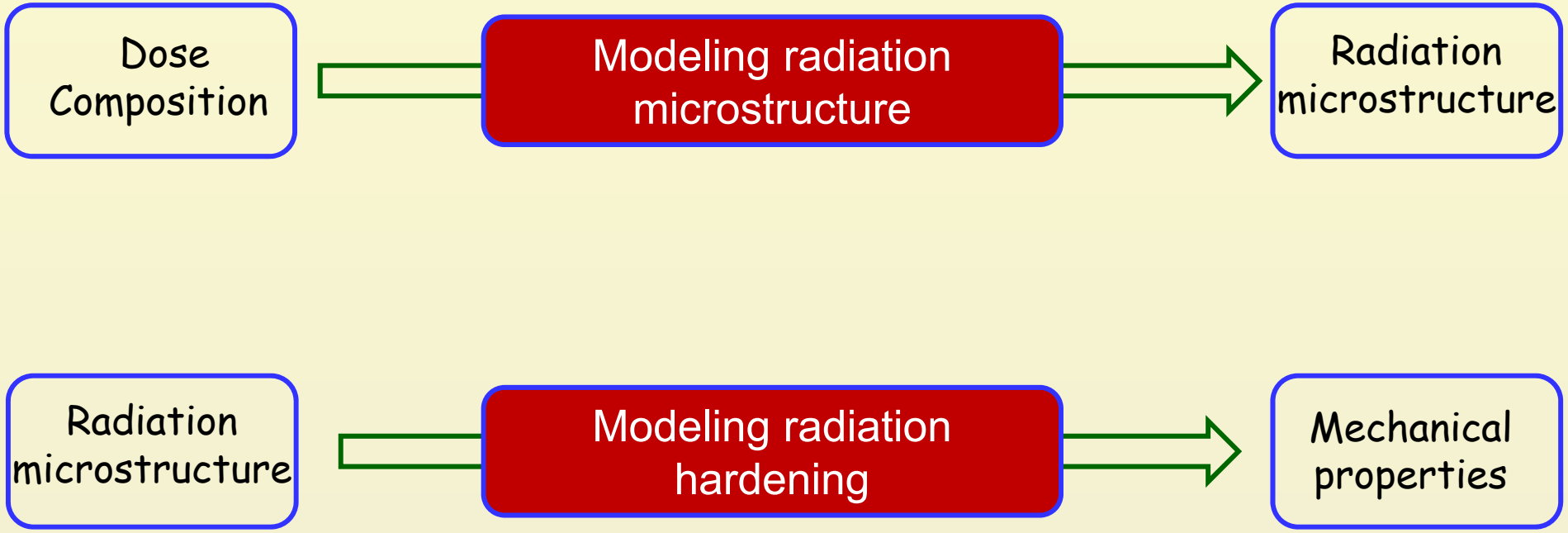
Transition temperature shift in RPV steels

Empirical (through microstructure) approach in predicting radiation

Multiscale modeling Irradiation induced hardening

From 2000, European projects on multiscale modeling : (REVE, SIRENA, PERFECT, PERFORM,..SOTERIA) with partners (EDF, CEA, SCK, …)

Modeling on physical basis of radiation effects on nuclear materails



Content

Two examples of multiscale modeling

Local obstacles

clusters and precipitates

Extended obstacles

Dislocation loops

Atomistic simulation results

Transition to the continuum level

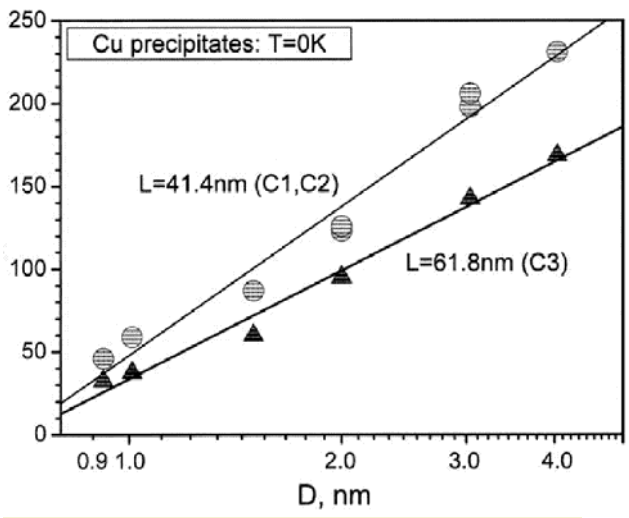
Prediction hardening at the grain scale

Conclusions and challenges

Atomistic results : interaction with solute clusters

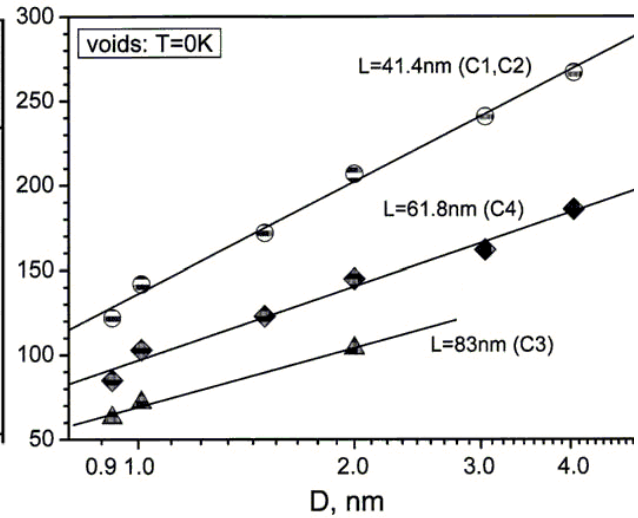
- Simulate dislocation-defect interaction
- Compute the critical stress necessary to unpin from defects
- Evidences of strong interaction with precipitates and voids
- Results depend on the atomistic simulation box

Cu precipitates



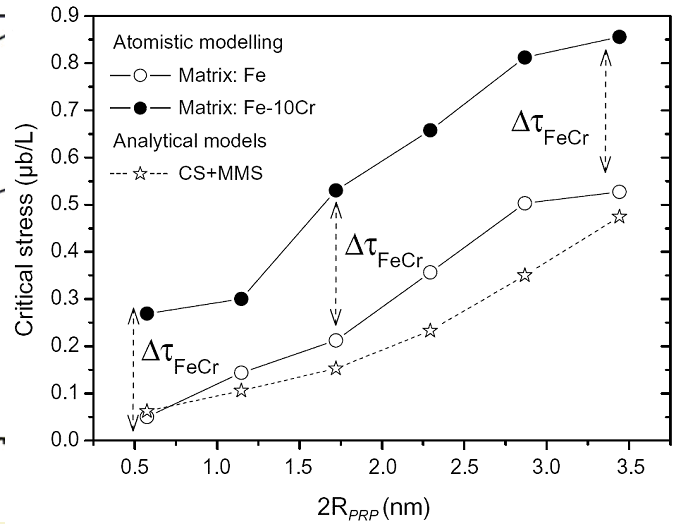
[Osetsky et al. JNM, 2003]

Voids



[Osetsky et al Phil Mag 2003]

Cr precipitates

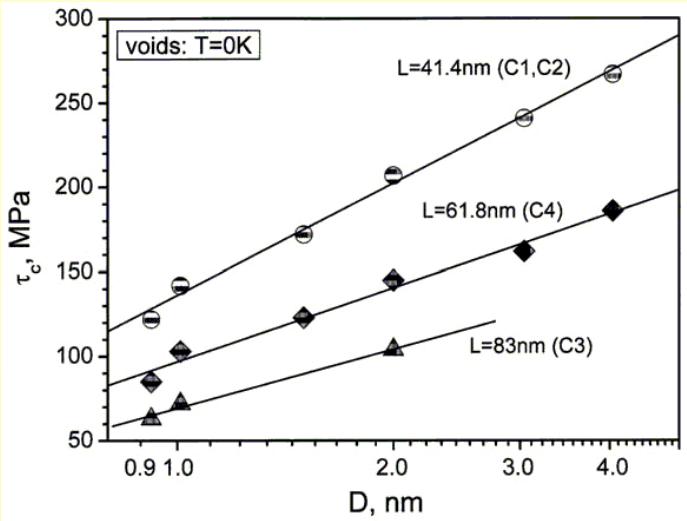


[Terentyev et al. Acta Mat 2008]

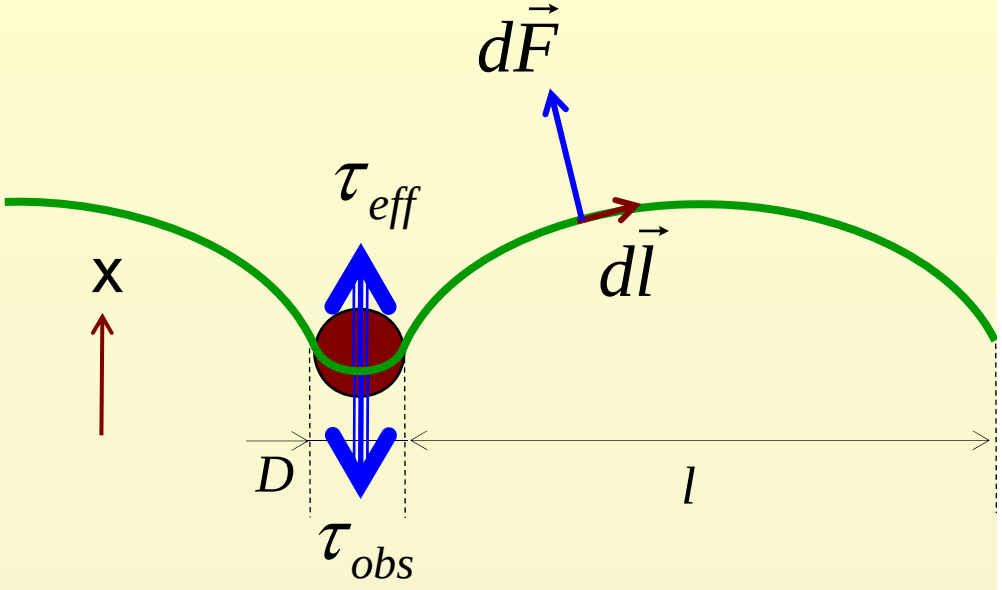
How to use these results at larger scale ?

Scale transition to continuum level

Voids



[Osetsky et al Phil Mag 2003]



- Mechanical equilibrium $$F_{obs} = \int_L b\,\tau_{app}\vec{e}_x \cdot d\vec{l} = b\,\tau_{app} L = b\,\tau_{eff} D$$
- Definition of obstacle resistance $$\tau_{obs} = \frac{L}{D}\tau_{\max}$$
- τ_{obs} accounts for all interaction mechanisms (lattice, chemical, modulus, etc.)
- τ_{obs} can be used in DD simulations

Scale transition to continuum level

Application to defects in RPV steels

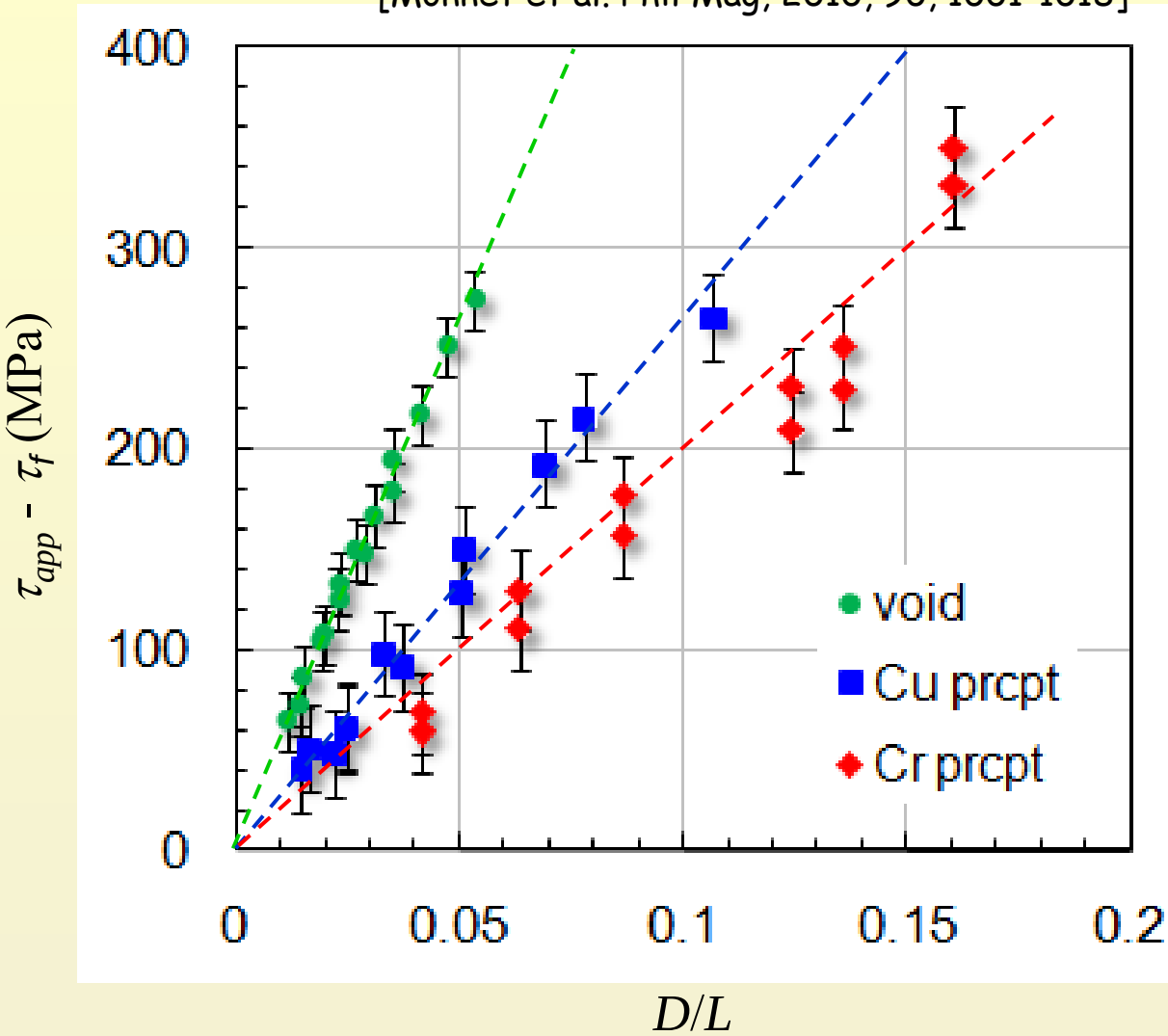
$$\tau_{\max} - \tau_f = \frac{D}{L}\tau_{obs}$$

$$\tau_{voids} = 4.7\ \text{GPa}$$

$$\tau_{Cu\ prcp} = 2.4\ \text{GPa}$$

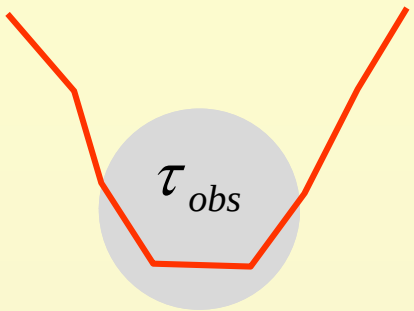
$$\tau_{Cr\ prcp} = 2.1\ \text{GPa}$$

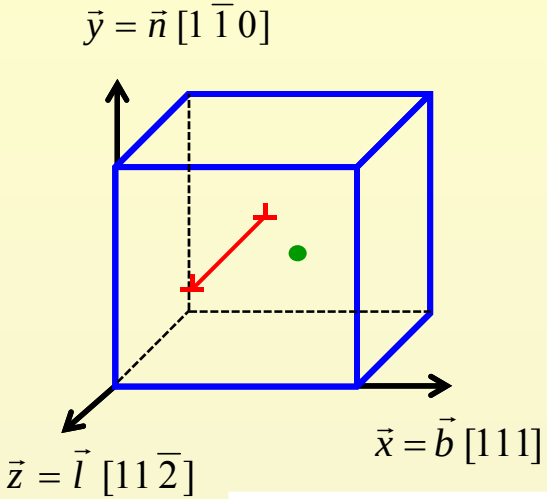
[Monnet et al. Phil Mag, 2010, 90, 1001-1018]

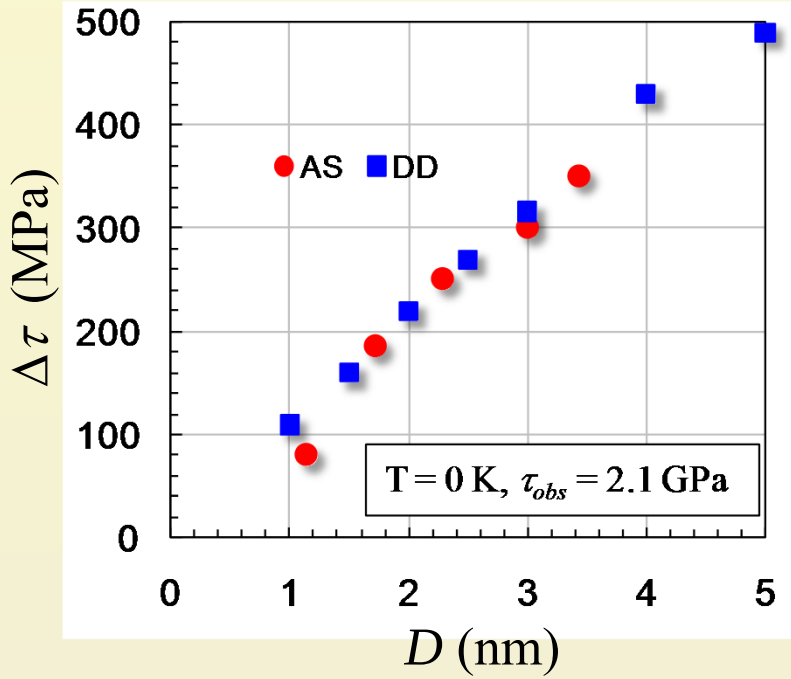


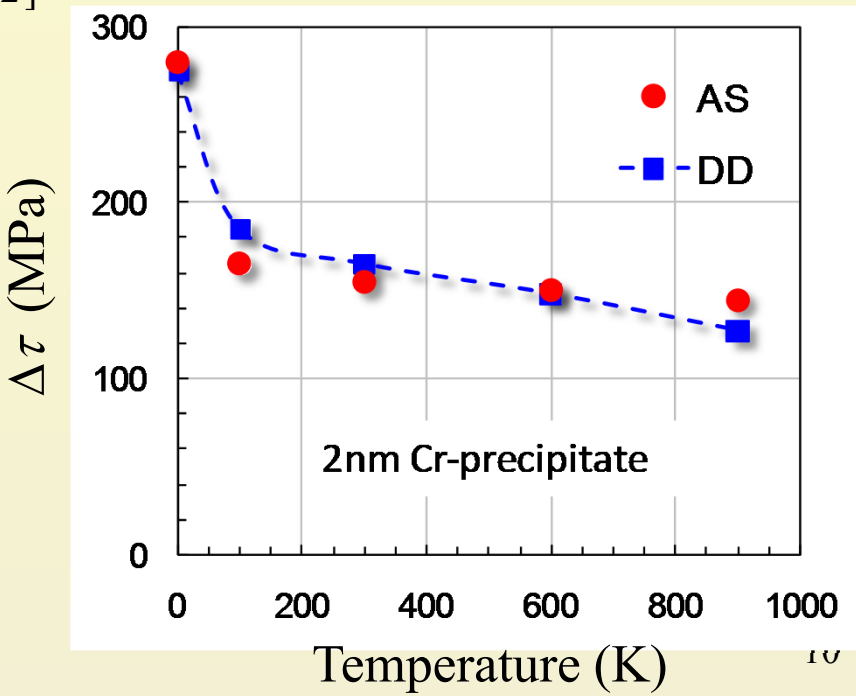
Scale transition to continuum level

Modeling of dislocation interaction with precipitates



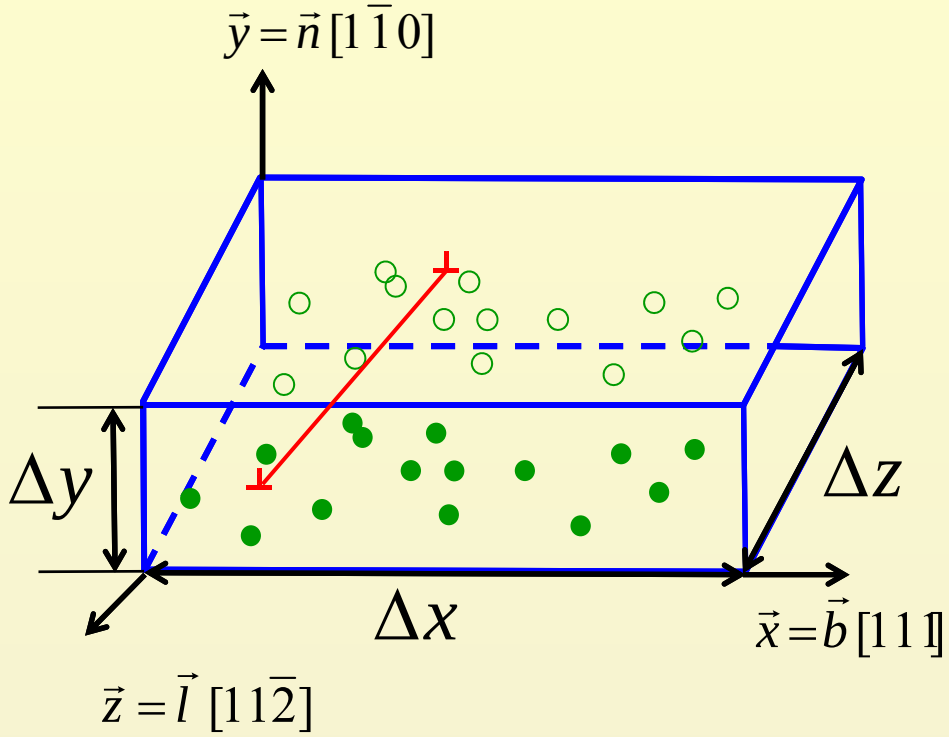






Modeling radiation hardening at the grain scale

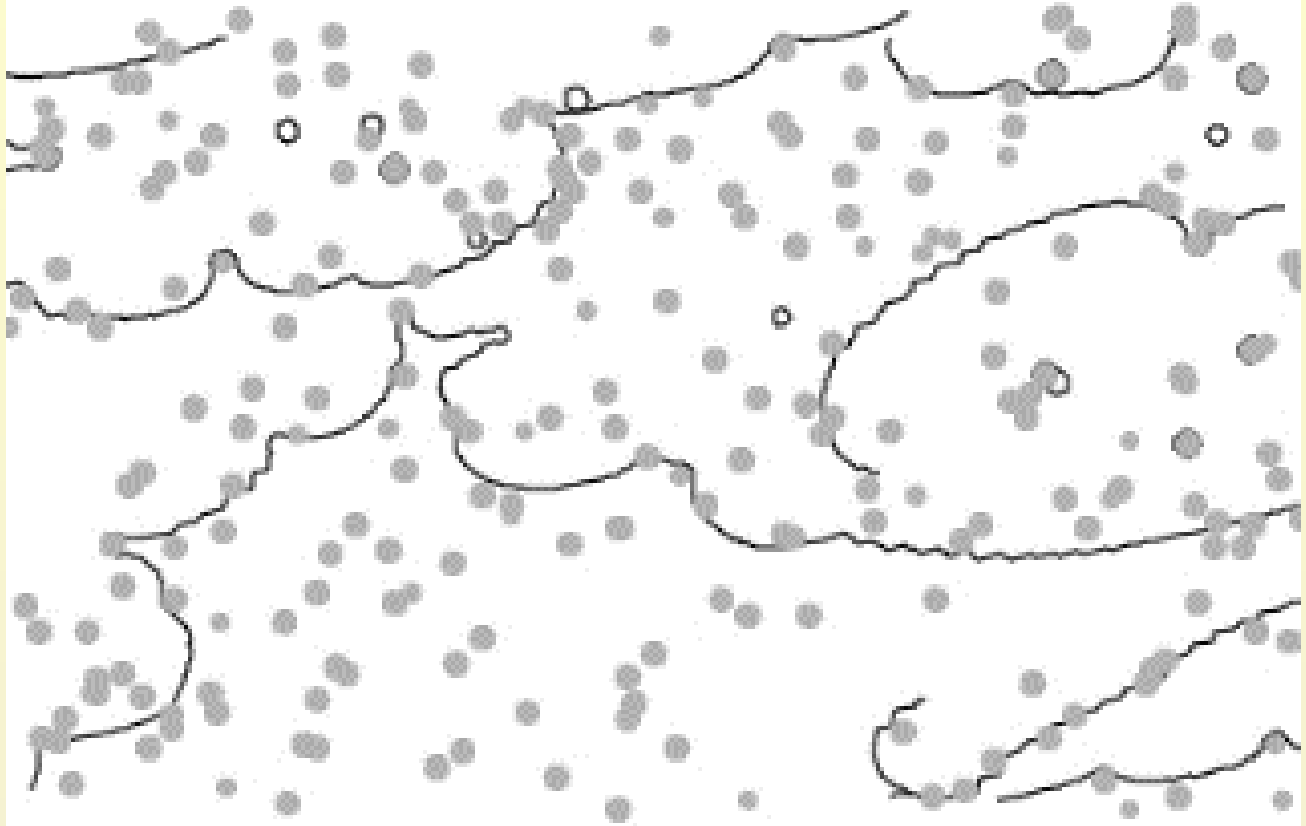
Modeling of dislocation interaction with precipitates



- 20 000 precipitates
- Random distribution
- Dislocation length > 20 l
- D = 1, 2, 4 nm
- C = 10^{23} – 810^{24} m^{-3}

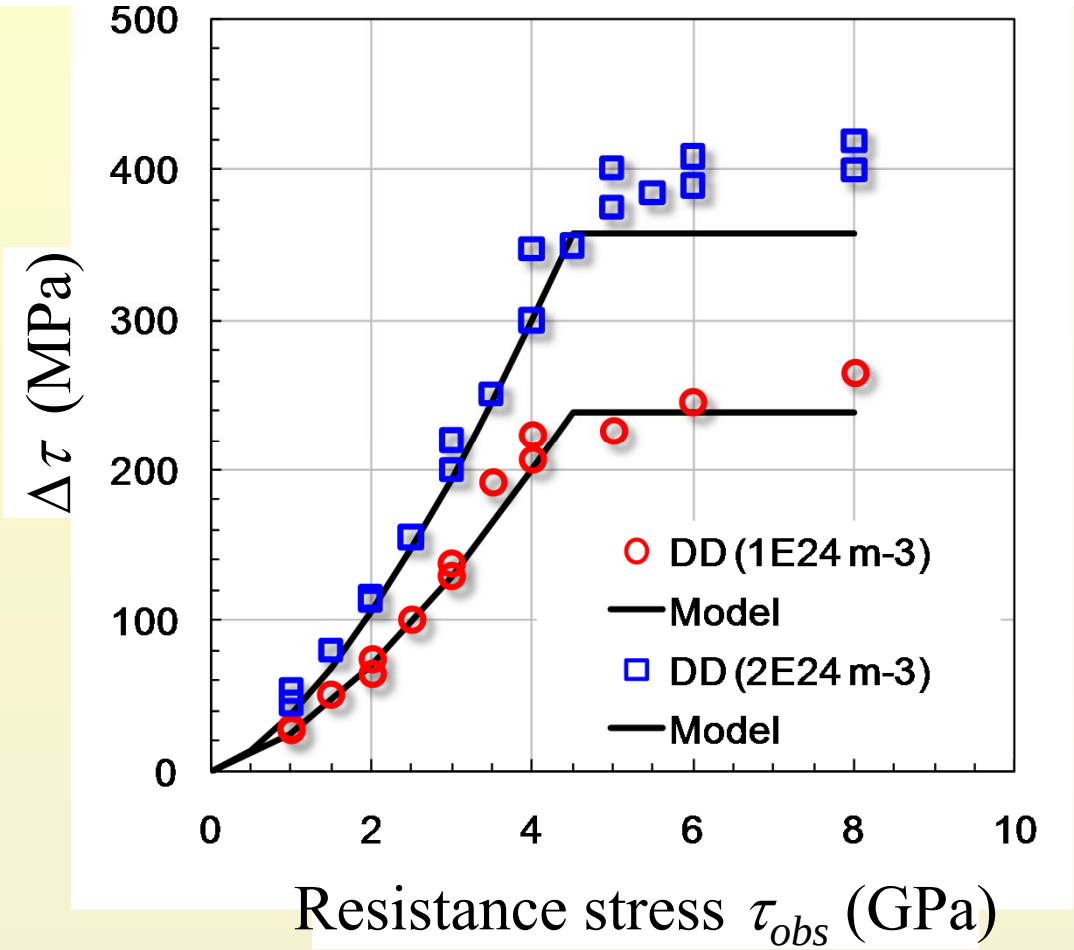
Modeling radiation hardening at the grain scale

Simulations of hardening induced by Orowan obstacles



Modeling radiation hardening at the grain scale

Constitutive equation for hardening induced by local obstacles

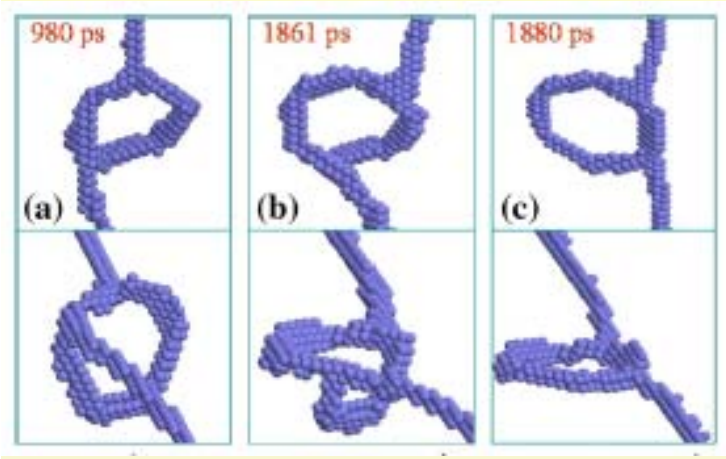


[Monnet, Acta Mat 2015]

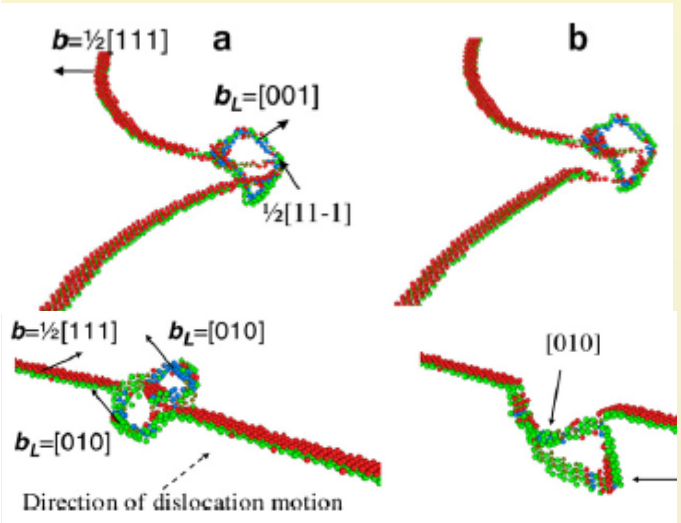
$$\Delta\tau = \left(\frac{\tau_{obs}}{\tau_\infty} \frac{\ln 2D}{\ln 2l} \right)^{3/2} \frac{\mu}{2\pi l} \ln(2l), \quad l = \frac{1}{\sqrt{DC}} - D$$

Atomistic results : interaction with dislocation loops

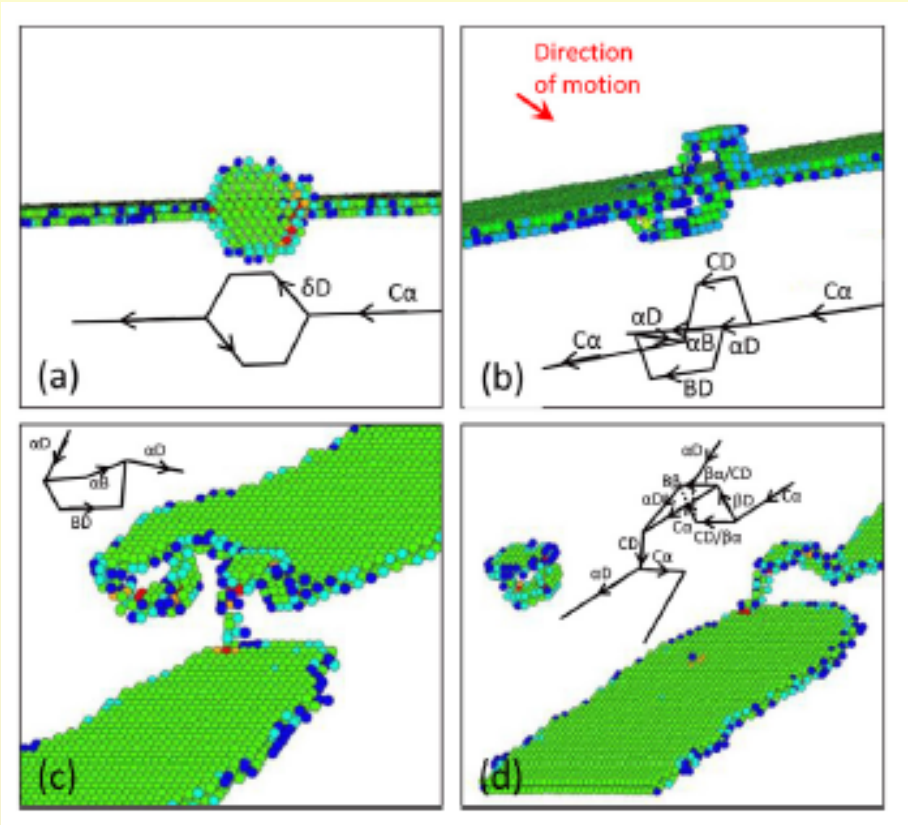
Screw vs $\frac{1}{2}$ [111] loop



Edge vs [100] loop



FeNiCr alloys



Edge vs Frank loops

[Liu et al. Scripta 2008]

[Terentyev et al. Acta Mat 2008]

[Baudouin et al, JNM 2015]

Scale transition to continuum level

Dislocation interaction with loops at the continuum level

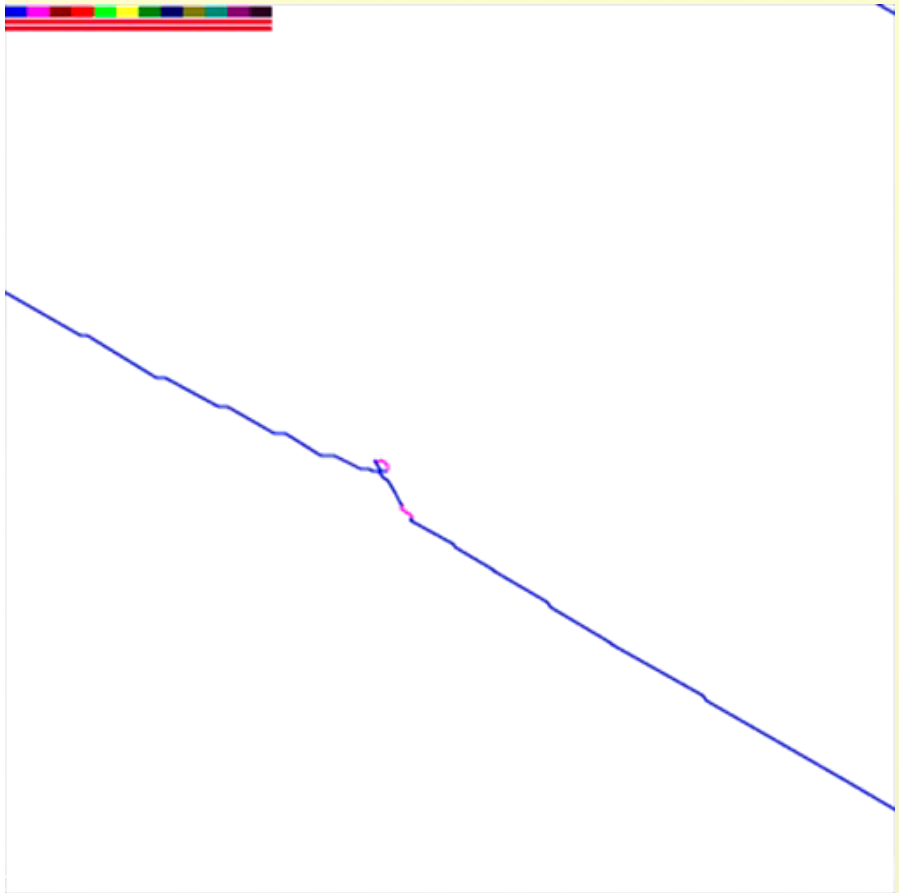
Large variety of interaction mechanisms depending on

- Effect of loop size, nature and orientation
- Effect of temperature and strain rate
- Effect of dislocation character

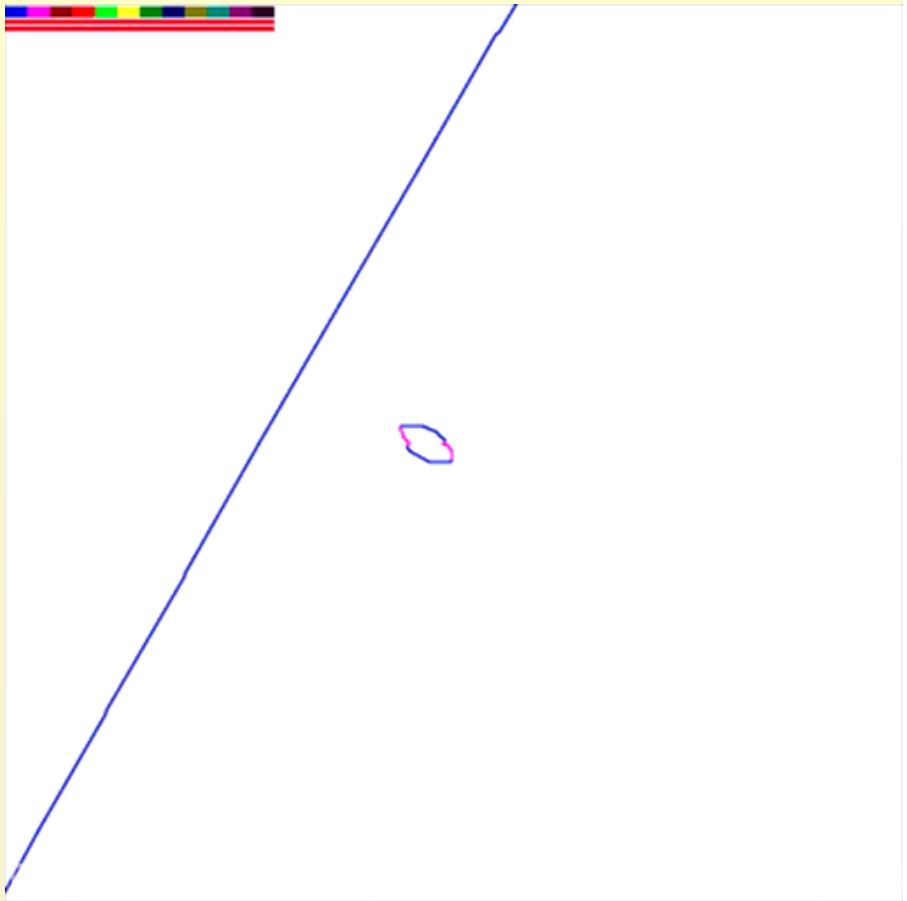
General trends

- Large dislocation loops are sheared
- Small dislocation loops are absorbed

Modeling radiation hardening at the grain scale

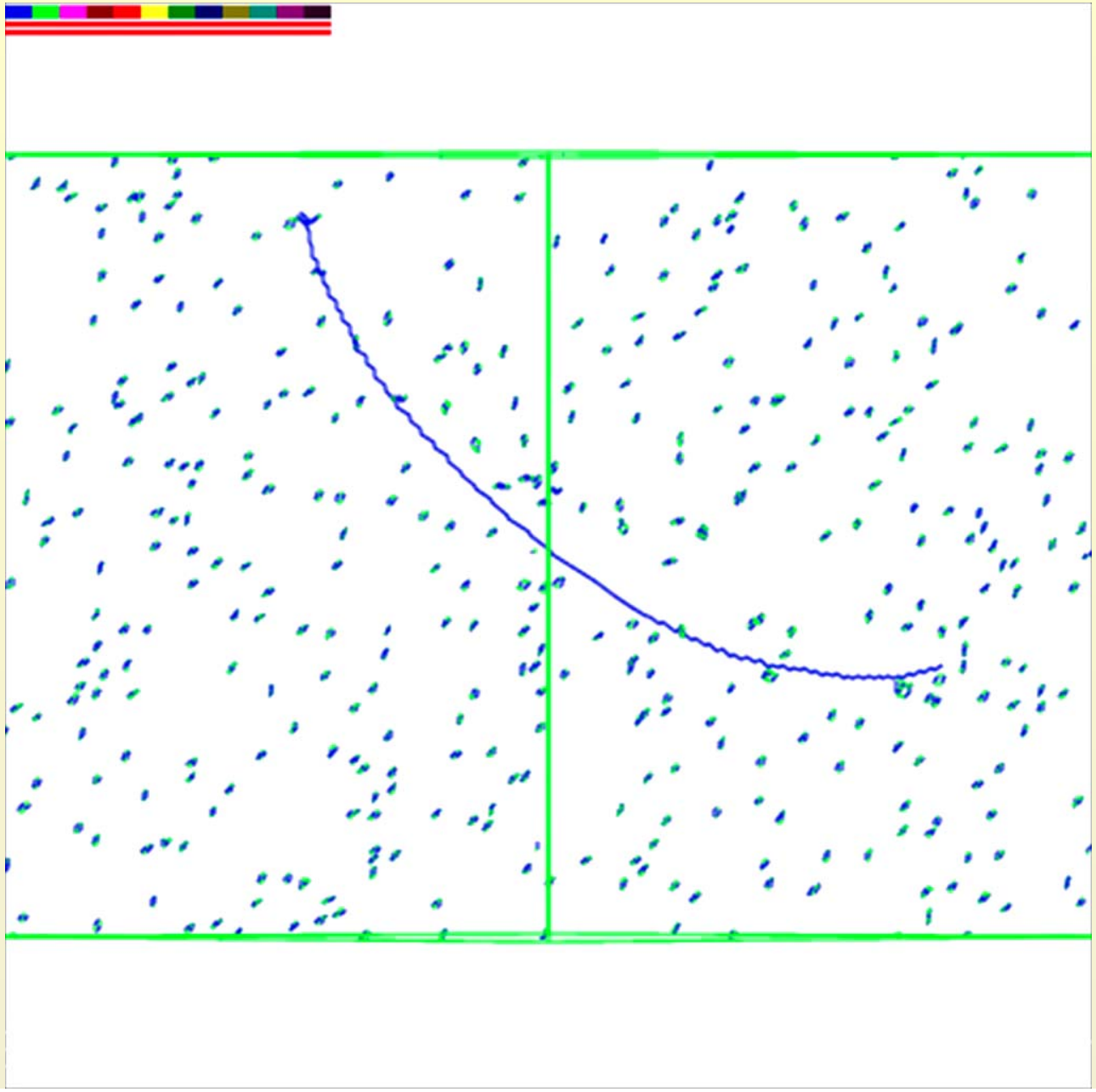


Absorption by edge dislocation



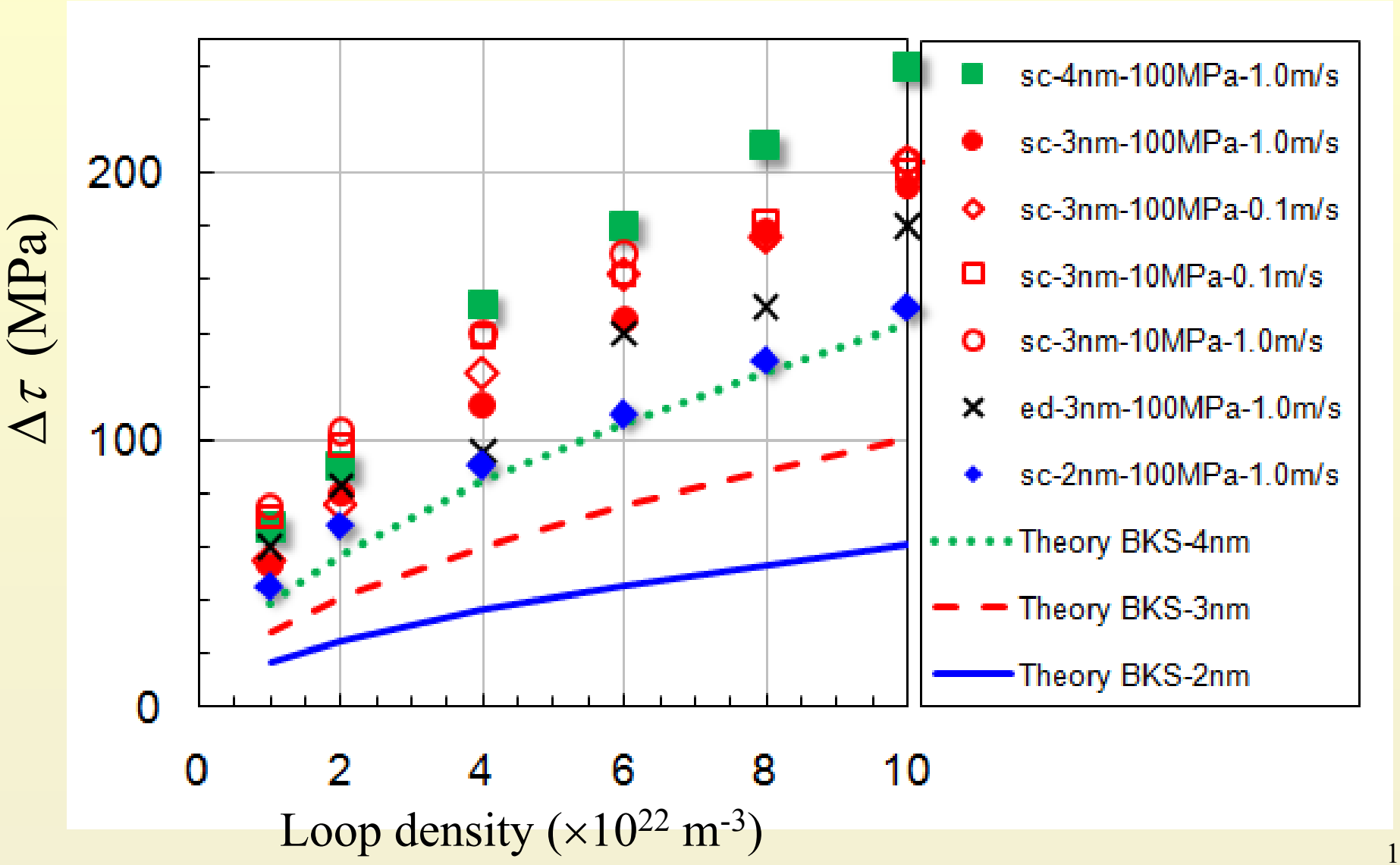
Absorption by screw dislocation

Modeling radiation hardening at the grain scale

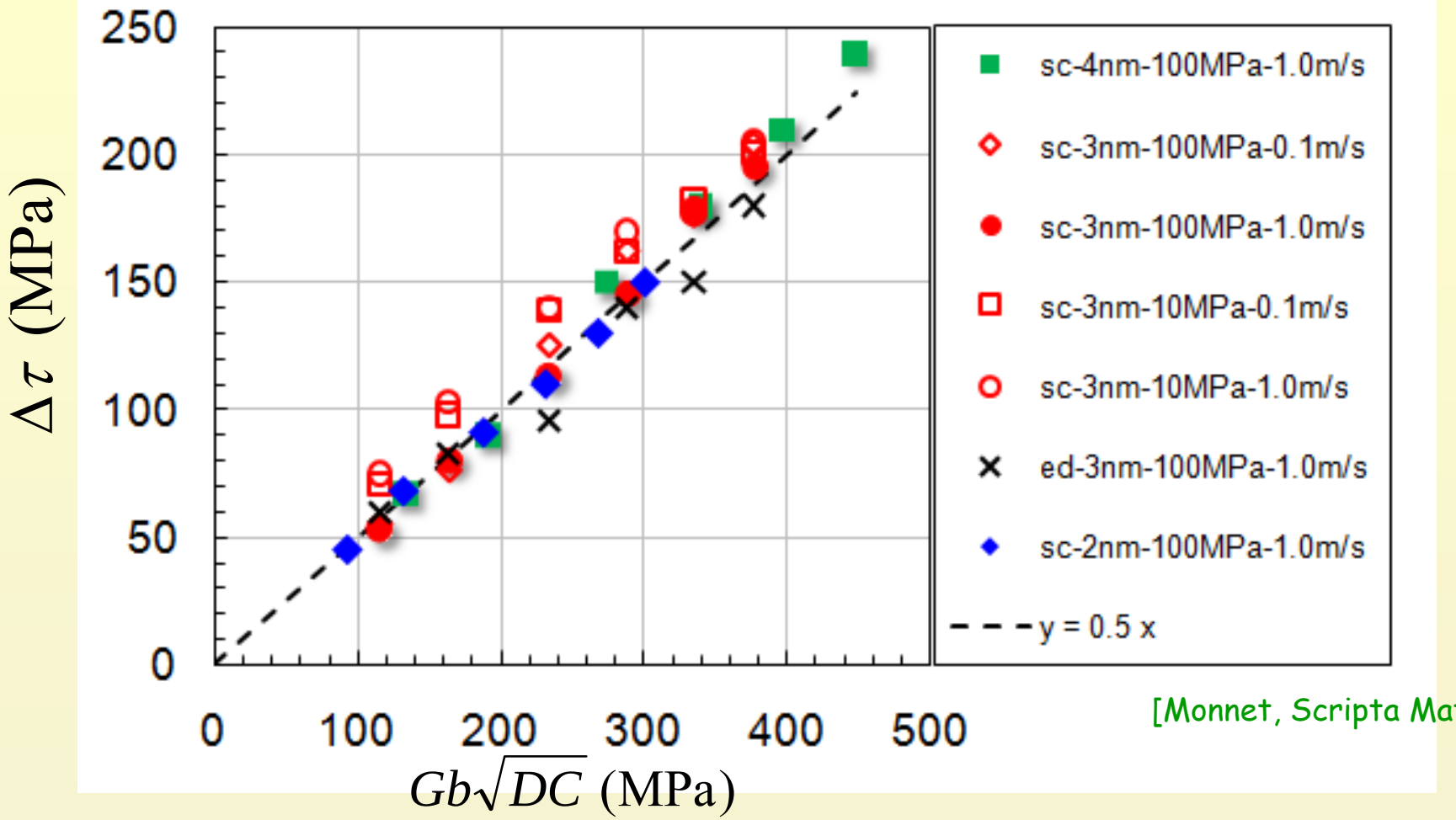


Modeling radiation hardening at the grain scale

[Monnet, Scripta Mat 2015]



Modeling radiation hardening at the grain scale



[Monnet, Scripta Mat 2015]

$$\Delta\tau = 0.5\,Gb\sqrt{DC}$$

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

Conclusions & challenges

Achievements of multiscale modeling:

- Atomistic simulations of edge dislocation
- Interactions with simple defects (Cr, Cr prcp, loops, voids, SFT, etc.)
- Dislocation Dynamics simulations of precipitation hardening
- DD simulations of hardening induced by small loops
- Construction of crystalline laws for RPV and internal steels

Future challenges:

- Prediction and modeling of radiation microstructure
- Investigating solute segregation effects (decoration, mobility, strength)
- Dislocation interaction with grain boundaries
- Accounting for softening in crystalline laws in macroscopic modeling
- Allowing for mesh-independent strain heterogeneity