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

Ghiath Monnet

MMC, EDF -R&D, Les Renardières, France
Irradiation induced hardening

Material + Dose

Mechanical properties

[Rawel 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

0.6 dpa neutron, Fe-12%Cr alloys

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

Cr- and NiSiPCr- clusters
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 materials
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

Voids

Cr precipitates


How to use these results at larger scale?
Scale transition to continuum level

**Voids**

Voids: $T=0K$

- 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
  \[ \tau_{obs} = \frac{L}{D} \tau_{max} \]

- $\tau_{obs}$ accounts for all interaction mechanisms (lattice, chemical, modulus, etc.)

- $\tau_{obs}$ can be used in DD simulations

[Osetsky et al Phil Mag 2003]
Scale transition to continuum level

Application to defects in RPV steels

\[ \tau_{\text{max}} - \tau_{f} = \frac{D}{L} \tau_{\text{obs}} \]

- \( \tau_{\text{voids}} = 4.7 \text{ GPa} \)
- \( \tau_{\text{Cu prcp}} = 2.4 \text{ GPa} \)
- \( \tau_{\text{Cr prcp}} = 2.1 \text{ GPa} \)

[Monnet et al. Phil Mag, 2010, 90, 1001-1018]
Scale transition to continuum level

Modeling of dislocation interaction with precipitates

\[ \tau_{\text{obs}} \]

\[ \bar{\gamma} = \bar{n} \{1 \overline{1} 0\} \]

\[ \bar{z} = \bar{l} \{11 \overline{2}\} \]

\[ \bar{x} = \bar{b} \{111\} \]

\[ \Delta \tau \text{ (MPa)} \]

\[ T = 0 \text{ K, } \tau_{\text{obs}} = 2.1 \text{ GPa} \]

\[ \Delta \tau \text{ (MPa)} \]

\[ 2\text{nm Cr-precipitate} \]

\[ \text{Temperature (K)} \]
Modeling radiation hardening at the grain scale

Modeling of dislocation interaction with precipitates

- 20,000 precipitates
- Random distribution
- Dislocation length > 20 \( \ell \)
- \( D = 1, 2, 4 \) nm
- \( C = 10^{23} - 8 \times 10^{24} \) 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

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

[Monnet, Acta Mat 2015]
Atomistic results: interaction with dislocation loops

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

**FeNiCr alloys**

**Edge vs [100] loop**

**Edge vs Frank loops**

[Liu et al. Scripta 2008]
[Terentyev et al. Acta Mat 2008]
[Baudouin et al., JNM 2015]
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

\[ \Delta \tau = 0.5 \, Gb \sqrt{DC} \]

\[ \dot{C}^s = -\lambda \frac{D}{b} C^s |\dot{\gamma}^s| \]

[Monnet, Scripta Mat 2015]
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