SOTERIA

POST-IRRADIATION STRESS-STRAIN AND FRACTURE RESPONSE EVOLUTION DESCRIPTION OF RPV STEELS: RECENT AND FUTURE DEVELOPMENTS

7TH SEPTEMBER 2018

Contribution to SOTERIA WP5
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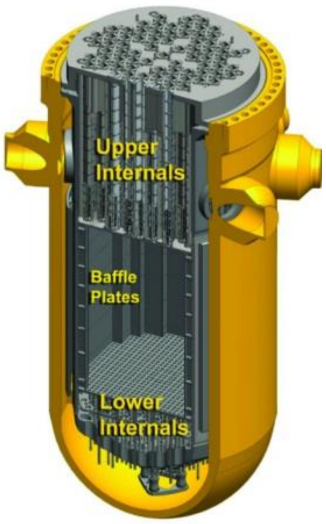
Speaker: **Christian Robertson**

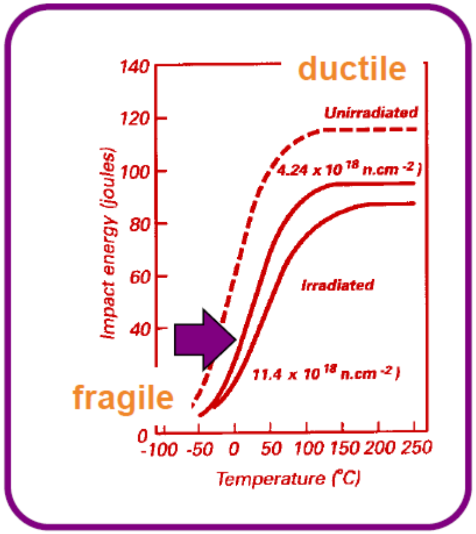
Long-term goal or vision: predicting dose-dependent fracture toughness response based on non-destructive post-irradiation examinations (material polycrystalline microstructures, i.e. grain sizes and orientations; irradiation defect microstructures) and physically based models

☞minimizing/optimizing time-consuming/costly mechanical testing of post-irradiated specimens in hot cells

Cross-cutting WP2/WP3/WP5 issue

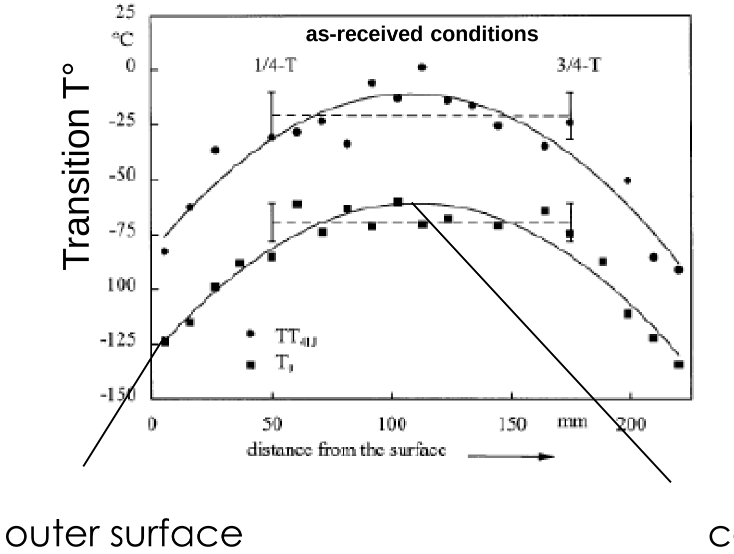
Thick-walled components: microstructure and fracture toughness variability





Initial microstructural variations: a major contributing factor

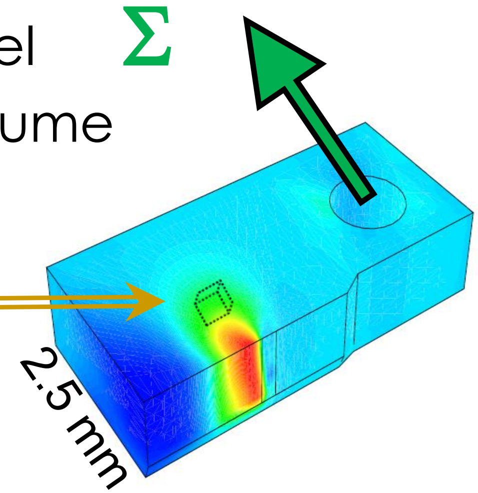
H.V. Viehrig et al. Nucl. Engi. Des. 212 (2002) 115-124

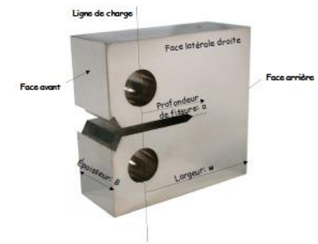


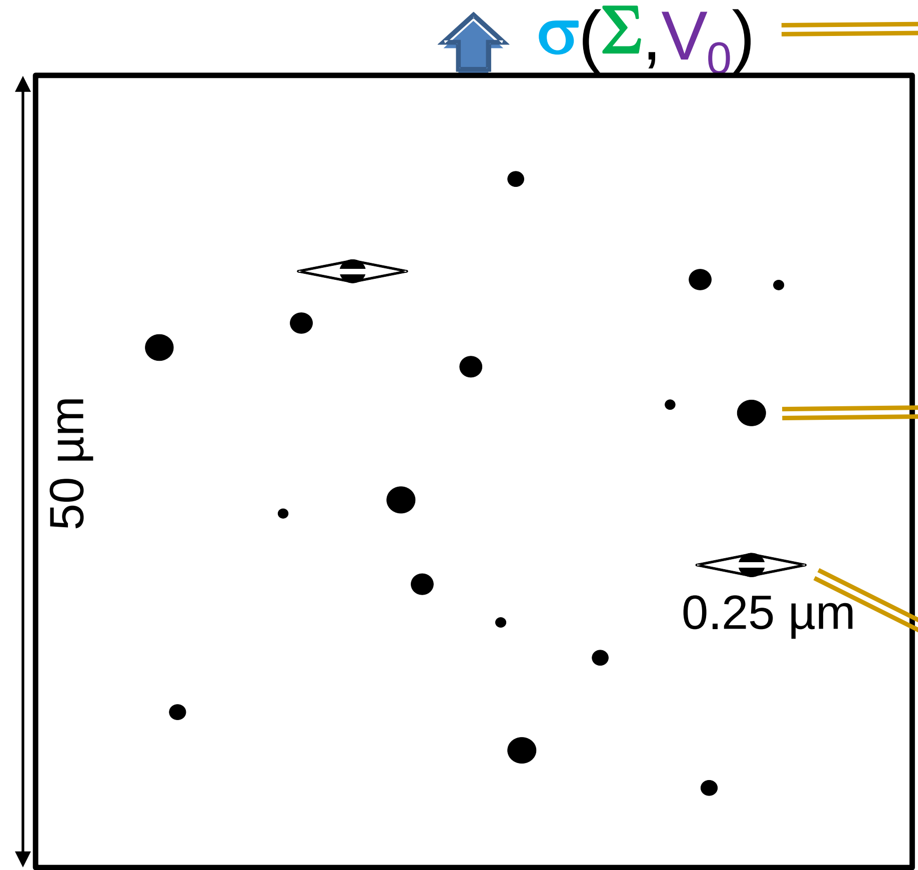
☞Modelling efforts adressing: dose-dependent fracture response and its scattering

«Local Brittle Fracture models»

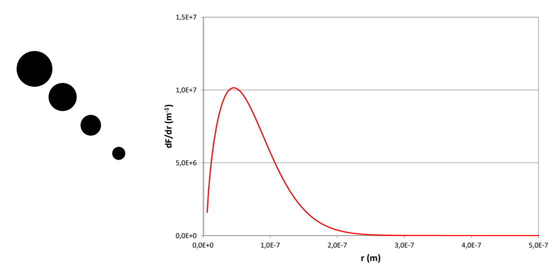
- Σ : CT specimen-scale loading level
- V_0 : representative elementary volume
- σ : stress level acting on $V_0(r)$







- Particle size distribution: f(r) = dF/dr:



- «Griffith» crack propagation criteria:

$$\sigma_c = \sqrt{\frac{\pi}{2(1-\nu^2)} \cdot \frac{E \cdot \gamma_f}{r}}$$

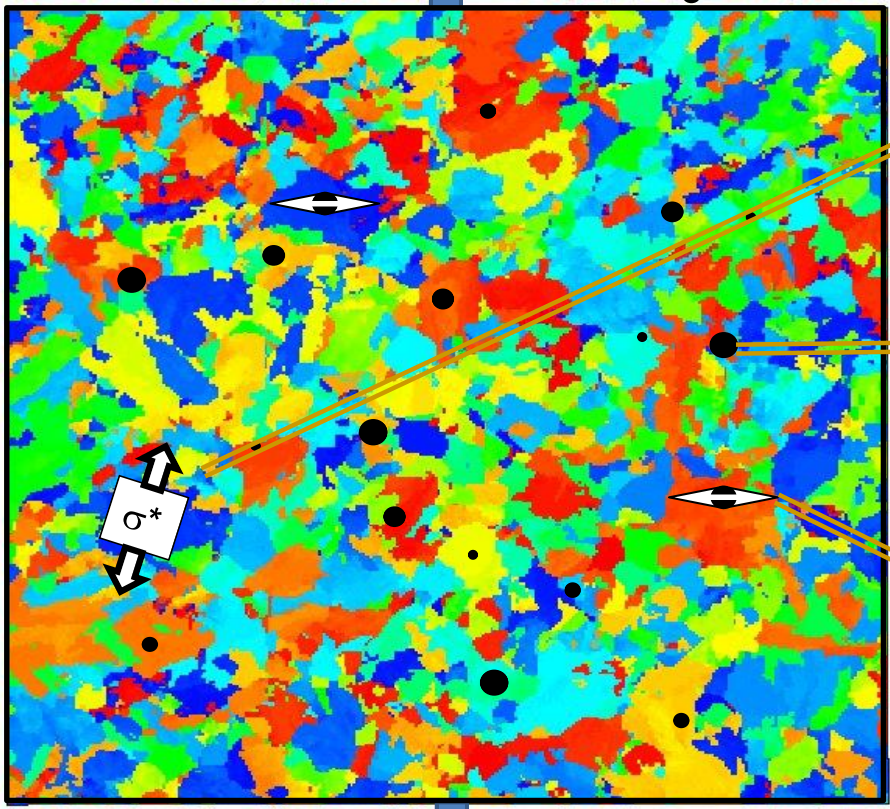
…including local stress distribution (MIBF)

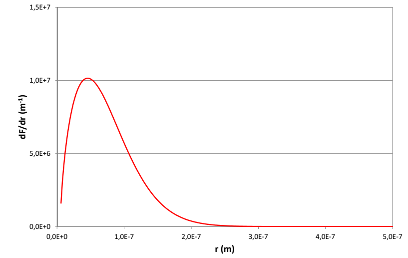
➢ **MIBF model INPUTS** : irradiation-induced hardening level, particle size distribution, surface energy, grain-size, grain orientation, grain-scale stress fields

J. Nucl. Mat. 406 (2010) 91-96

RPV steel microstructure
$\Rightarrow$ local stress distribution σ^* inside V_0

$\sigma(\Sigma, V_0)$

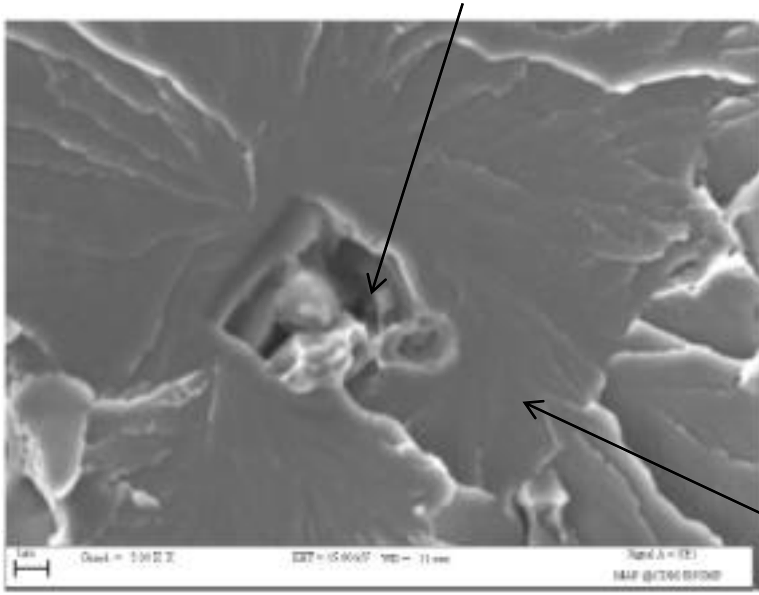




$$\sigma_c = \sqrt{\frac{\pi}{2(1-\nu^2)} \cdot \frac{E \cdot \gamma_f}{r}}$$

Weakest link assumption

Cracked inclusion: brittle fracture initiator



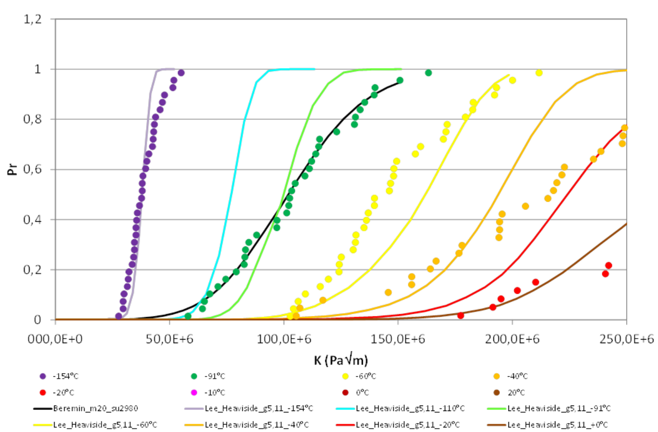
Cleavage fracture surface

<u>Weakest leak assumption</u>

I- all inclusions/particles break down, for $\varepsilon > \varepsilon_{p0}$
II- micro-cracks grow (or not) according to a definite criteria
III- first micro-crack develops $\rightarrow$ the whole specimen fails

IV- **fracture toughness then directly relates to plastic zone size a_0, near the micro-crack initiators**

Failure probability



load

$\Rightarrow$ Transition curves, DBT shift

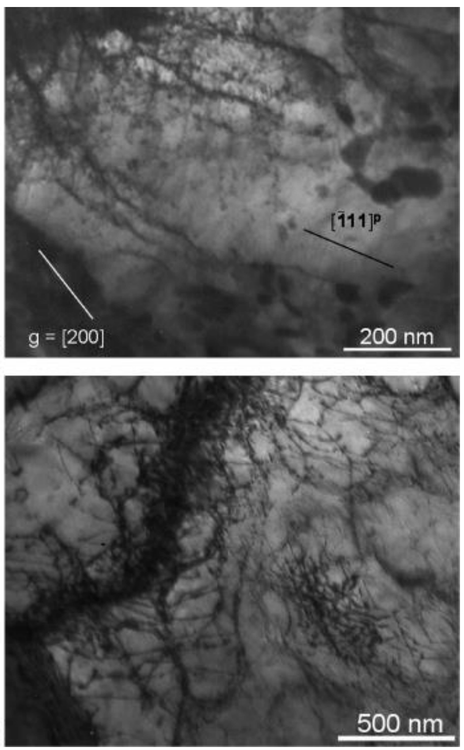
Micro-crack induced plastic zone?

Q. Effect of straining temperature on a_0?
Q. Grain size and orientation effect on a_0?
Q. Dose effect, irradiation temperature effect, on a_0?

R. Crack-induced plasticity: dislocation-mediated

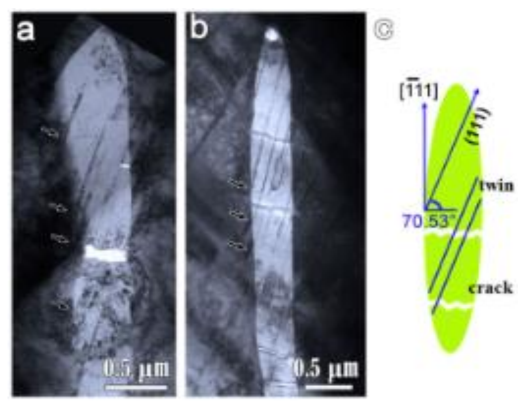
☞ **«Statistical, investigation of post-irradiation plasticity mechanisms using, 3D DD simulations»**

☞Dislocation Dynamics simulations?



(a)
(b)

Modelling Simul. Mater. Sci. Eng. **18** (2010) 025003



MnS in steel, Sci. Reports 4, 5118 (2014)

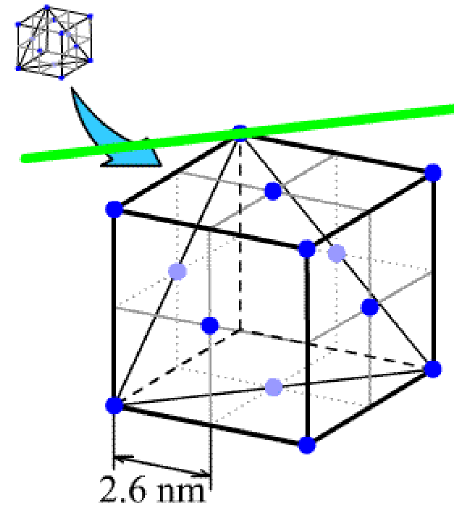
Dislocation dynamics simulations?

« TRIDIS » code

Model. Simul. Mater. Sci. Eng. 6 (1998) 755-770

Dislocation Model

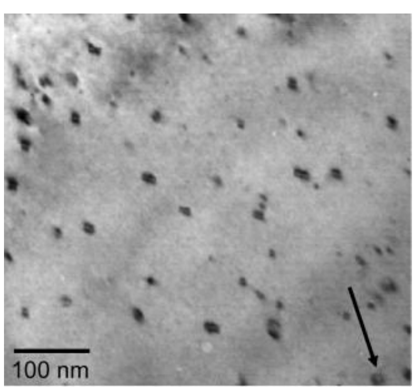
- Discrete dislocation lines
- Discrete time steps: 10^{-10} s
- Discrete bcc lattice



Stress → **D**islocation **D**ynamics code → Dislocation microstructures, Plastic strain

Dislocation theory

→ Dislocation mobility (stress and T° dependent)
→ Interaction with radiation defects, other dislocations, GB…
→ Cross-slip



Dislocation stress-velocity response

FCC models (Cu, FCC Fe)

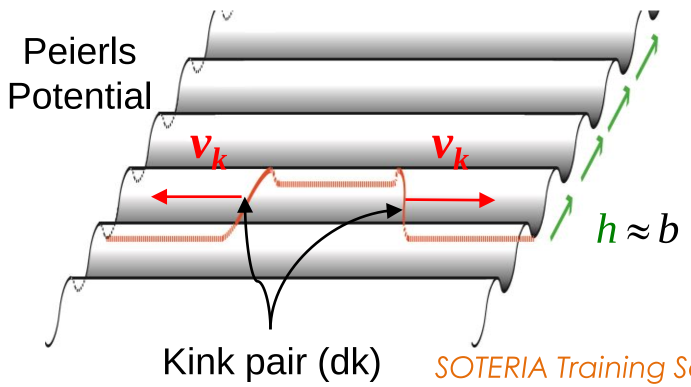
Screw ~ Edge

Negligible Peierls barrier (τ_p~10 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 and Fe alloys

Screw ≠ Edge

Velocity anisotropy depends on T°

Low temperature

Significant Peierls barrier (τ_p~1GPa)

Thermally activated mobility

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

High temperature

Athermal regime

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

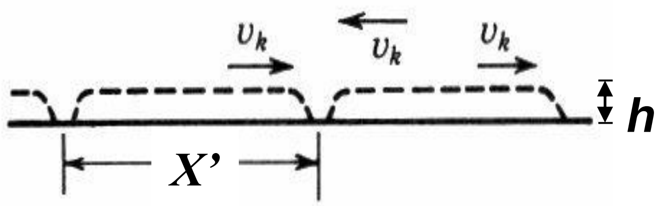
Low-T screw dislocation mobility mechanism

- **Nucleation** of a kink pairs (thermally activated)
- Kink pair **propagation** $v_k \propto \tau$ « effective » $B_k < B_{edge}$

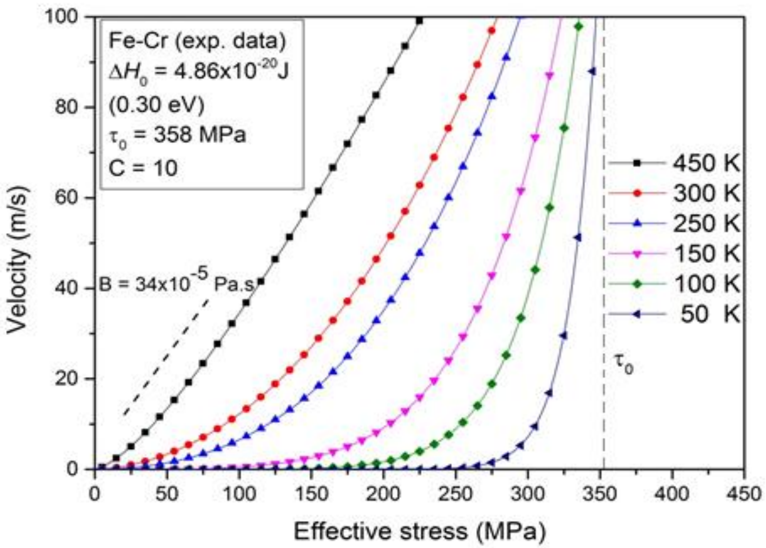
Dislocation mobility rules for RPV steels

Journal of Nuclear Materials 504 (2018) 84-93

$$v_{screw} = hJX'$$



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



$$v_{screw}(\tau^*, T) = \underbrace{\frac{8\pi b(\tau^*)^2}{\mu B h}}_{} X' \exp\left(-\frac{\Delta G(\tau^*, T)}{k_B T}\right)$$

Stress-dependent pre-factor

☞ **Progressive transition from Low-T to Room-T**

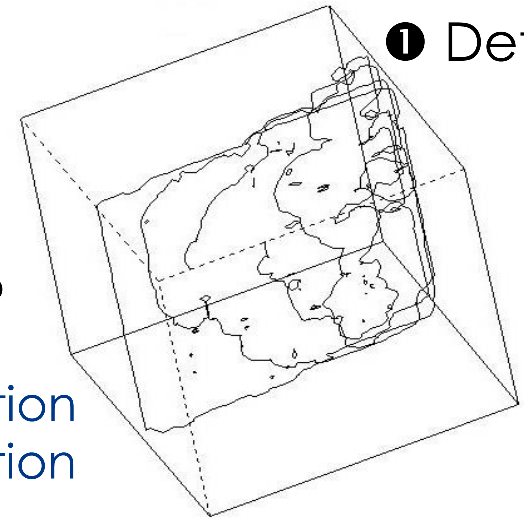
DD simulation setup

1μm³ ferritic grains (Fe-C or Fe-Cr):

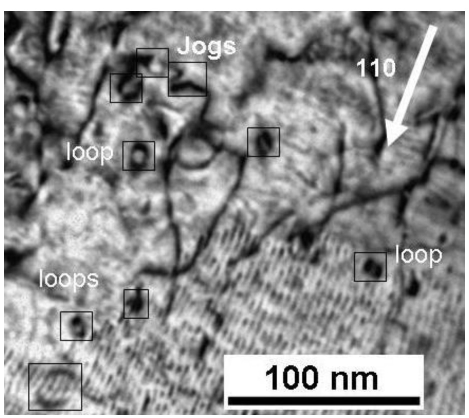
- Defect number density and defect size depend on selected dose and T_{irr} condition
- Uni-axial tension, strain-rate controlled conditions, fixed straining T°, presence of cross-slip

- **Model INPUTS**: grain size, kink-pair activation energy, phonon drag coefficient, irradiation defect size, and number density

❶ Defect-free

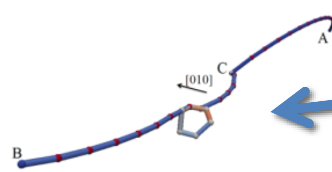


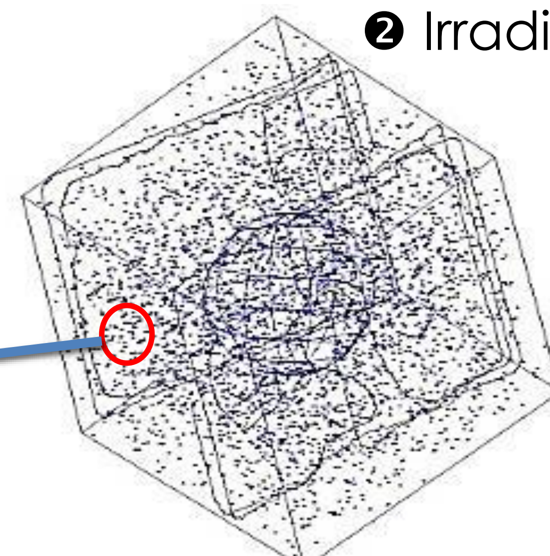
❷ Irradiated



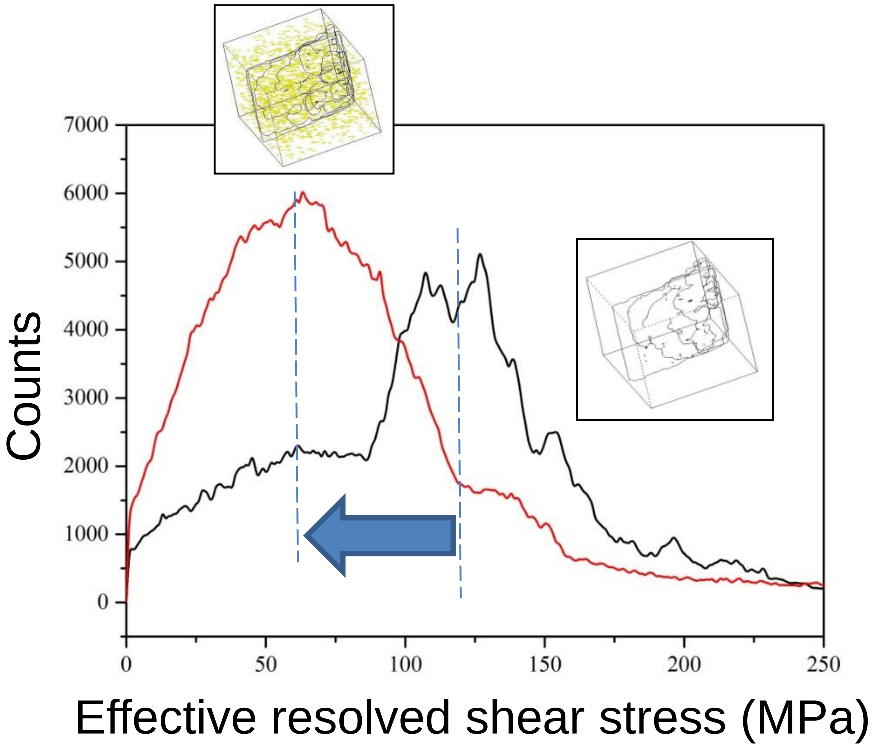
T_{irr}=400°C, dose = 1 dpa, defect size D = 50 nm

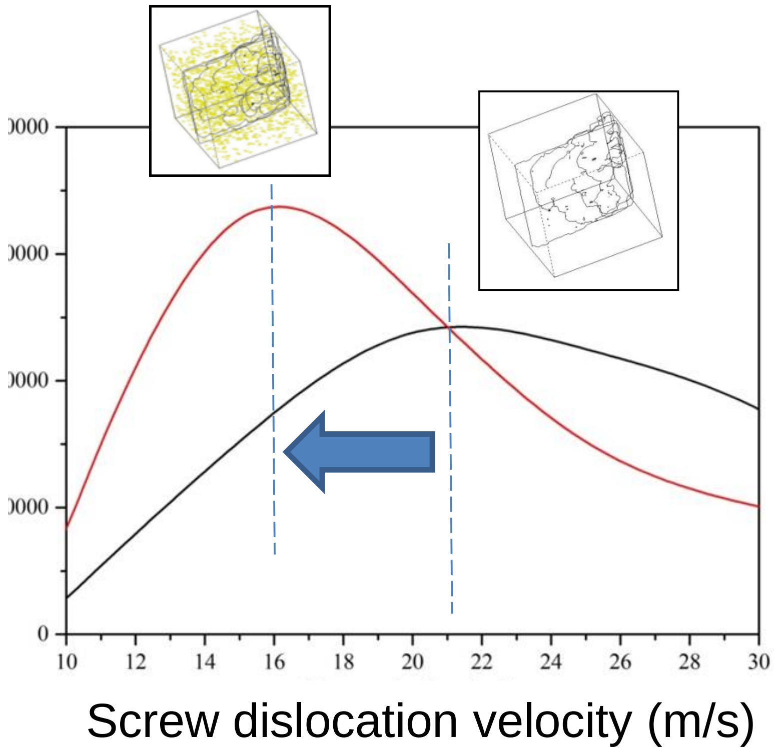
dislocation/defect interactions





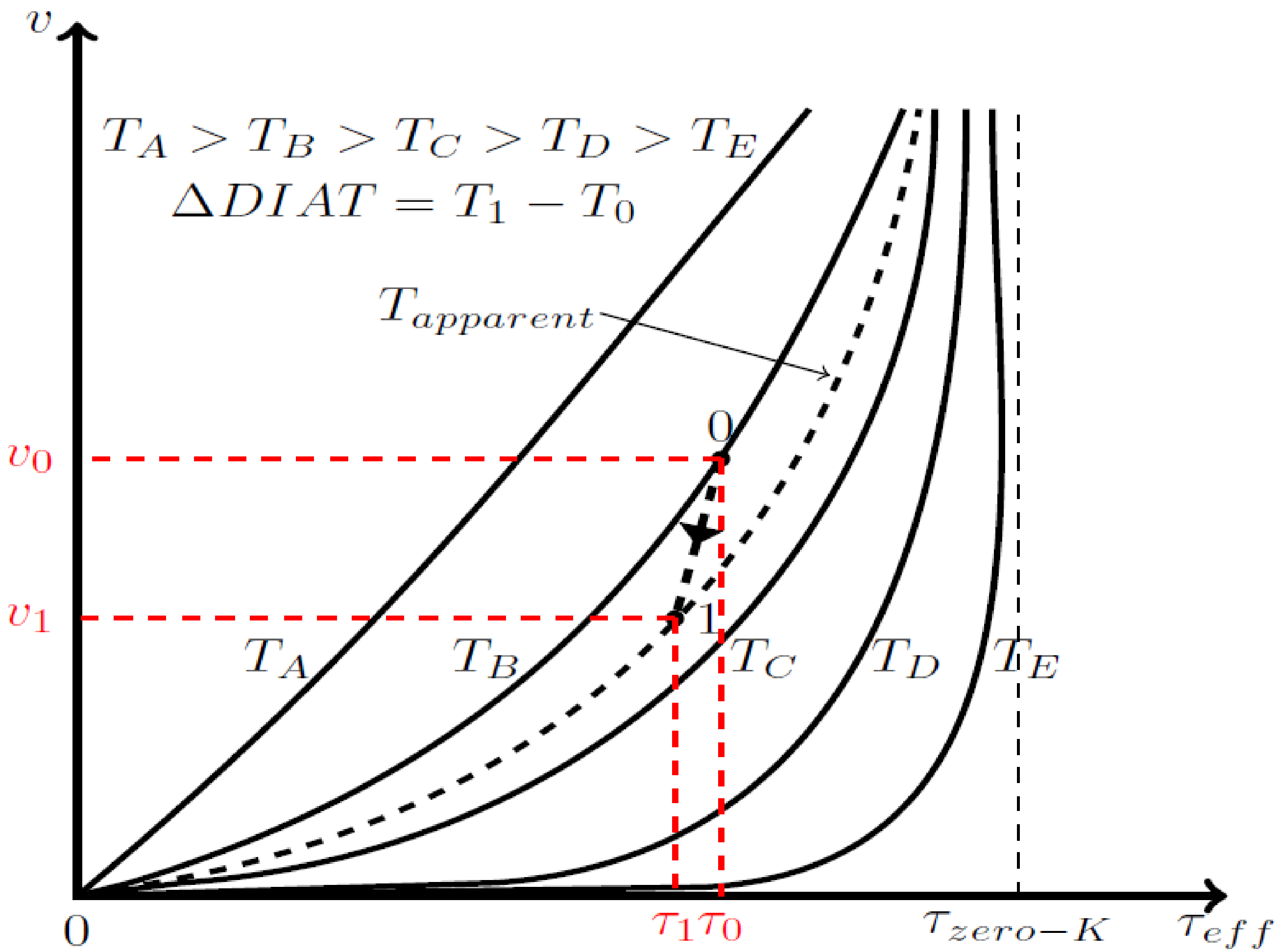
Predicted defect-induced evolutions





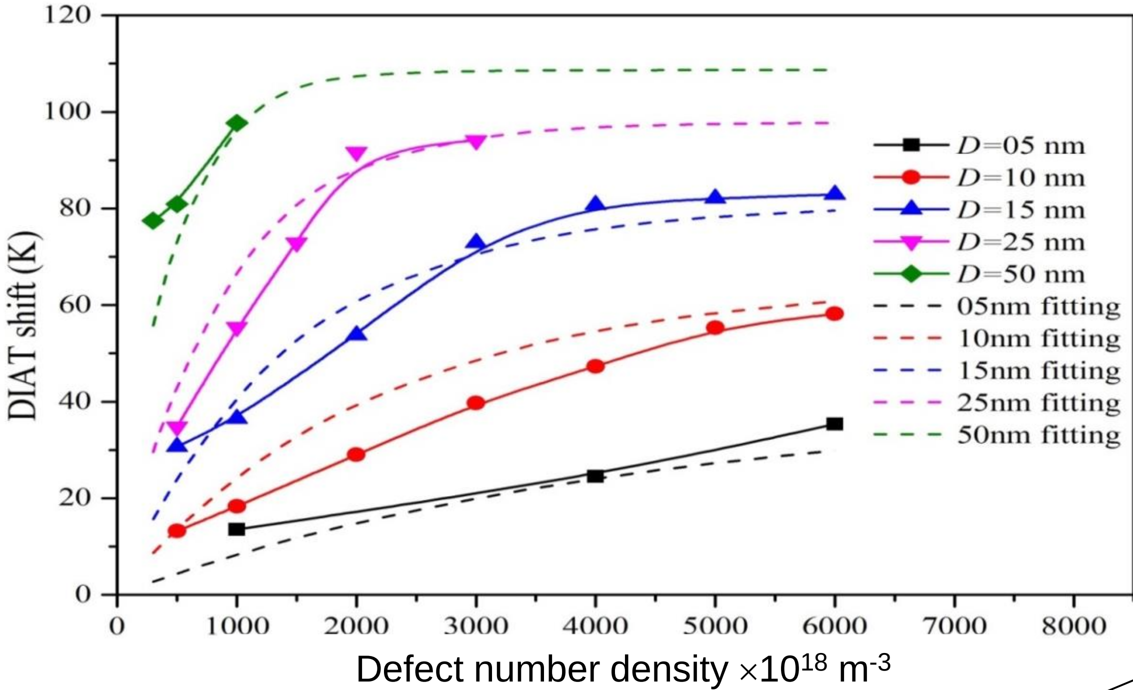
- ❑ Defect-induced effect on effective screw dislocation mobility :
  - **statistically significant.** Why it matters?

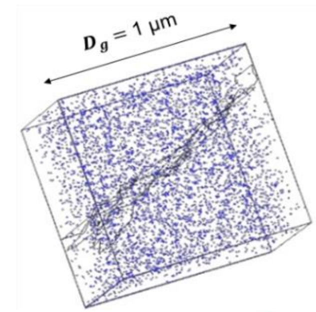
DIAT shift: interpretation

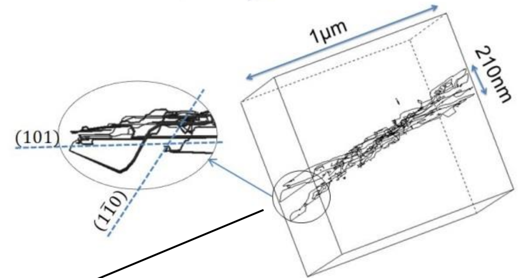


$T_{apparent} - T_0$ = Defect-Induced Apparent straining Temperature shift (ΔDIAT)

ΔDIAT: a systematical investigation







$$\Delta\mathrm{DIAT} = \Delta T_{max}\left(1 - exp\left(-\frac{D}{\lambda}\right)\right)\left(1 - exp(-\boldsymbol{d}^2 DN)\right) \approx \Delta\mathrm{DBTT}$$

N: defect number density (in nm^{-3}); D: defect size (in nm);
3 material-dependent scaling parameters (ΔT_{max}, d and λ)

ΔDIAT: a simple, predictive DBT shift indicator

$$\Delta \mathrm{DBTT} \approx \Delta \mathrm{DIAT} = \Delta T_{max} M$$

$\Delta T_{max} \rightarrow$ first principles elasticity theory & **dislocation statistics**

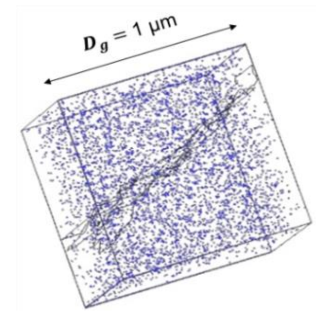
ΔH_0 (Joules)
$\tau_{Peierls}$ (MPa)
μ (MPa)
B (MPa.s)
T_0 (K)
[n] and D <u>at saturation</u>
effective τ_1(Orowan)
effective τ_0 (at T_0 = 300K)

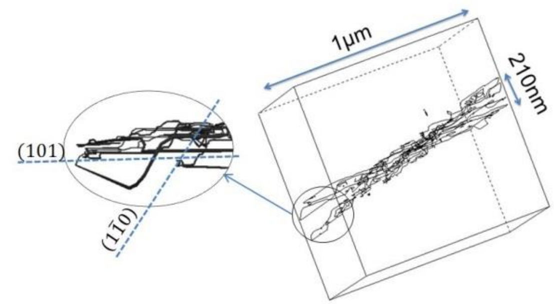
No adjustable variable/parameters

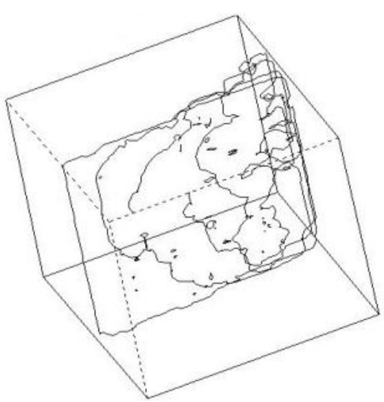
$0 < M < 1$:
dimensionless «mitigation» term

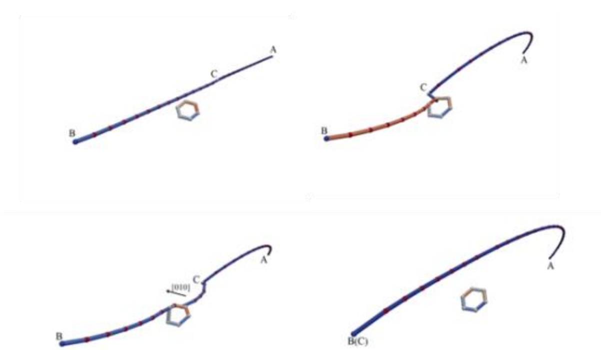
$M \propto$ «stress landscape» associated with shear band structures

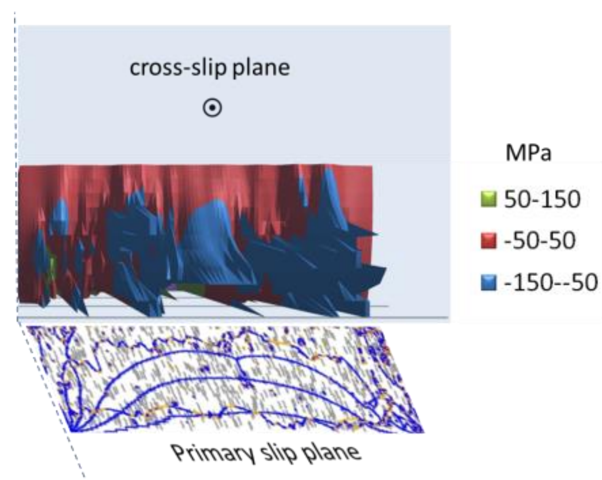
Controls cross-slip activity → *effective* defect interaction strength (τ^*) and dislocation length (*X'*)











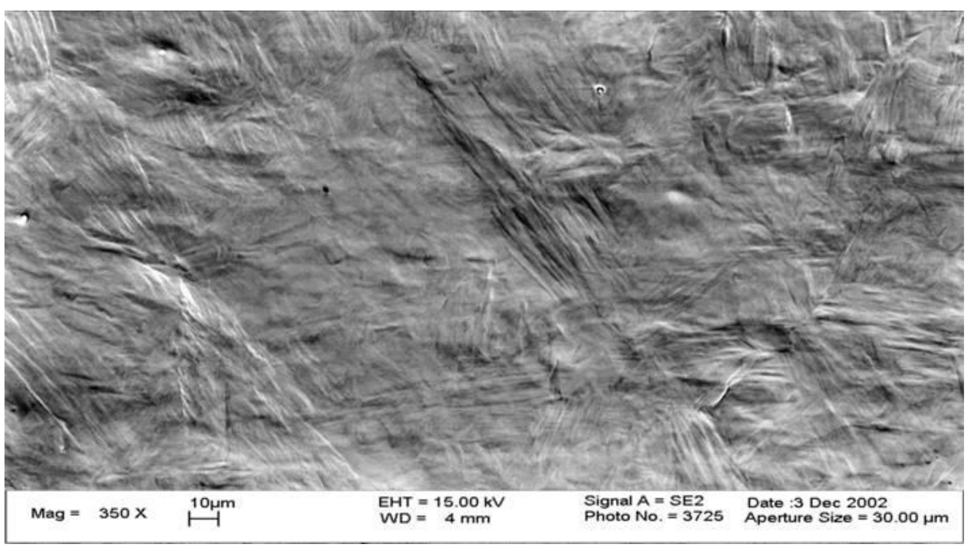
ΔDIAT: a simple, predictive DBT indicator

Stress landscape ↔ shear band spreading

Grain size and grain orientation
Dose-dependent τ_{YS} (MPa)
Strain per shear band
[n] and D at considered dose, irradiation-T°
Defect strength (MPa)
Dislocation accumulation rate with ε_p

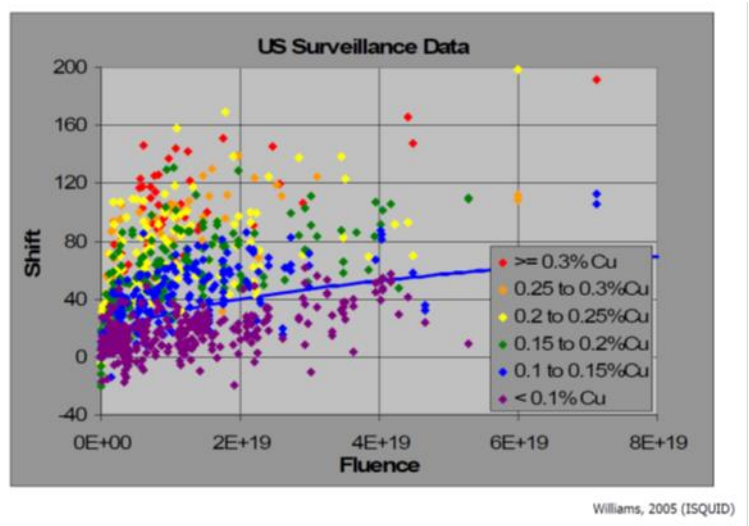
Shear band spacing and thickness: micro-model based on **DD simulation results**

Micro-model validation based on comparison with experimental observation of strained specimens



ΔDIAT/ΔDBTT comparison: data collection

Dose-dependent DBT shift



Defect number density

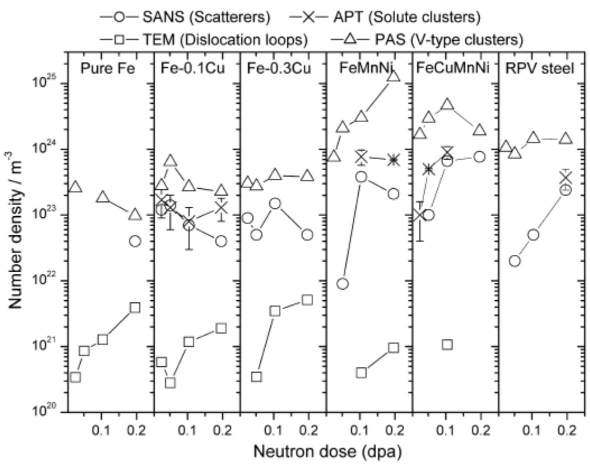
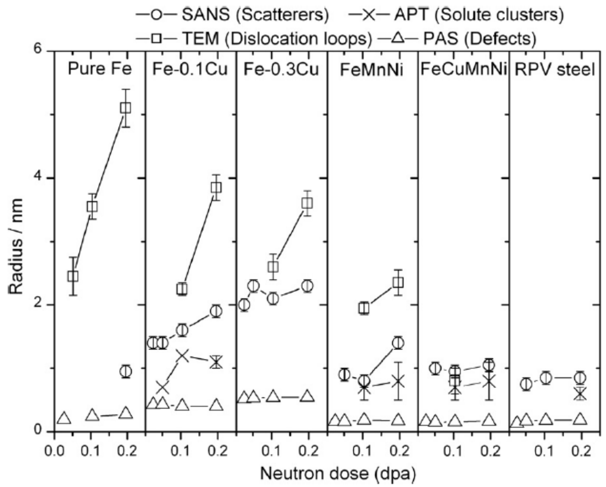


Fig. 3. Number density of radiation-induced damage as functions of dose from APT, SANS, TEM and PAS measurements.

Defect size



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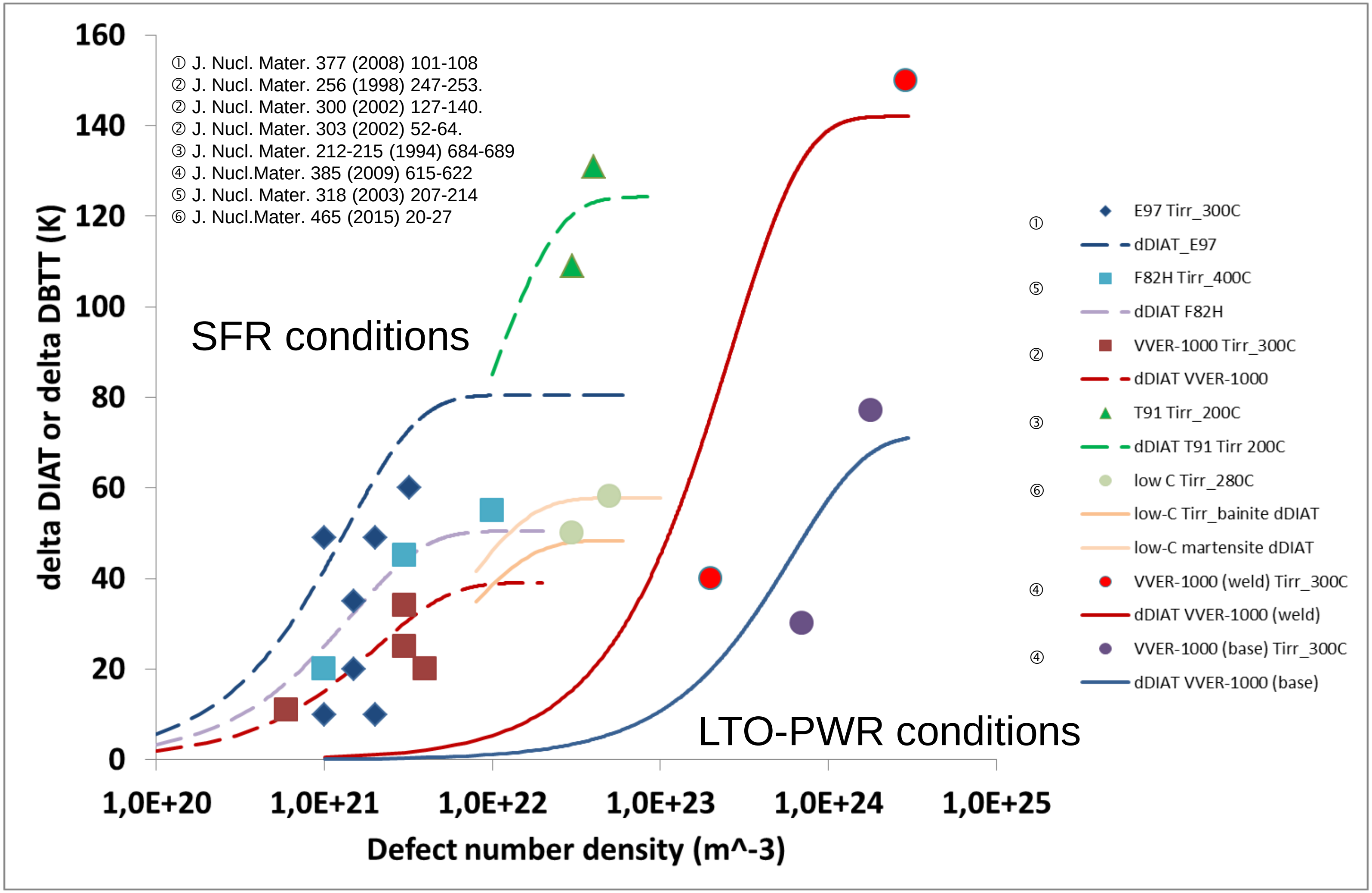
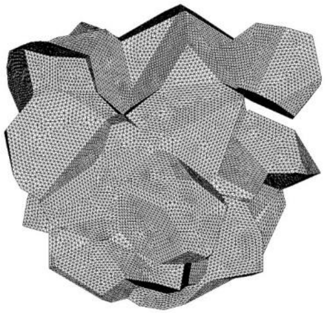
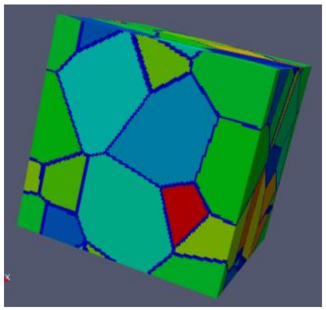
ΔDIAT/ΔDBTT comparison

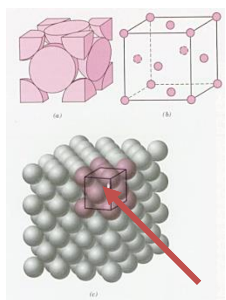


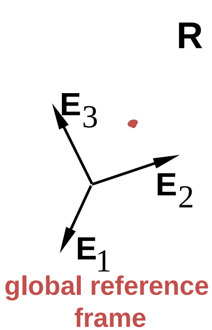
- ΔDIAT ≈ ΔDBTT [irradiation conditions: little or no segregation at fracture initiators (particles or GB)]
- Absolute toughness levels: link with local approach of fracture/MIBF approach/models
- Support/link dose-dependent crystal plasticity…

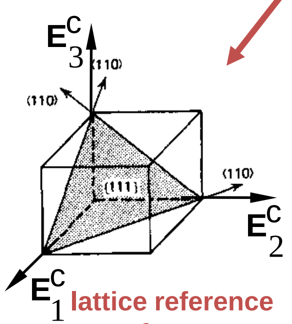
Crystal plasticity approach











- Explicitly models discrete grains and slip systems, accounting for anisotropy of single crystal properties and crystallographic texture.
- Slip system level constitutive equations for dislocations with use of Internal state variables for various parameters at each slip system
- Approach used to study aggregate of crystals to obtain a better understanding of single-crystal or poly-crystal behavior.
  - **Support from DD-based simulations**
- Physically based stress-velocity rules, system-system interaction strength
- Evolution of irradiation defect population with increasing strain, mobile dislocation density evolution

Modified T°-dependent mobility rule

$$\frac{1}{\dot{\gamma}_{total}} = \frac{1}{\dot{\gamma}_{nuc}} + \frac{1}{\dot{\gamma}_{prop}} \quad (1)$$

$\dot{\gamma}_{nuc}$ accounts for thermally activated kink pair nucleation. The stress-independent l_s term assumes that each nucleated kink-pair sweeps the whole dislocation line, while a given screw dislocation moves from one Peierls valley to the next one.

Inverse of strain rate sensitivity parameter

Reference shear strain rate

$$\dot{\gamma}_{prop1} = \dot{\gamma}_0 \left(\frac{\tau_{RSS}}{\tau_c} \right)^n$$

High value of n limits its numerical applicability

$$\dot{\gamma}_{prop2} = \rho_m b v_k = \rho_m b . \frac{\tau_{eff} b}{B} \quad (2)$$

$$\dot{\gamma}_{nuc2} = \rho_m b \frac{8\pi \tau_{eff}^2}{\mu B} exp\left[-\frac{\Delta H_0}{k_B T} \left(1 - \left[\frac{\tau_{eff}}{\tau_0} \right]^p \right)^q \right] X_\infty$$

$$X_\infty = 2\sqrt{\frac{v_k}{J}}$$

Formulations (1)&(2) yield comparable results at the strain rate 10^{-4} for $\Delta H_0 > 0.6$ eV

Formulation (2) is however able to handle a **larger range of strain rate and material parameters**.
It is also found to be more robust in terms of convergence in finite element formulation.

Modified dislocation/defect interaction rule

- τ_{eff} depends on many different contributions, including irradiation defects, acting as obstacles cutting the dislocation glide planes hence, treated as forest obstacles to the glide of dislocations.

- Dose level controls the number of loops N_{irr} formed and temperature controls the size of the loop d_{irr}

$$\rho_{irr} = N_{irr} d_{irr}$$

Irradiation defect density evolution

$$\dot{\rho}_{irr} = -\xi \rho_{irr} \dot{\gamma}$$

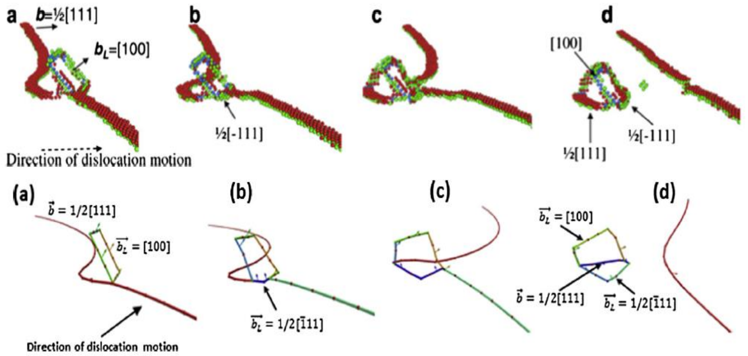
0 < ξ < 1: loop annihilation parameter

Affects τ_{eff} in eq. (2)

Modified dislocation/defect interaction rule

Through DD simulations → significant dose-dependent increase in total and mobile dislocation density.

This increase is ascribed to interaction of screw dislocations with irradiation defects → dislocation pinning, multiplication.



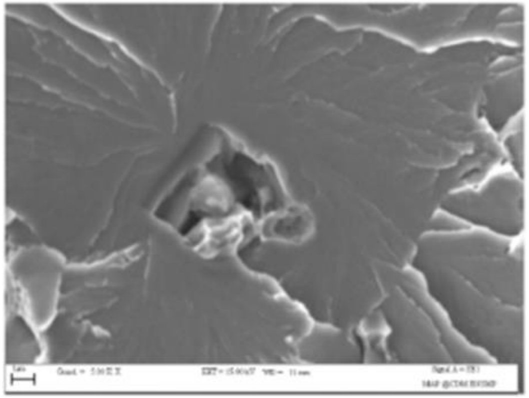
X.J. Shi et al. *J. Nucl. Mat.* 460 (2015) 37-43

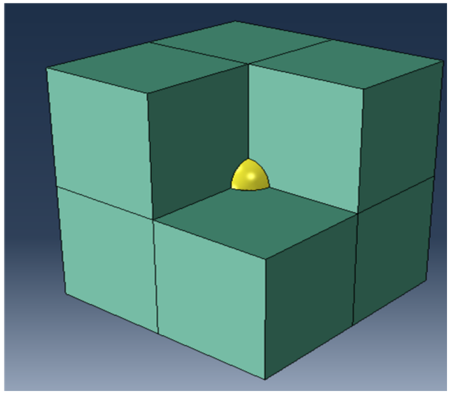
$$\dot{\rho_m} = \frac{\kappa\xi}{r_0}\rho_{irr(t)}\dot{\gamma}$$

affects gamma-dot in eq. (2)

☞ Interaction means dislocation pinning, which subsequently act as source of mobile dislocation for their further generation.
☞ This mechanism/term is defect-size dependent (irradiation temperature)

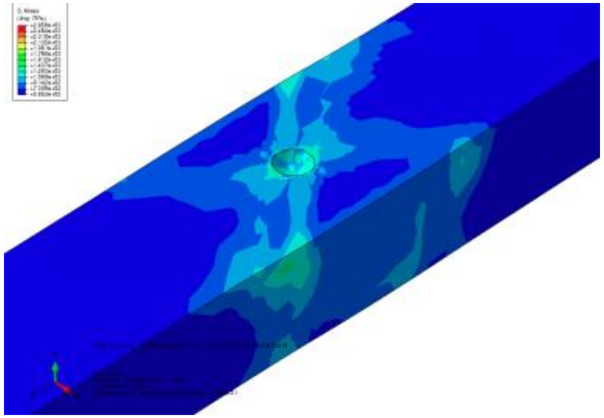
Preliminary results: FEM model

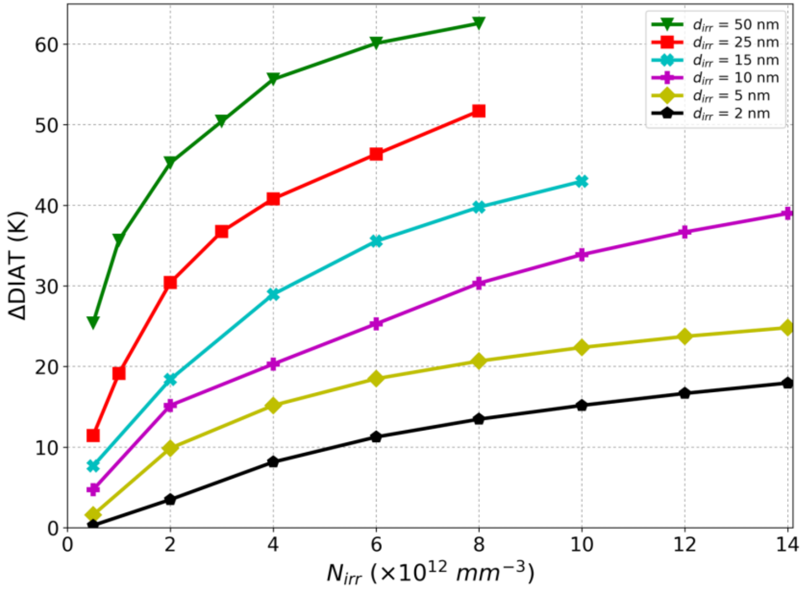




To predict stress field near fracture initiator and its dose-dependent evolutions

☞ Link with DD calculations: ΔDIAT prediciton
☞ Link with MIBF model





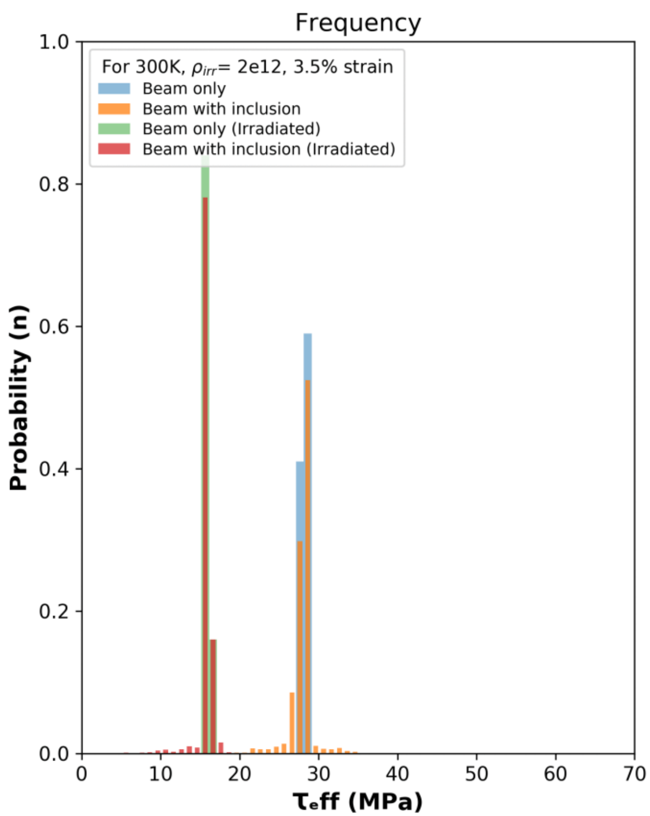
Stress field near fracture initiator:
Weibull statistics description

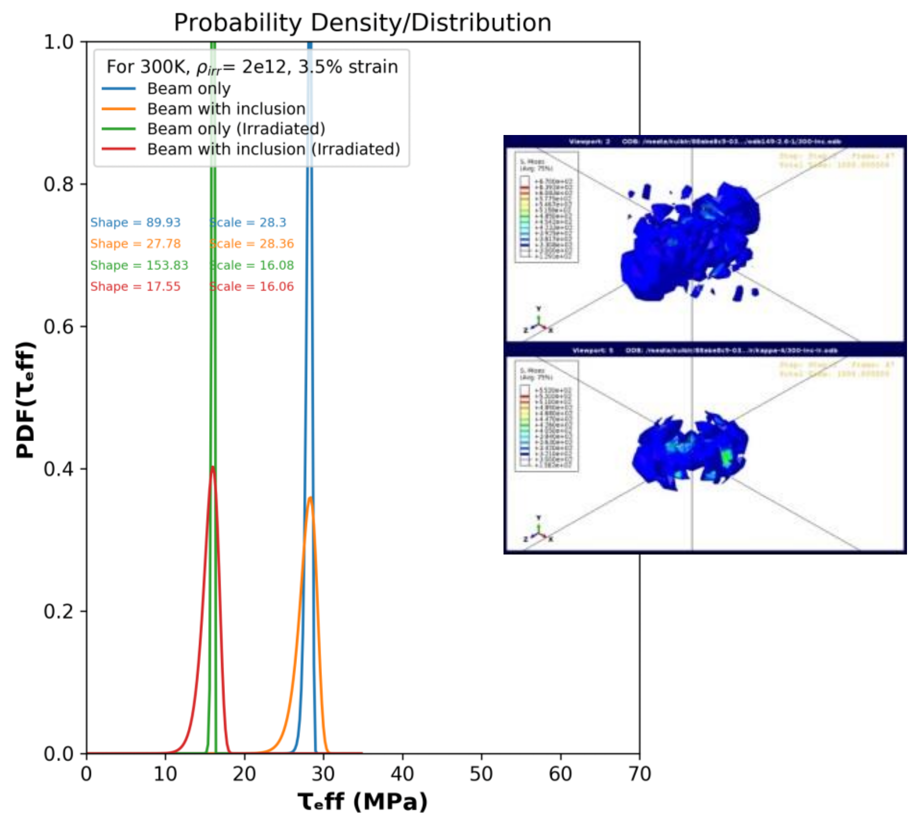
$$f(\tau_{eff}) = \frac{\beta}{\eta}\left(\frac{\tau_{eff} - \gamma}{\eta}\right)^{\beta-1} exp^{-\left(\frac{\tau_{eff}-\gamma}{\eta}\right)^{\beta}}$$

Scale Parameter

Shape Parameter

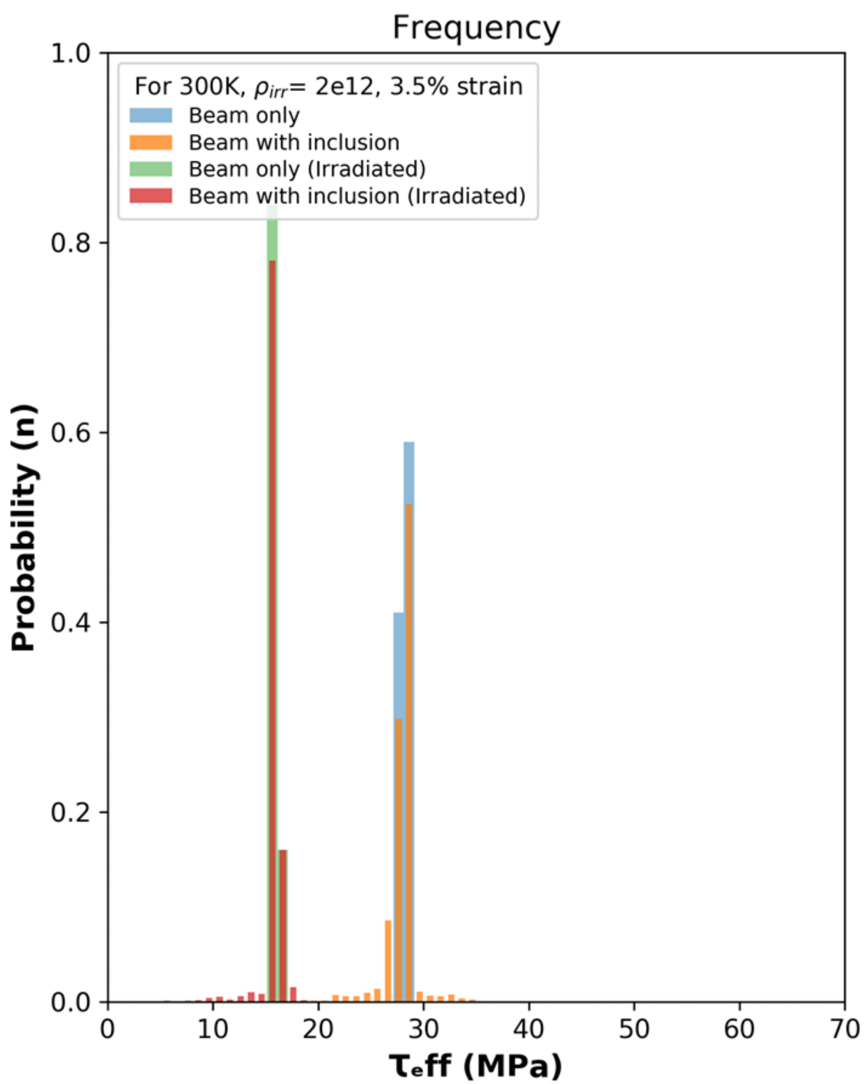
Position Parameter

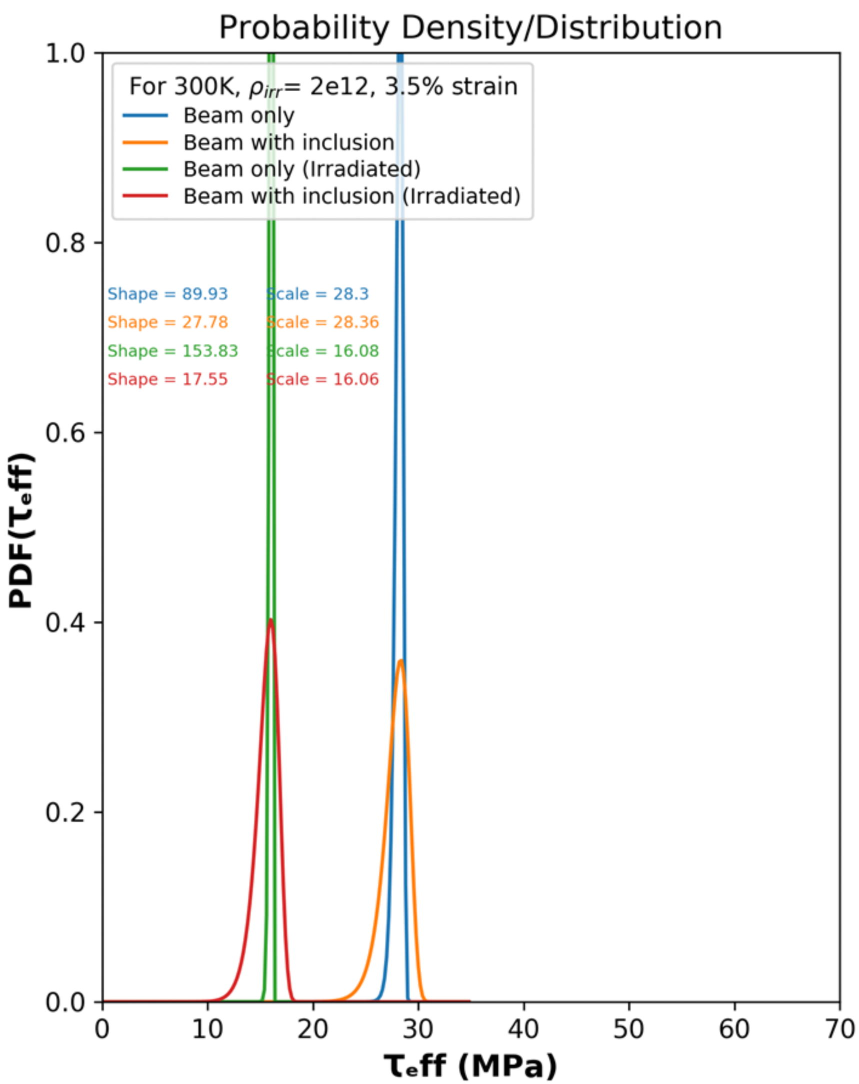




Preliminary results: dose-dependent stresses

Irradiation defect size - 15 nm

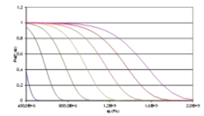


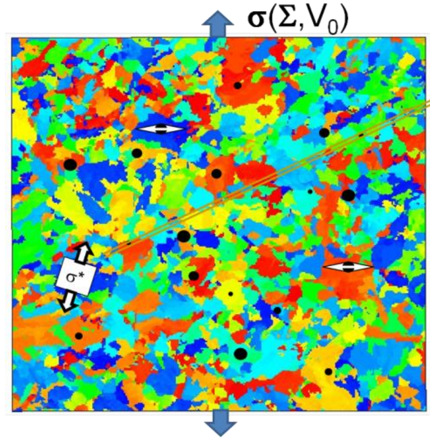


Preliminary results: link with MIBF model

Ongoing: to compare ΔDIAT and ΔDBTT based on MIBF prediction

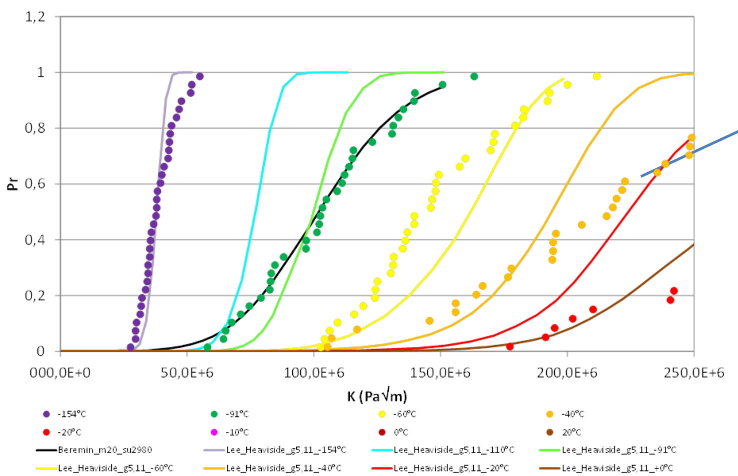
RPV steel microstructure
⇒ local stress distribution σ^* inside V_0.





+Δσ or dose-dependent change of Weibull grain stress distribution parameters

$$P_f\left(V_p,\Sigma\right) = 1 - \exp\left(\int_{V_p} \ln\left(1 - P_f\left(V_0,\sigma\right)\right)\frac{dV}{V_0}\right)$$



Example: as-received (0 dpa) conditions
Solid line: without grain plasticity
Solid symbols: accounting for grain plasticity

Summary

- In presence of disperse defect populations:

- «Weakest link» fracture model framework: toughness level is controlled by the **plastic zone size «a_0»**, near the BF initiators (particles or GB)
- Plastic zone size «a_0» is **dose-dependent** and scales with the **apparent (screw) dislocation mobility**
- Apparent dislocation mobility depends on dispersed defect populations and can be estimated using the **statistical ΔDIAT concept**
- Calculated ΔDIAT levels are comparable to DBT transition <u>shifts</u>, for a given disperse defect microstructure (*N*, D)
- DD and ΔDIAT approach used in support of crystal plasticity calculation framework
- Corresponding dose-dependent stress distributions to feed MIBF model, predicting DBT <u>shift and level</u>

- Perspectives:

- To apply ΔDIAT method to a broader range of materials and irradiation conditions
- To predict dose-dependent evolutions of upper shelve level