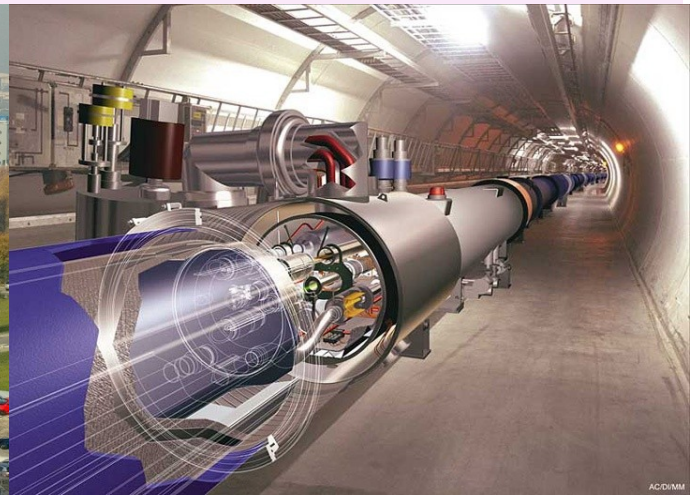
Evolution of radiation induced micro-damage in the materials used in particle accelerators design

Błażej Skoczeń, Aneta Ustrzycka
Centre for Particle Accelerators Design, Cracow University of Technology



Outline

I. Typical components subjected to irradiation (LHC, EUROnu, ITER)

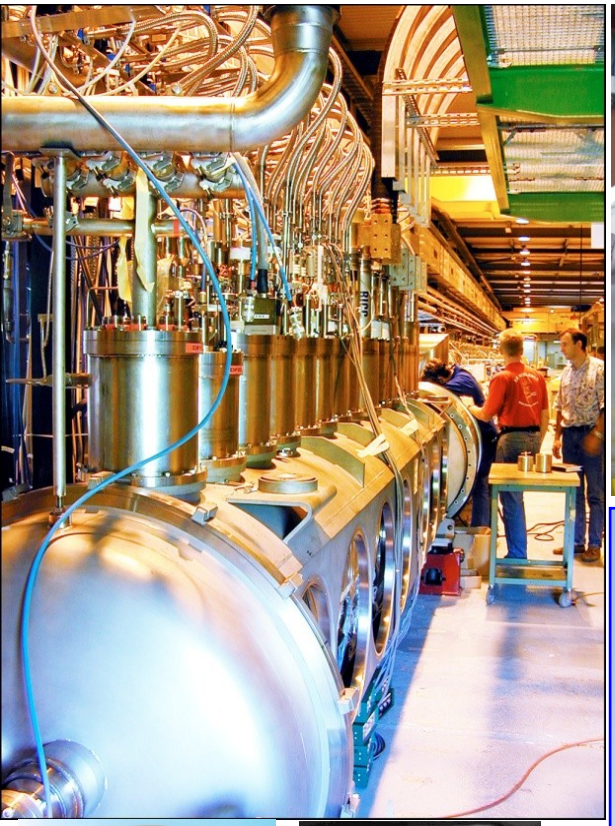
II. State of the art in radiation induced damage

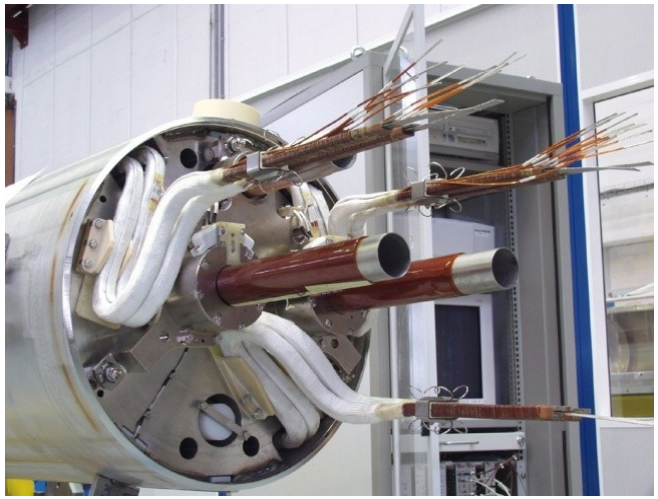
III. Evolution of radiation induced damage under mechanical loads

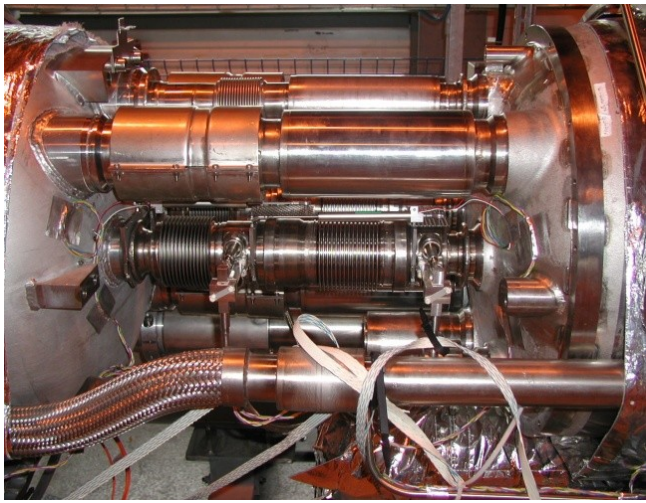
IV. Example of lifetime estimation for irradiated components

V. Specific coupled fields problems

Materials used in particle accelerators design







304L, 316L, 316LN, P506

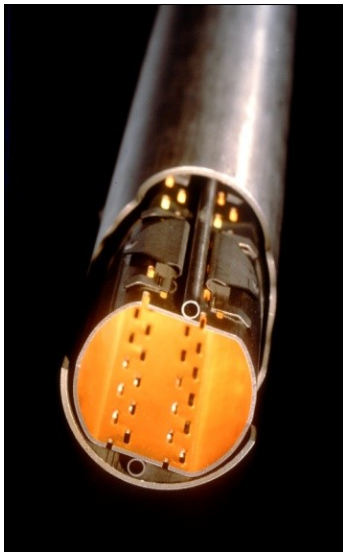
Fe, Cu, Al, Sn, Au, Ag,

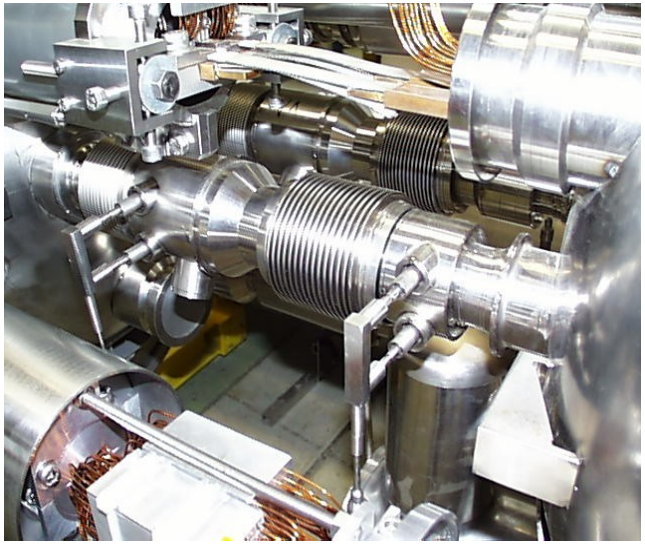
NbTi, Nb_3Sn,

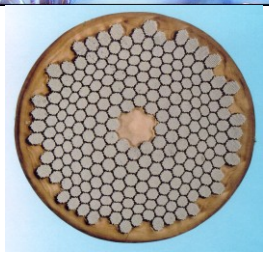
NbAl, MgB_2,

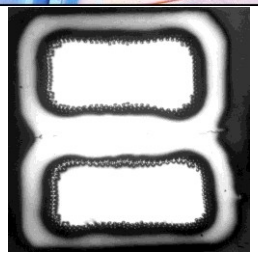
BSCCO2223,

G10, G11









The main task of the research

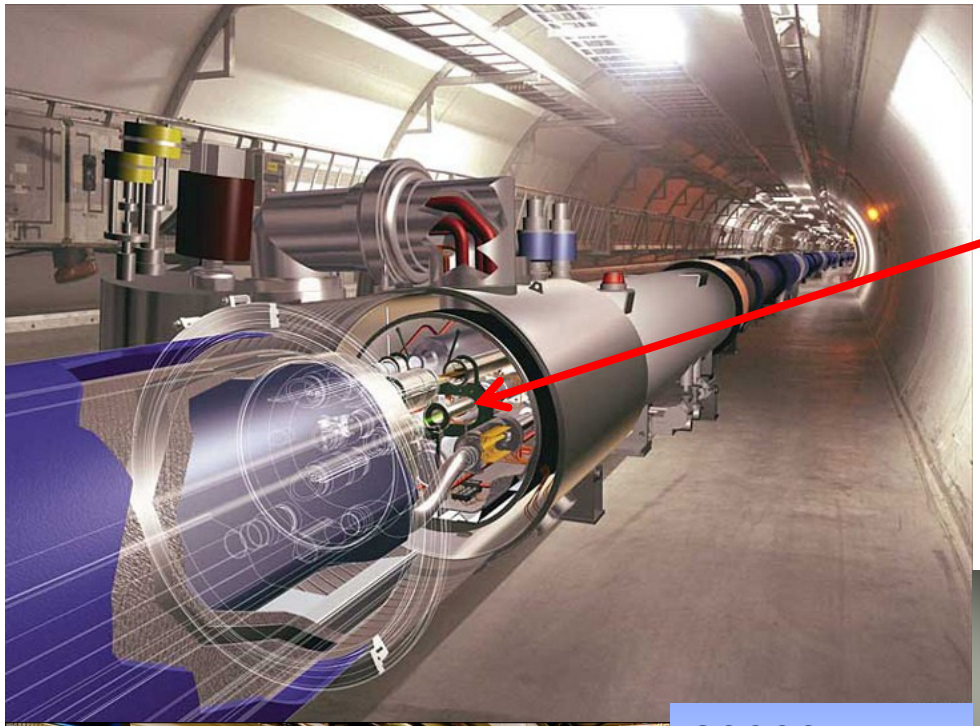
Task

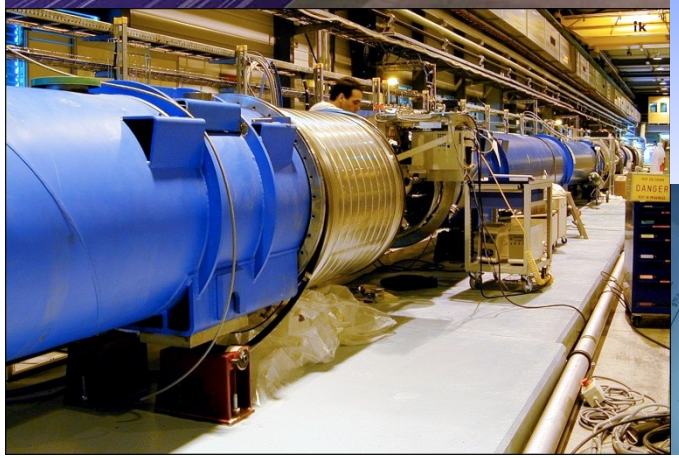
We need to determine the lifetime of irradiated components, subjected to periodic thermo-mechanical loads in the course of their service

Method

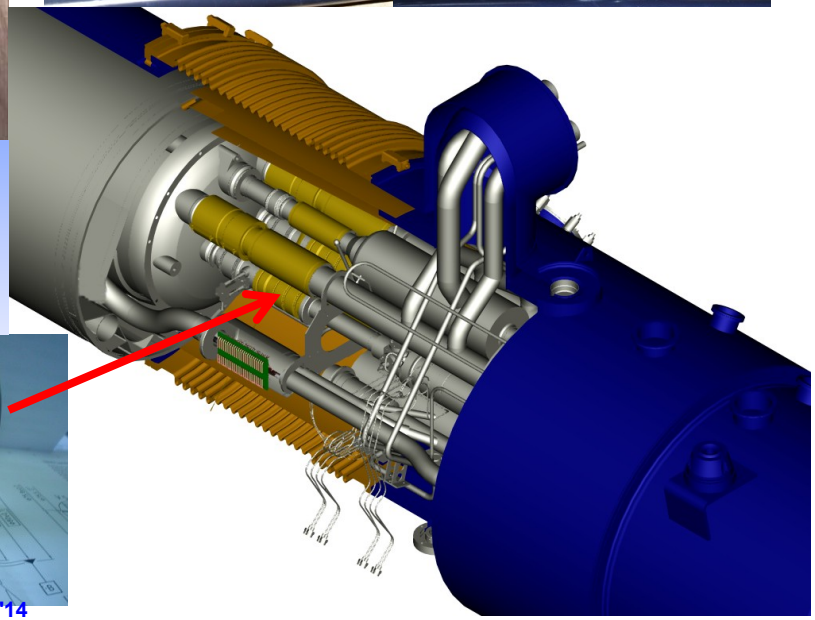
Well calibrated constitutive model of micro-damage evolution in the irradiated components

Typical components subjected to irradiation in the LHC

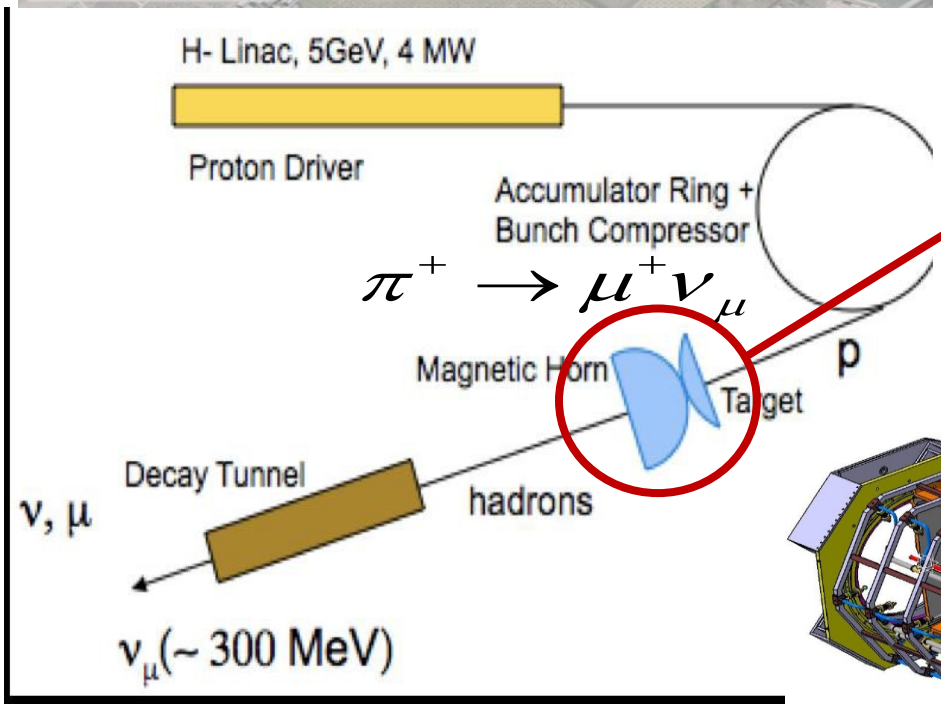


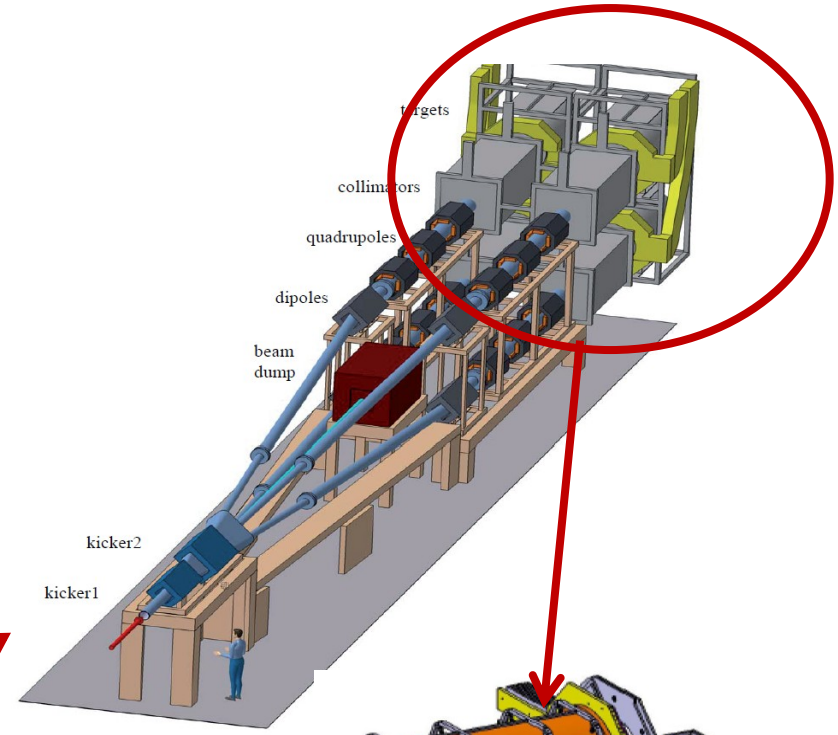


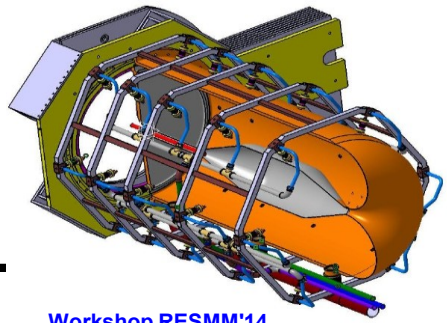
20000 expansion bellows

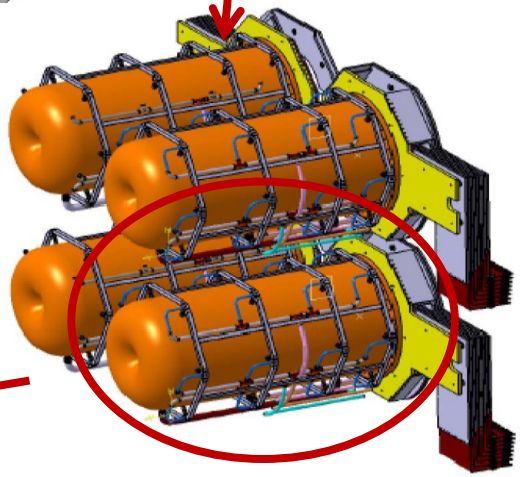


EUROnu: High Intensity Neutrino Oscillation









Int. Thermonuclear Experimental Reactor ITER

Central Solenoid
Nb_3Sn, 6 modules

Toroidal Field Coil
Nb_3Sn, 18,

Poloidal Field Coil
NbTi, 6

Correction Coils
NbTi, 18

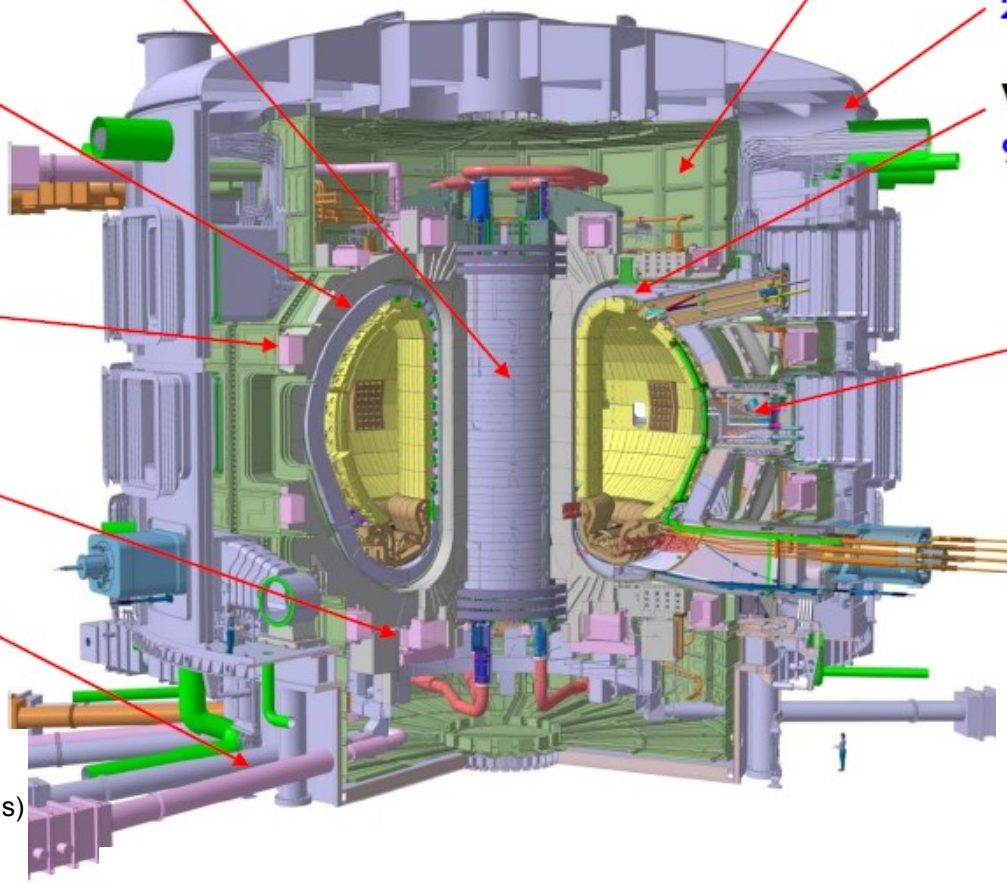
Feeders
NbTi, 31

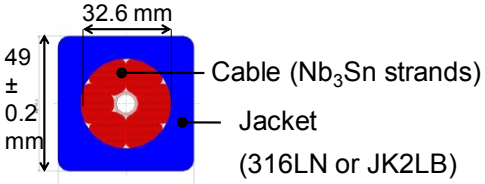
Cryostat Thermal shields

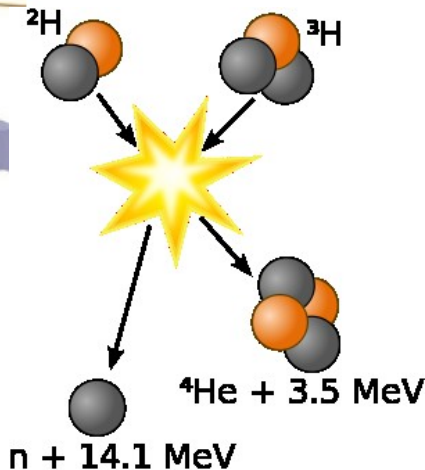
Cryostat
24 m high x 28 m dia.

Vacuum Vessel
9 sectors

Port Plug
heating/current drive, test blankets limiters/RH diagnostics

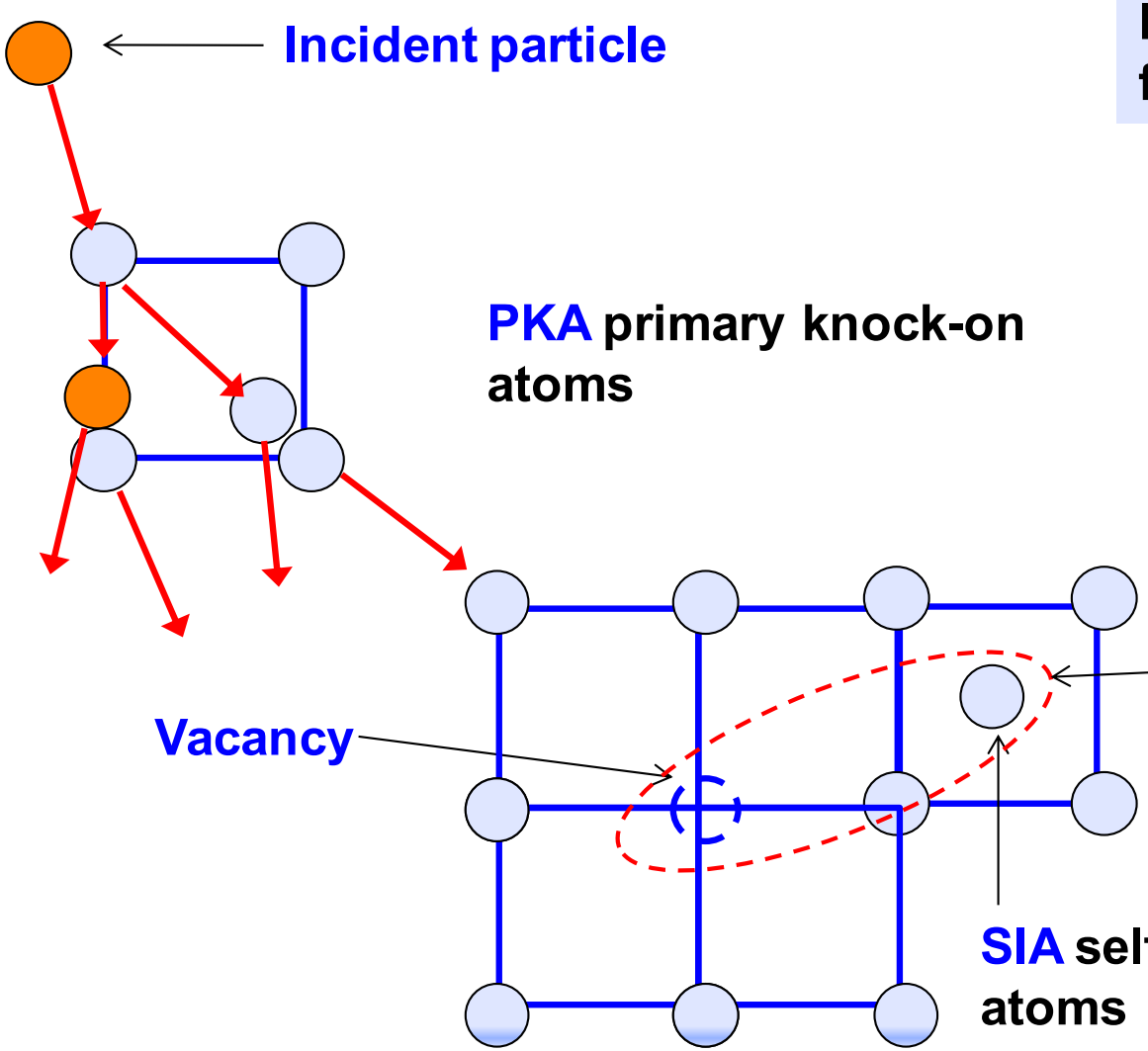






State of the art in radiation induced damage

Irradiation induced defects in the lattice



Displacement cascade and formation of Frenkel pairs

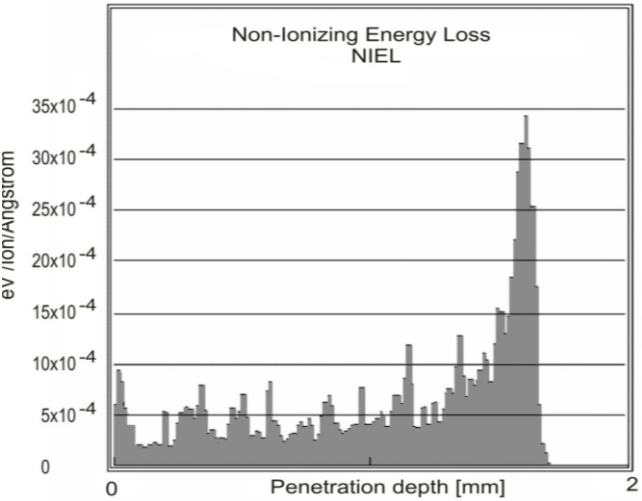
Kinchin & Pease, 1955

Norgett, Robinson, Torrens, 1975

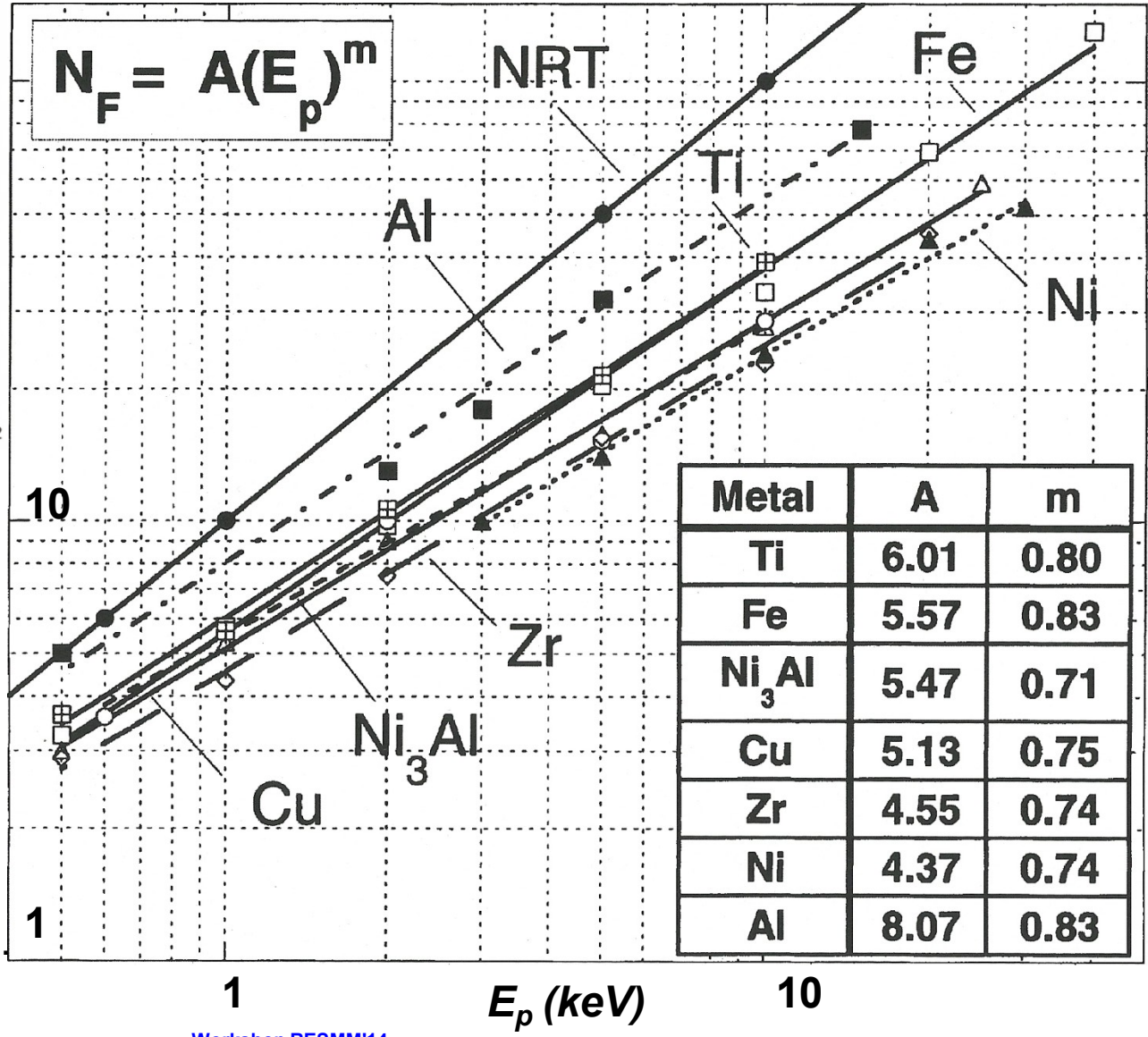
$$N_{NRT} = \frac{0.8 E_{dam}}{2 \overline{E}_d}$$

$$E_{dam} = NIEL$$

Irradiation induced defects in the lattice



NIEL profile for copper irradiated by hydrogen 30MeV ions

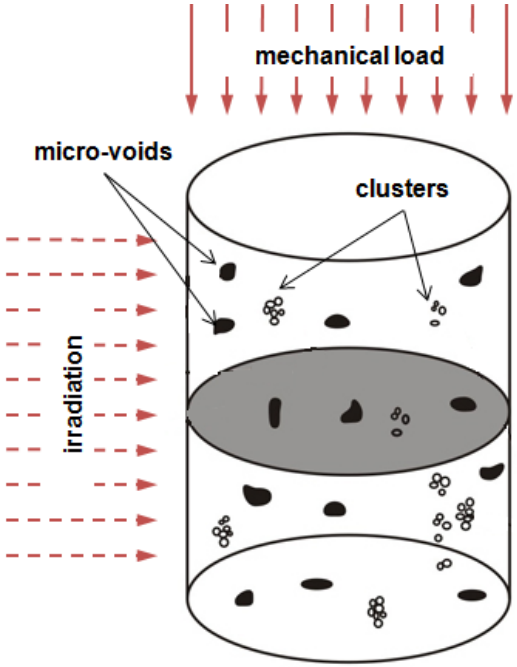


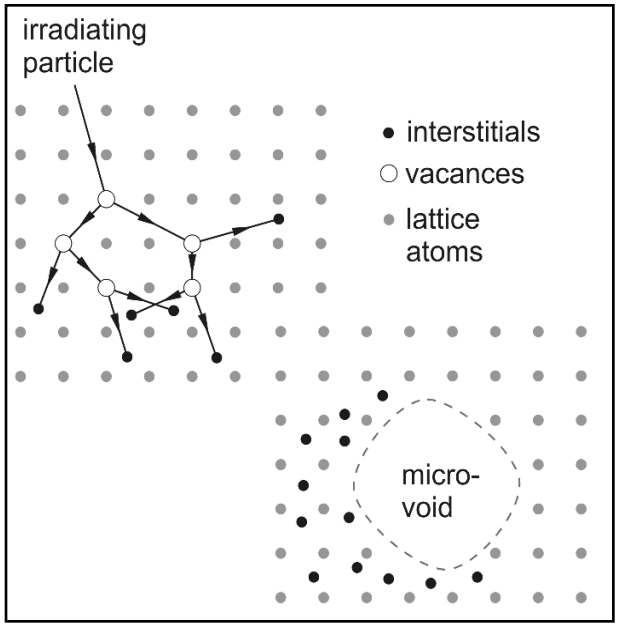
Metal	A	m
Ti	6.01	0.80
Fe	5.57	0.83
Ni_3Al	5.47	0.71
Cu	5.13	0.75
Zr	4.55	0.74
Ni	4.37	0.74
Al	8.07	0.83

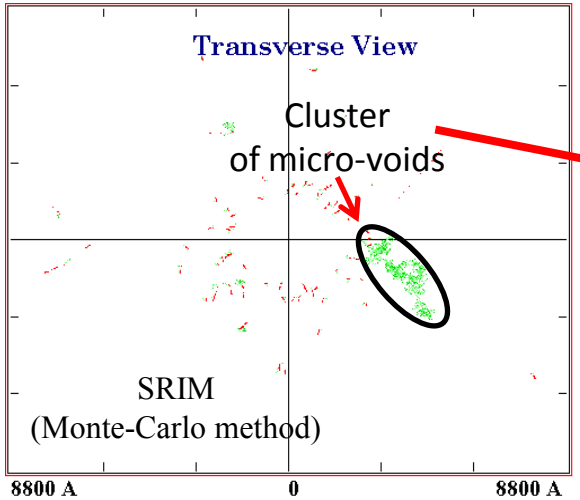
Number of Frenkel defects created by a cascade as a function of kinetic energy of primary knock-on atoms

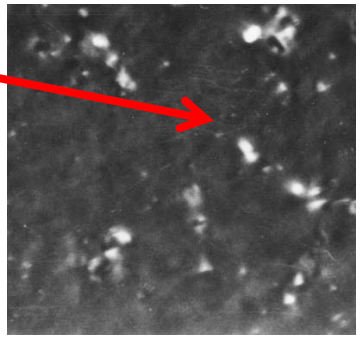
Source: D.J. Bacon, F. Gao, Yu.N. Osetsky, JNM 276, 2000

Irradiation induced micro-damage – types of defects





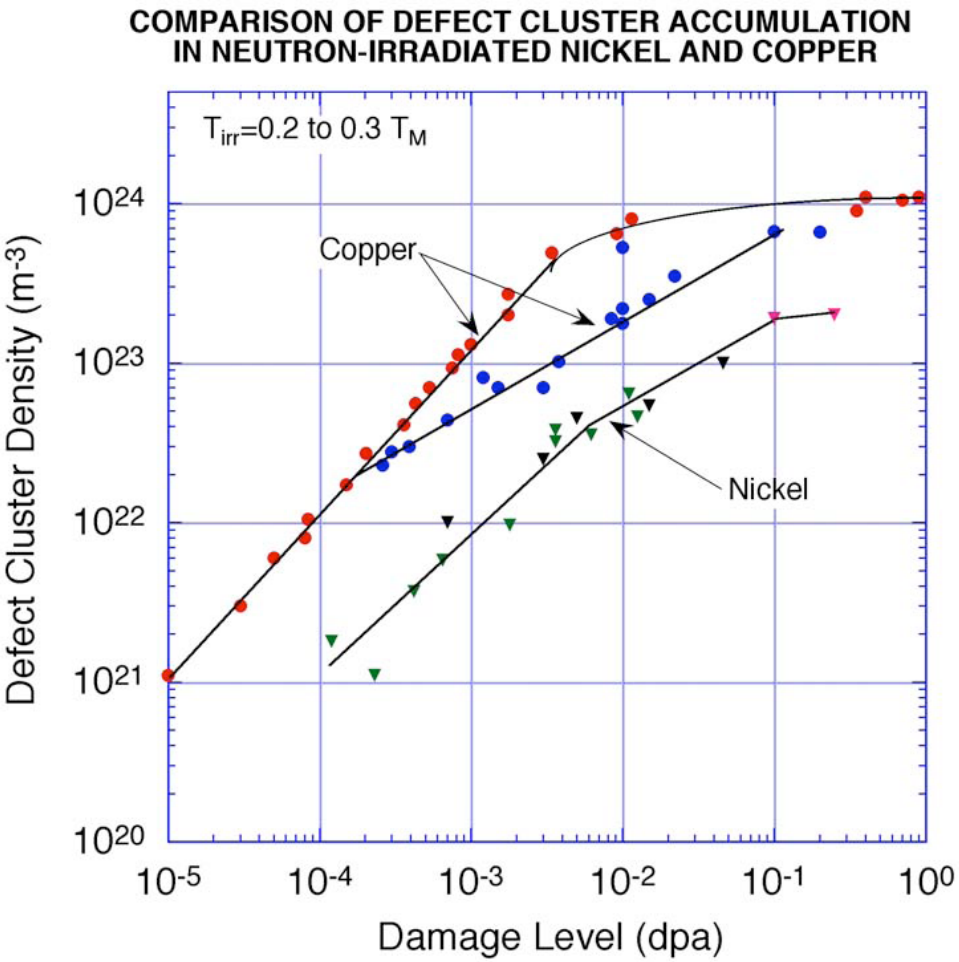


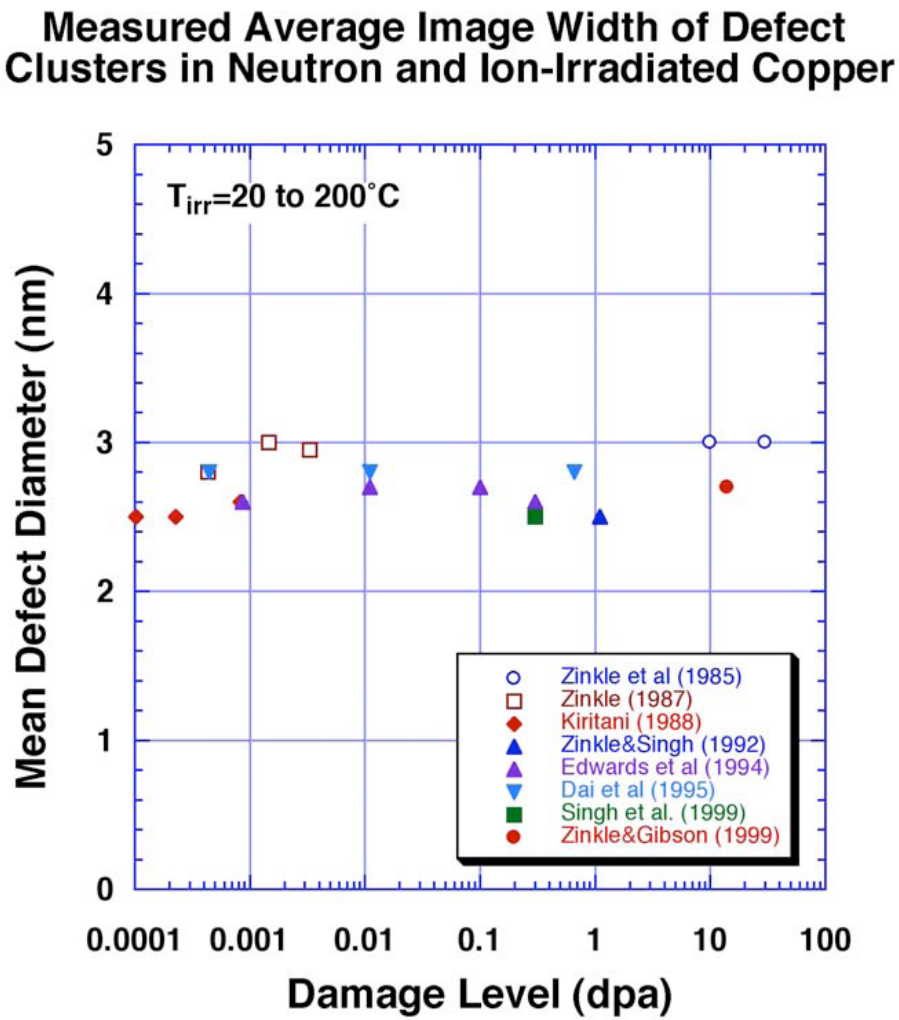


Defects due to irradiation:

1. **SFT – stacking fault tetrahedron**
2. **Faulted or perfect dislocation loops**
3. **Voids – 3D vacancy clusters**
4. **Cavities – 3D vacancy clusters with impurities (He)**

Irradiated metals and alloys: Copper

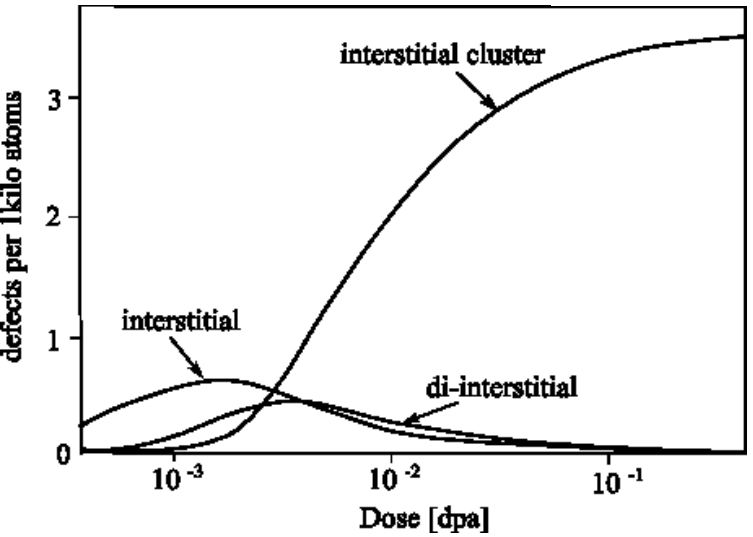


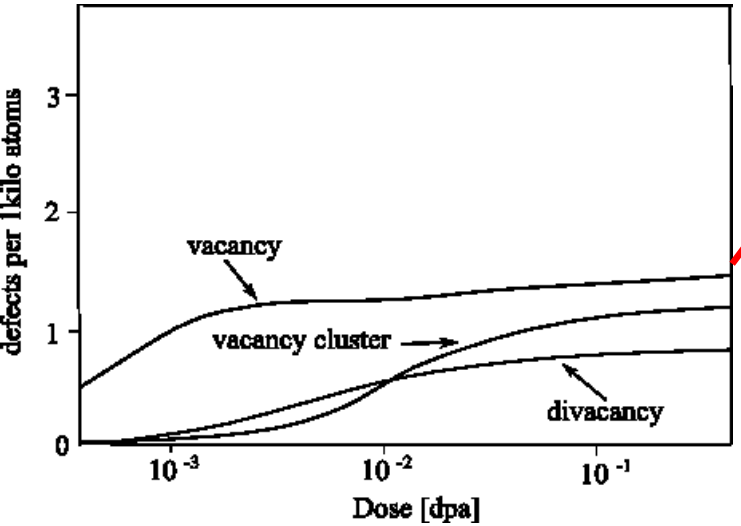


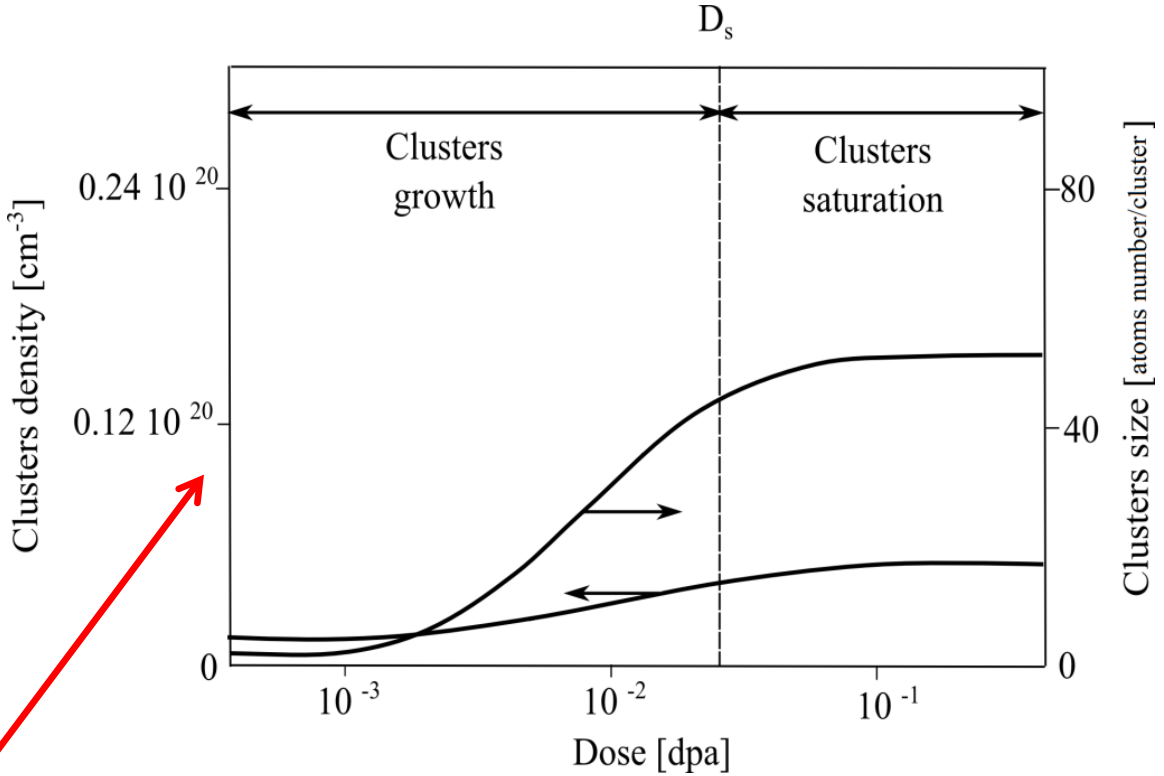
Source: S.J. Zinkle „Microstructure evolution in irradiated metals and alloys: fundamental aspects", Italy, 2004

Defect concentration during irradiation - Aluminium

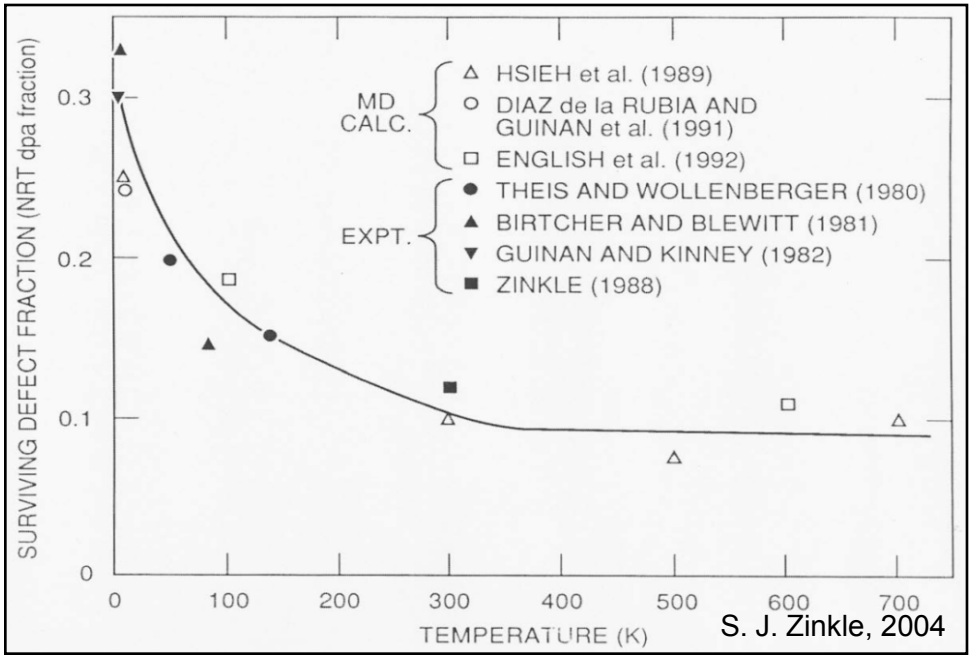
(for Al, after Verbiest and Pattyn, 1982)



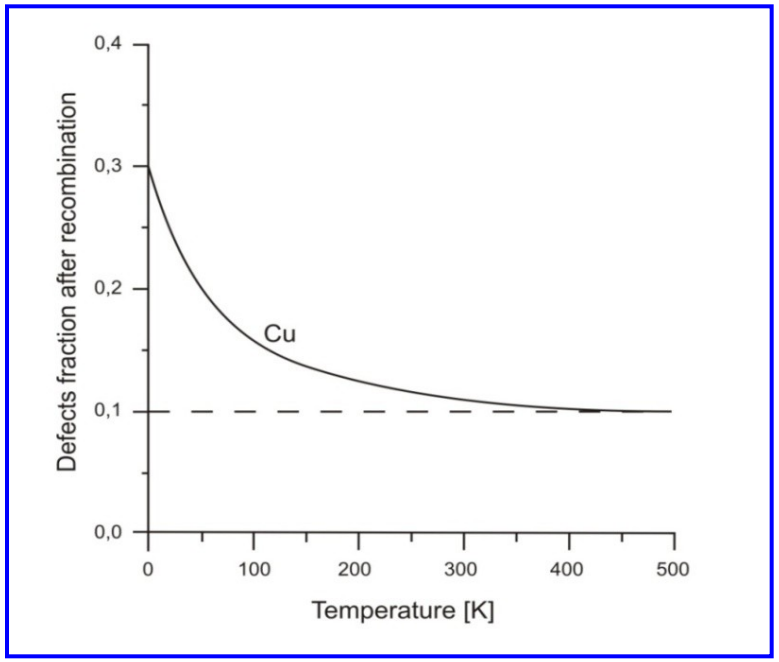




Recombination ratio



S. J. Zinkle, 2004



Much smaller recombination ratio at extremely low temperatures!

The fraction of surviving defects in the proximity of absolute zero is 3 times higher than at room temperature

Evolution of radiation induced damage under mechanical loads: experiments

Research programme

Experiments including neutron irradiated samples subjected to multiple loading/unloading technique

↓

Building well calibrated multi-scale 3D constitutive models of damage evolution in the irradiated components in the framework of CDM

↓

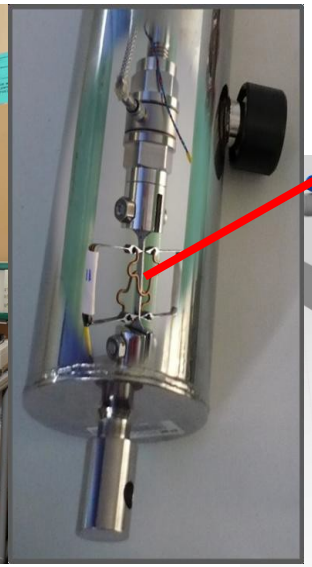
Combining CDM with fracture mechanics in order to predict transition from critical damage to fracture

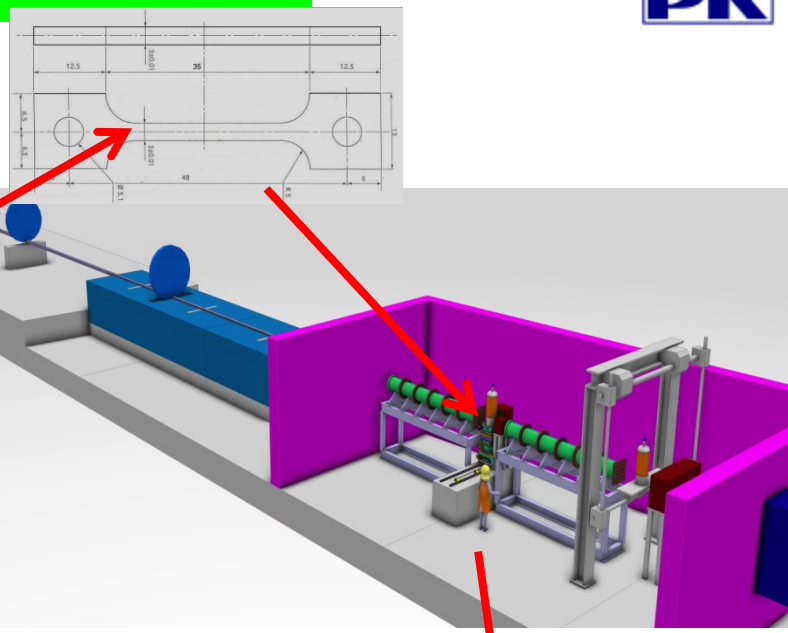
↓

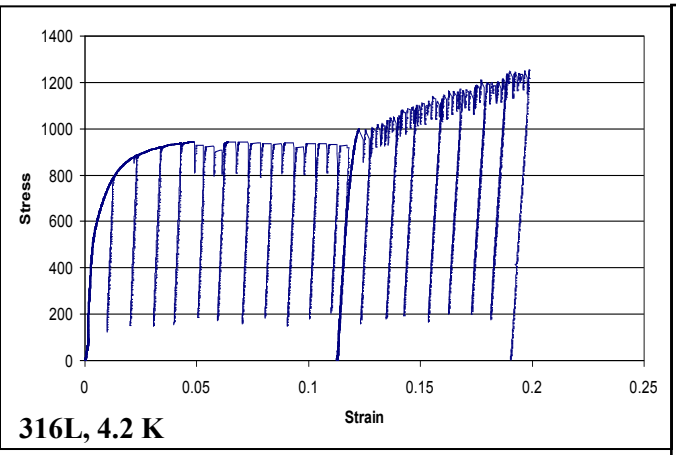
Computing evolution of nano/micro damage fields and macro-crack propagation in the irradiated components

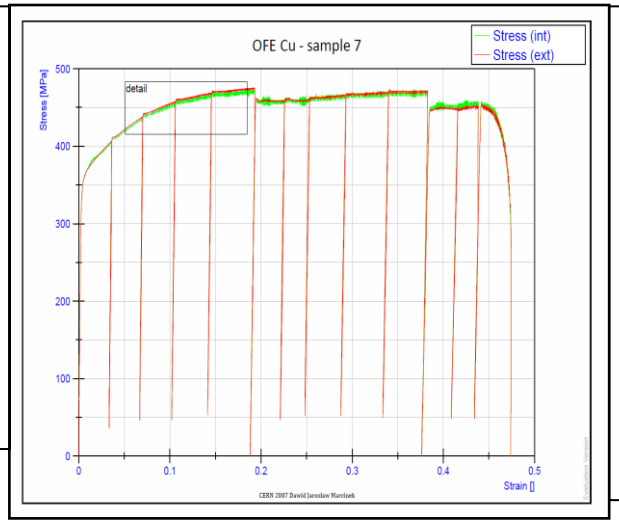
Lifetime prediction

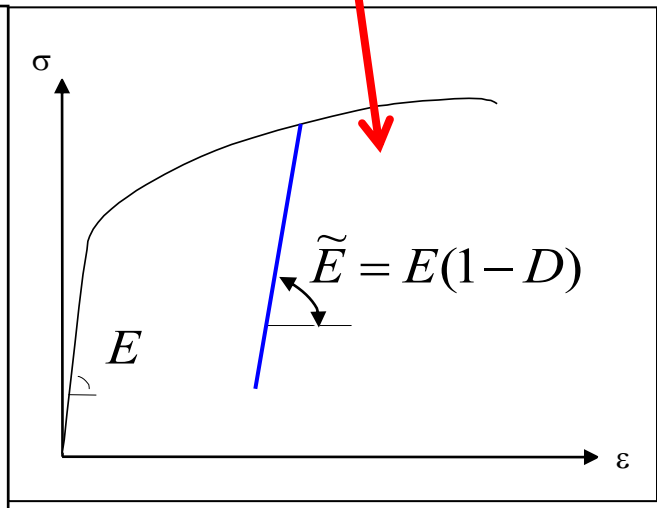
ESS facility – proposal of experiments







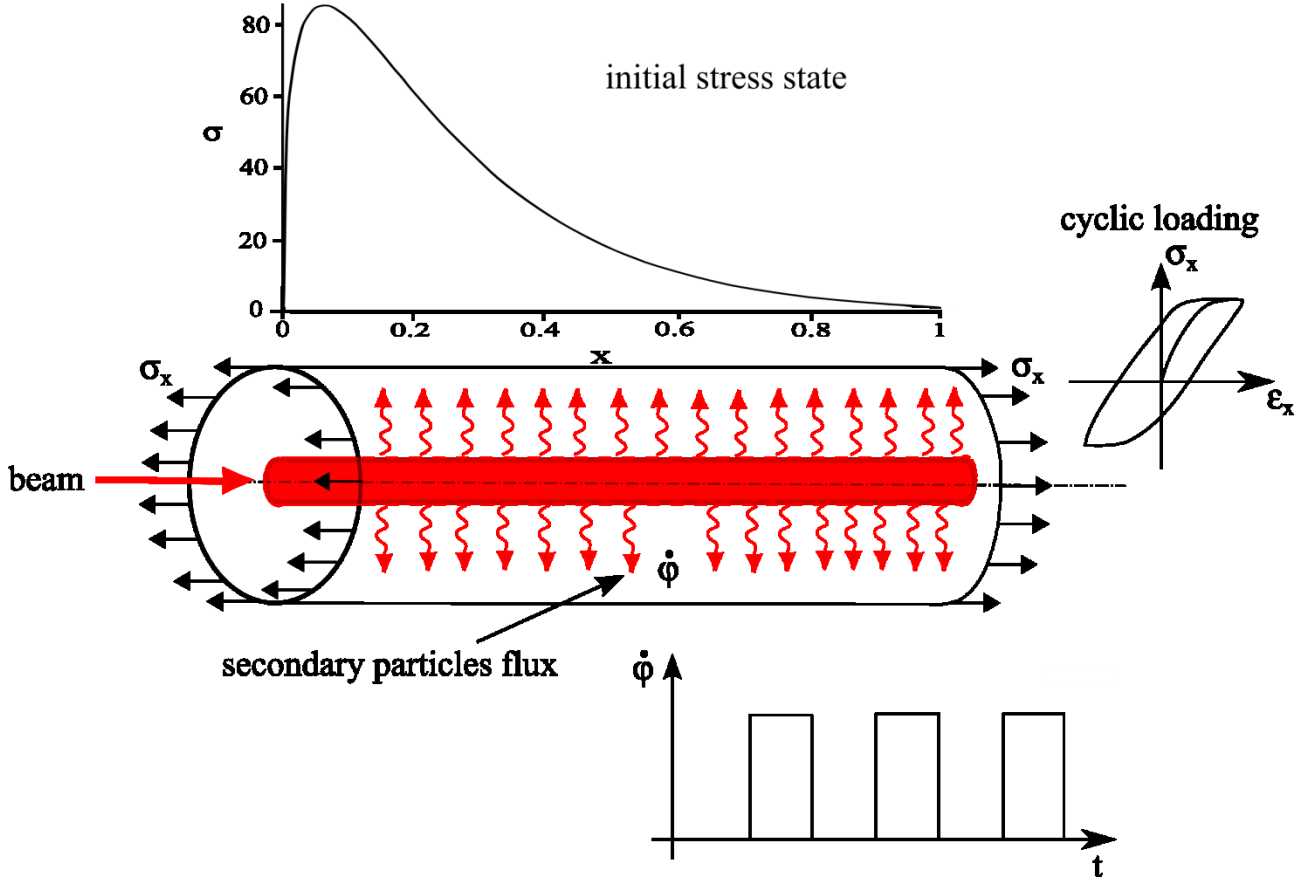




Identification of damage evolution is based on analysis of unloading modulus

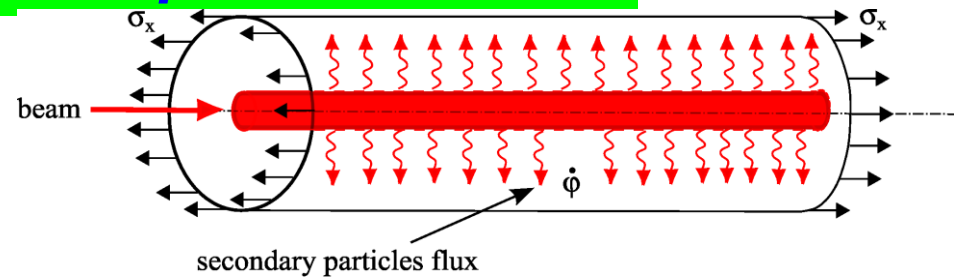
Examples

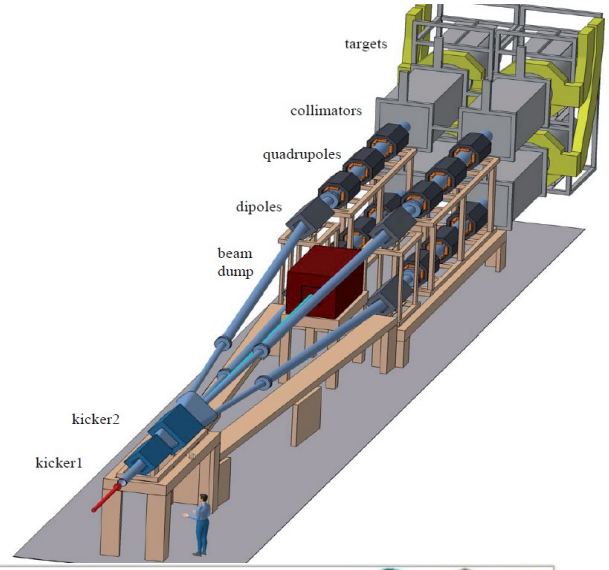
Example of lifetime estimation for irradiated components

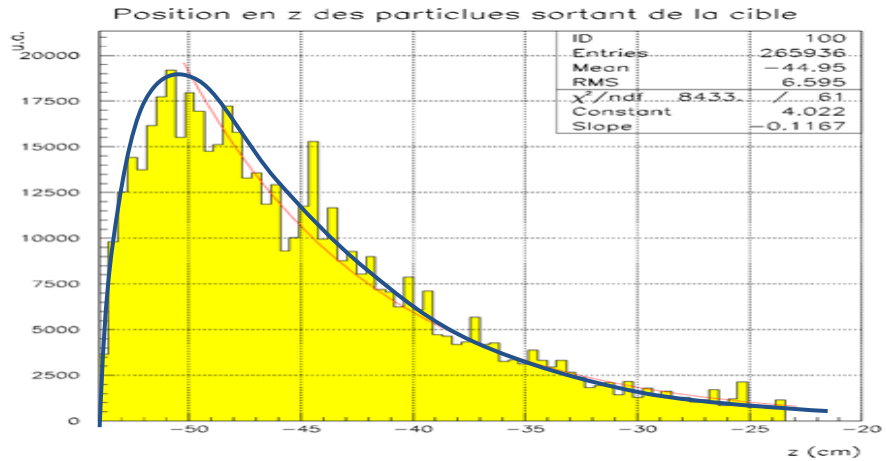


Typical distribution of *dpa* in the horn

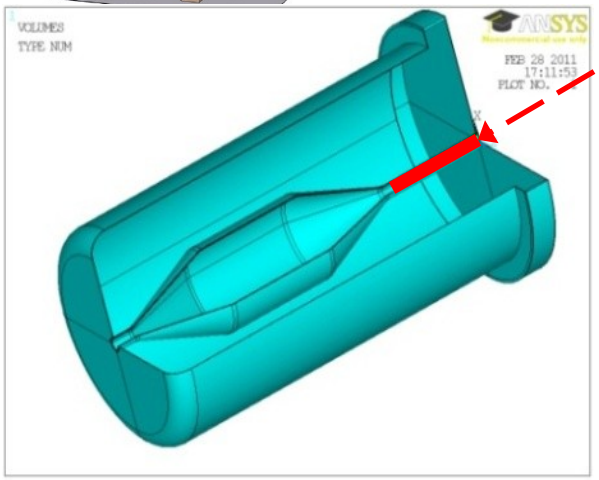
Secondary particles flux:
γ, **n**, p+, π± and e±

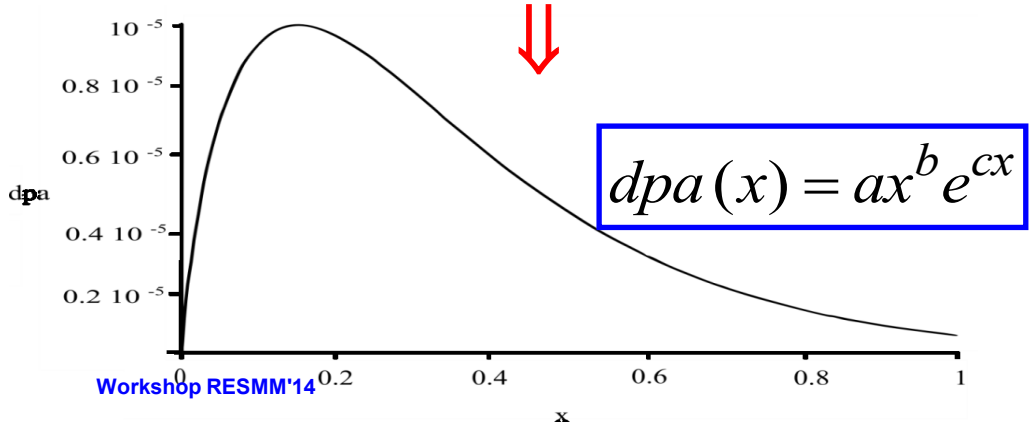






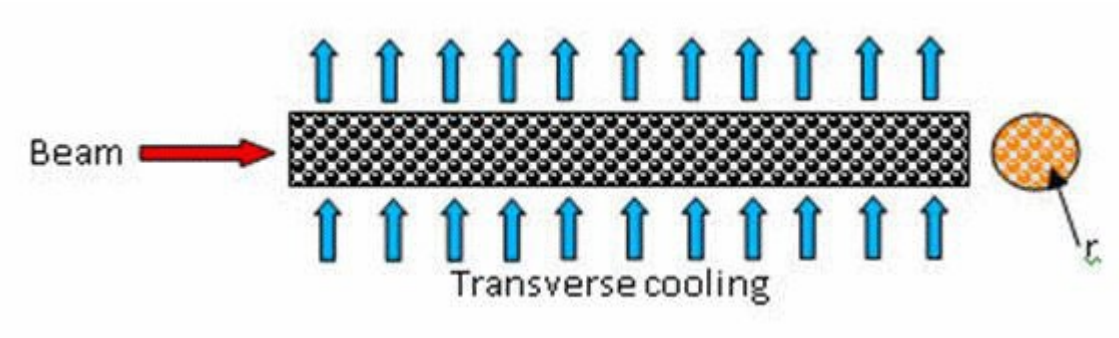
Typical distribution of particle flux along the target axis

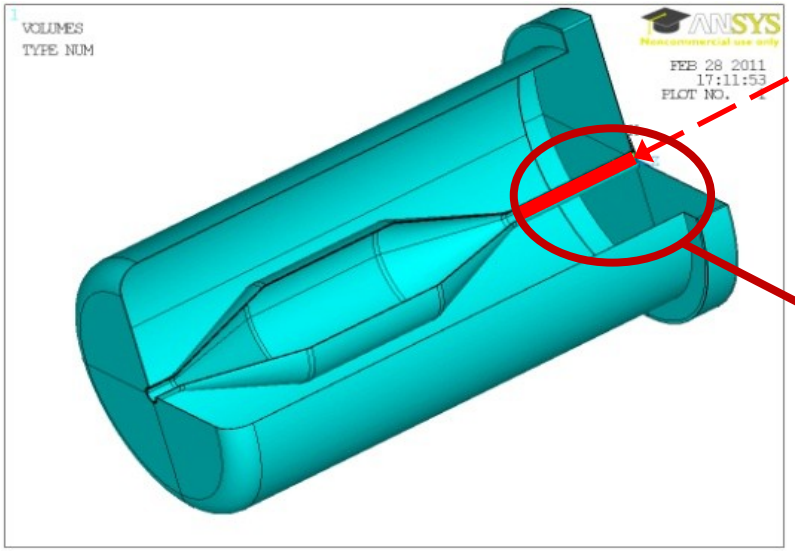


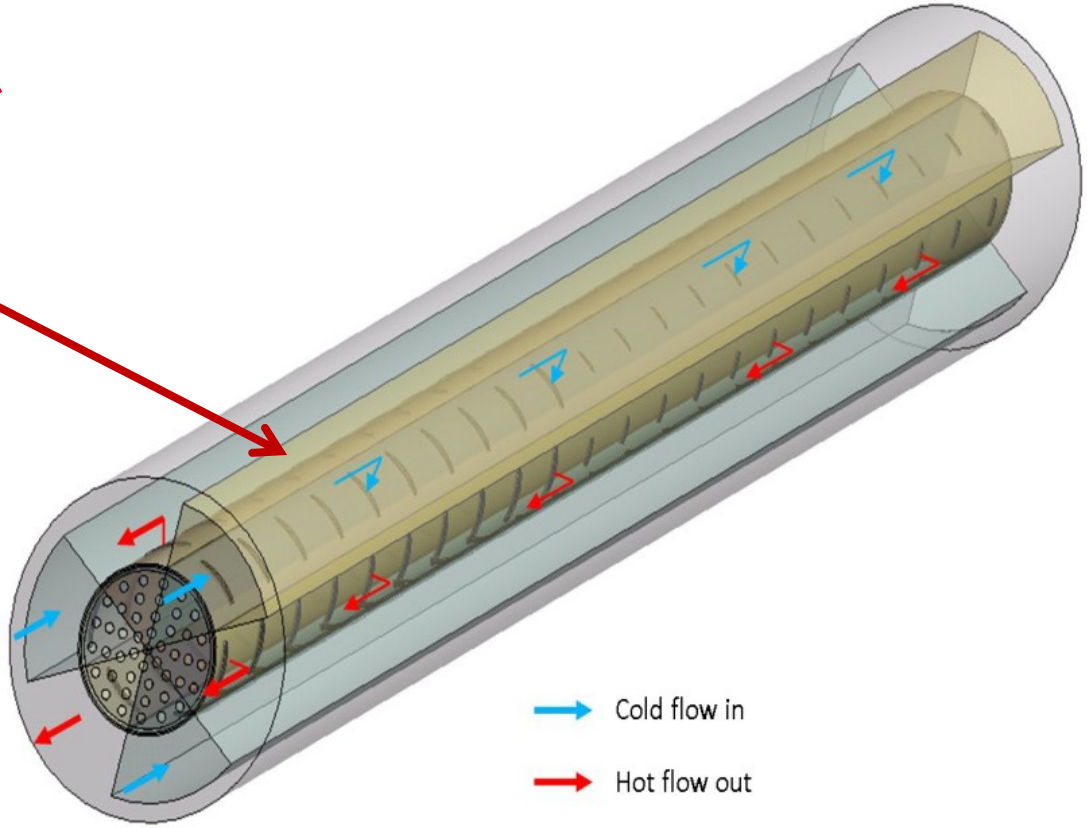


$$dpa(x) = ax^b e^{cx}$$

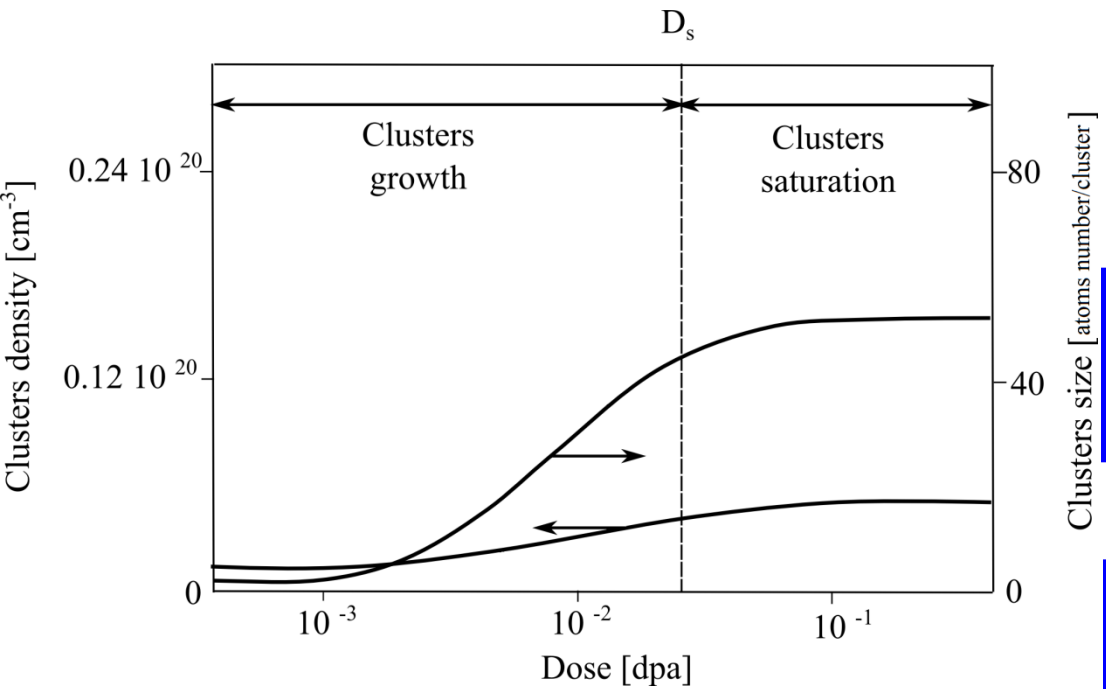
Target – Packed Bed (titanium spheres)







Clusters density and average cluster size after irradiation



$$dpa$$

$$q_c = \begin{cases} C_{qI}(dpa)^{n_{qI}} & for \quad dpa < D_S \\ C_{qII}(dpa)^{n_{qII}} & for \quad dpa \geq D_S \end{cases}$$

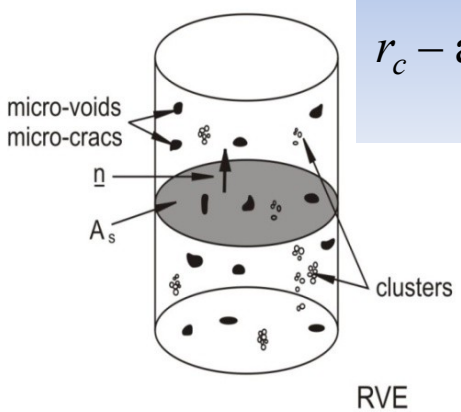
$$r_c = \begin{cases} C_r(dpa)^{n_r} & for \quad dpa < D_S \\ r_{cr} & for \quad dpa \geq D_S \end{cases}$$

$$q_A = \left(\sqrt[3]{q_V}\right)^2 = q_c^{\,2/3}$$

$$D_{r0} = q_A \pi r_{c0}^{\,2}$$

q_c – number of clusters per unit volume

r_c – average radius of clusters



$$D = \frac{dS_D}{dS} \quad ; \quad 0 \leq D \leq 1$$

$$\xi = \frac{dV_D}{dV} \quad ; \quad 0 \leq \xi \leq 1$$

Kinetics of clusters evolution

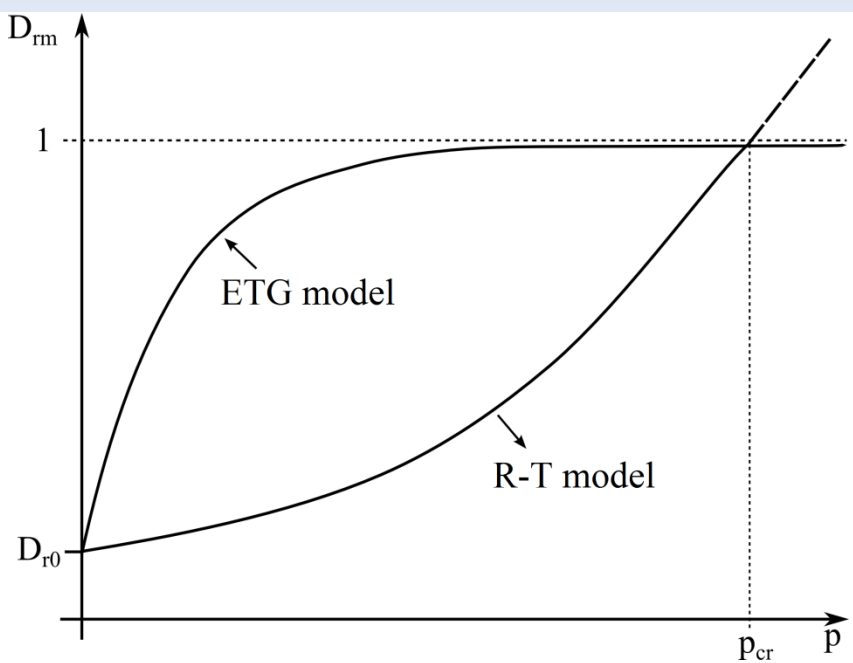
Kinetics of evolution of radiation induced micro-damage (clusters of voids) under mechanical loads

Rice&Tracey (R-T) model:

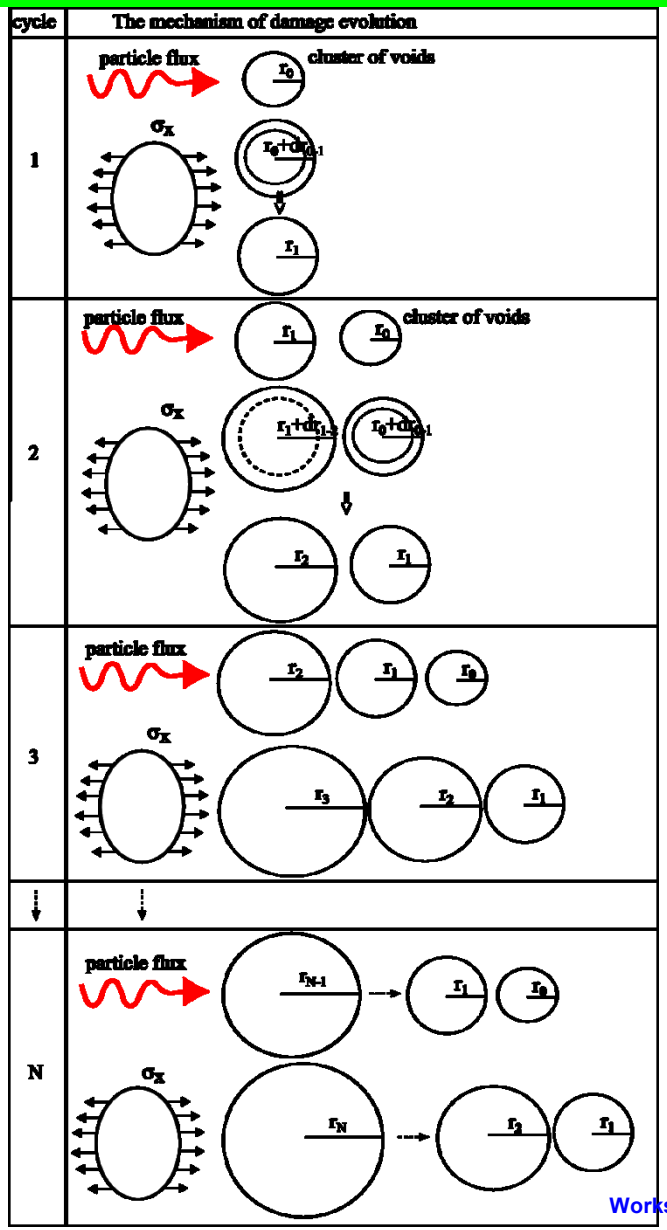
$$dr_c = r_c \alpha_r \exp\left(\frac{3\sigma_m}{2\sigma_{eq}}\right) dp$$

Gurson (ETG) model:

$$d\xi = (1-\xi)dp \qquad \dot{p} = \sqrt{\frac{2}{3}\dot{\varepsilon}_{ij}^{p}\dot{\varepsilon}_{ij}^{p}}$$



Mechanism of damage evolution under periodic irradiation



Description based on the **Rice & Tracey law**

$$\int_{D_i}^{D_{i+1}} dD = q_A 2\pi \int_{r_i}^{r_{i+1}} r\,dr$$

$$\Delta D_{i\to i+1} = q_A \pi \left(r_{i+1}^2 - r_i^2\right)$$

$$\int_{r_i}^{r_{i+1}} \frac{dr_c}{r_c} = \alpha_r \exp\left(\frac{3\sigma_m}{2\sigma_{eq}}\right) \int_0^{\tilde{p}} dp$$

$$r_{i+1} = r_i\, e^{A\tilde{p}}$$

$$\Downarrow$$

$$\Delta D_{i\to i+1} = q_A \pi r_i^2 \left(e^{2A\tilde{p}} - 1\right)$$

$$A := \alpha_r \exp\left(\frac{3\sigma_m}{2\sigma_{eq}}\right)$$

Analytical solution in the uniaxial stress state

$$D_{r0} = q_A \pi r_{c0}^2$$

$$D_{rm1} = D_{r0} + \Delta D_{rm(0\to1)} = D_{r0} + q_A \pi r_{c0}^2 \left(e^{2A\tilde{p}} - 1\right)$$

$$D_{rm2} = D_{rm1} + \Delta D_{rm(1\to2)} + D_{r0} + \Delta D_{rm(0\to1)} = 2D_{r0} + q_A \pi r_{c0}^2 e^{2A\tilde{p}} + q_A \pi r_{c0}^2 e^{4A\tilde{p}} - 2q_A \pi r_{c0}^2$$

$$\vdots$$

$$D_{rm_{i+1}} = D_{rm_i} + D_{r0} + \Delta D_{rm(i\to i+1)} + \Delta D_{rm(i-1\to i)} + \ldots + \Delta D_{rm(0\to1)}$$

$$\boxed{D_{rmN} = \underbrace{q_A \pi r_{c0}^2 e^{2A\tilde{p}} + q_A \pi r_{c0}^2 e^{4A\tilde{p}} + q_A \pi r_{c0}^2 e^{6A\tilde{p}} + \ldots + q_A \pi r_{c0}^2 e^{2NA\tilde{p}}}_{\text{Geometric series}}}$$

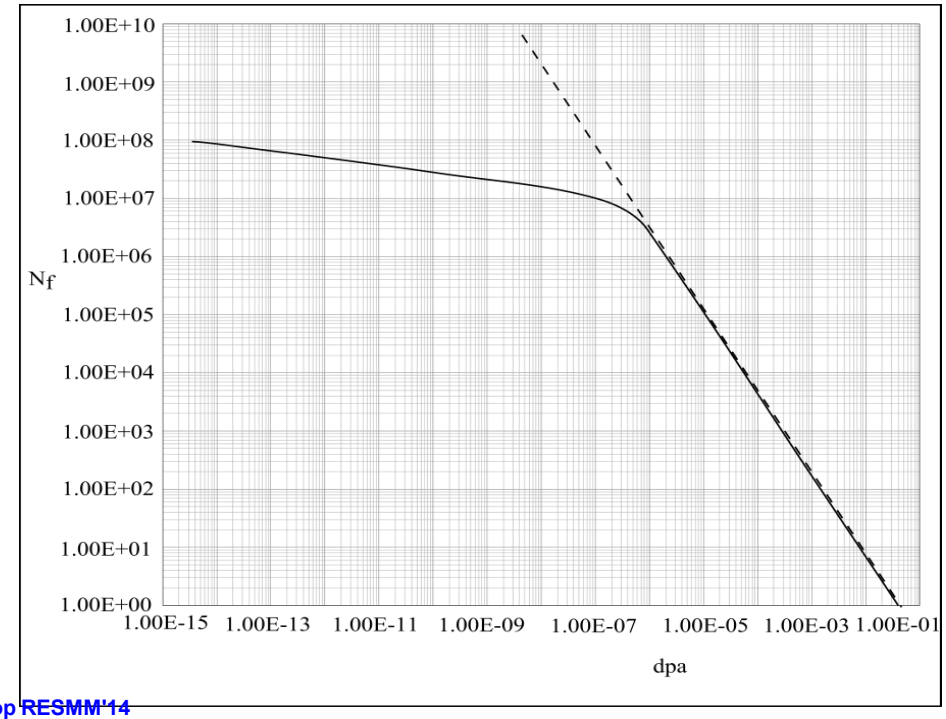
Number of cycles to failure N_f based on the critical damage criterion $D_{rm}=D_{cr}$

$$D_{rmN} = q_A \pi r_{c0}^2 \sum_{n=1}^{N} e^{2nA\tilde{p}}$$

$$S_N = a_1 \frac{1-q^N}{1-q} \qquad S_N = q_A \pi r_{c0}^2 e^{2A\tilde{p}} \frac{1-e^{2ApN}}{1-e^{2Ap}}$$

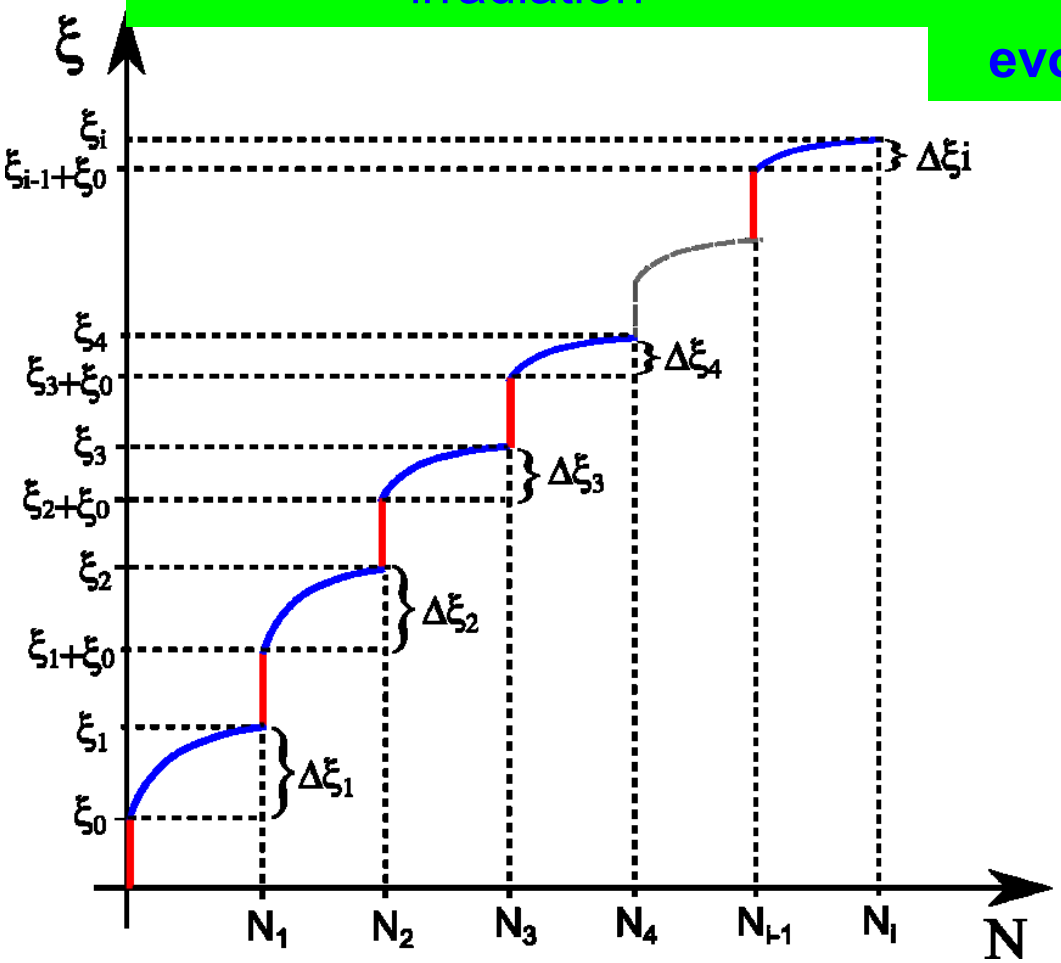
$$\boxed{D_{rmN} = q_A \pi r_{c0}^2 e^{2A\tilde{p}} \frac{1-e^{2ApN}}{1-e^{2Ap}}}$$

$$\boxed{D_{rmN_f} = q_A \pi r_{c0}^2 e^{2A\tilde{p}} \frac{1-e^{2A\tilde{p}N_f}}{1-e^{2A\tilde{p}}} = D_{cr}}$$



Mechanism of damage evolution under periodic irradiation

Description based on the **Gurson law evolution of porosity parameter ξ**



$$d\xi = (1-\xi)\,dp$$

$$\int_{\xi_i+\xi_0}^{\xi_{i+1}} \frac{d\xi}{1-\xi} = \int_0^{\tilde{p}} dp \qquad K := e^{-\tilde{p}}$$

$$\boxed{\xi_{i+1} = 1-(1-\xi_0-\xi_i)K}$$

Porosity parameter ξ_i increases from cycle to cycle by ξ_0 due to emission of secondary particles flux

Analytical solution for the uniaxial stress state

$$\xi_1 = 1-(1-\xi_0)K = 1+\xi_0 K - K$$

$$\xi_2 = 1-(1-\xi_0-\xi_1)K = 1+\xi_0 K + \xi_0 K^2 - K^2$$

$$\xi_3 = 1-(1-\xi_0-\xi_2)K = 1+\xi_0 K + \xi_0 K^2 + \xi_0 K^3 - K^3$$

$$\xi_4 = 1+\xi_0 K + \xi_0 K^2 + \xi_0 K^3 + \xi_0 K^4 - K^4$$

$$\vdots$$

$$\xi_i = \left(1-K^i\right) + \xi_0 \sum_{n=1}^{i} K^n$$

$$\boxed{\xi_N = 1+\underbrace{\xi_0 K + \xi_0 K^2 + \xi_0 K^3 + \xi_0 K^4 + \ldots + \xi_0 K^N}_{\text{Geometric series}} - K^N}$$

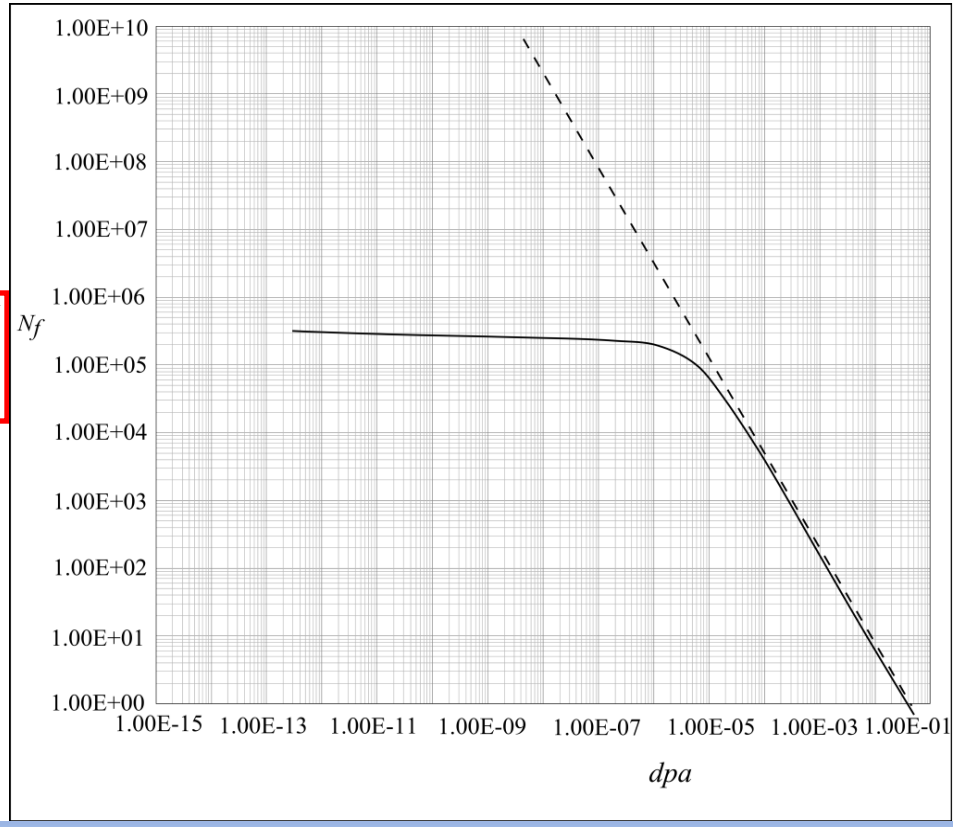
$$\xi_N = \left(1-K^N\right) + \xi_0 \sum_{n=1}^{N} K^N$$

$$S_N = \xi_0 K \frac{1-K^N}{1-K}$$

$$\boxed{\xi_N = 1+\xi_0 K \frac{1-K^N}{1-K} - K^N}$$

$$\boxed{\xi_N = 1+\xi_0 K \frac{1-K^N}{1-K} - K^N = \xi_{cr}}$$

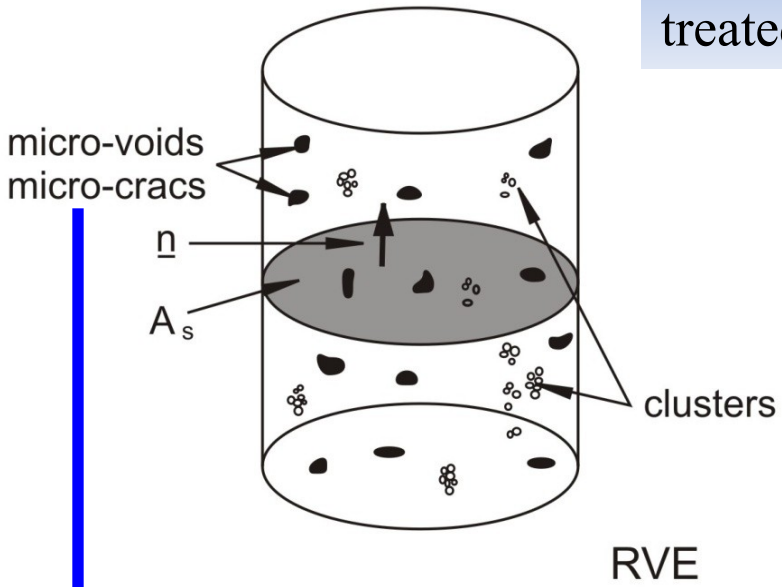
Number of cycles to failure N_f is based on the criterion $\xi_N = \xi_{cr}$



Mechanical loads have significant impact below $dpa \approx 10^{-5}$

Radiation and mechanical damage components: additive formulation

Postulate: both micro-damage components are treated in additive way



$$D_r = D_{r0} + \int_0^{\hat{p}} dD_{rm}$$

radiation induced damage

$$\underline{\underline{D}}_r = \frac{D_r}{3} \underline{\underline{I}}$$

isotropic

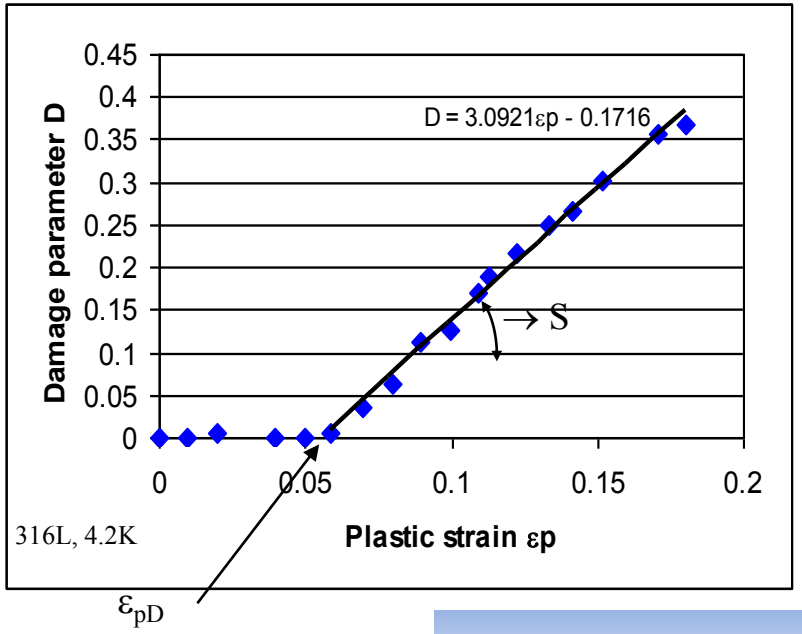
$\underline{\underline{I}}$ - identity tensor

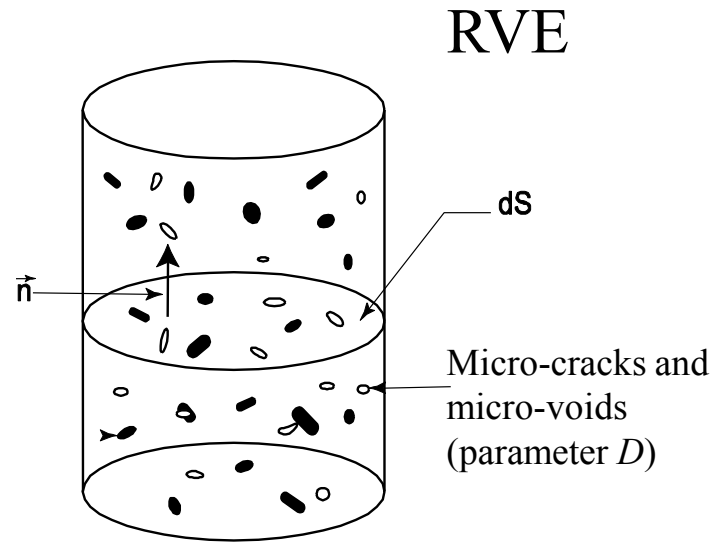
$$d\underline{\underline{D}}_m = \underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T dp$$

anisotropic

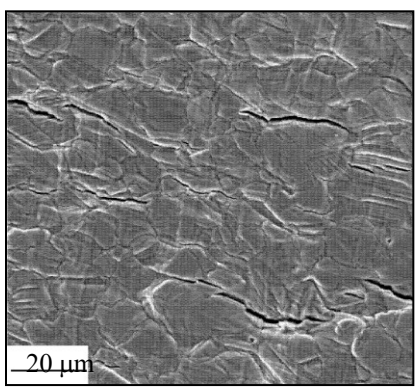
$$\underline{\underline{D}} = \underline{\underline{D}}_m + \underline{\underline{D}}_r = \underline{\underline{D}}_m + \frac{1}{3} D_r \underline{\underline{I}}$$

Kinetics of mechanically induced micro-damage





D – surface fraction of micro-cracks and micro-voids



$$D = \frac{dS_D}{dS} \quad ; \quad 0 \le D \le 1 \quad \longrightarrow \quad \underline{\underline{D}} = \sum_{i=1,3} D_i \, \underline{n}_i \otimes \underline{n}_i$$

$$\boxed{\dot{D} = \left(\frac{Y}{S}\right)^s \dot{p} H(p - p_D)} \quad \longrightarrow \quad \boxed{\dot{\underline{\underline{D}}} = \underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T \dot{p} H(p - p_D)}$$

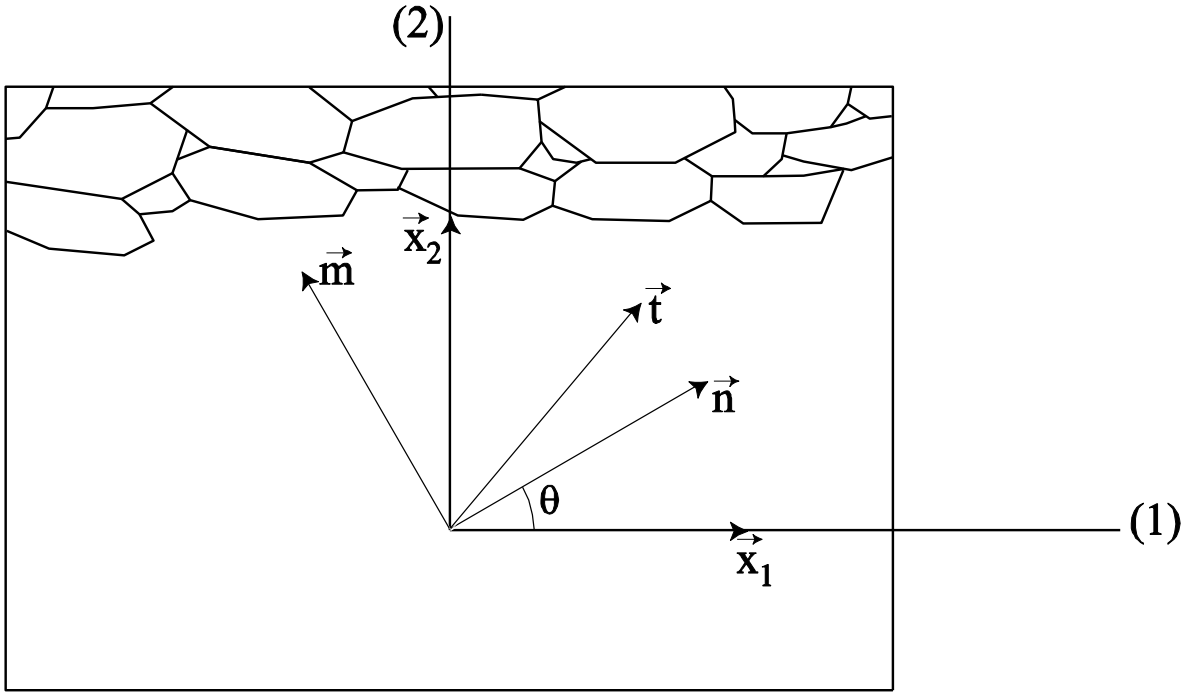
Chaboche, 1988; Lemaitre, 1992

Garion, Skoczeń; Int. J. Dam. Mech., 2003

Isotropic versus anisotropic model

Isotropic model	Anisotropic model
Helmholtz free energy	
$\Psi = \frac{1}{2\rho}\underline{\underline{\varepsilon}}^e : \underline{\underline{\underline{\underline{E}}}}(1-D) : \underline{\underline{\varepsilon}}^e + \Psi_p$	$\Psi = \frac{1}{2\rho}\underline{\underline{\varepsilon}}^e : \underline{\underline{\underline{\underline{M}}}}(\underline{\underline{D}}) : \underline{\underline{\underline{\underline{E}}}} : \underline{\underline{\varepsilon}}^e + \Psi_p$
Effective stress	
$\underline{\underline{\sigma}} = (1-D)\underline{\underline{\tilde{\sigma}}}$	$\underline{\underline{\sigma}} = \frac{1}{2}\left((\underline{\underline{I}} - \underline{\underline{D}})\underline{\underline{\tilde{\sigma}}} + \underline{\underline{\tilde{\sigma}}}(\underline{\underline{I}} - \underline{\underline{D}})\right)$ $\Leftrightarrow \underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{M}}}}(\underline{\underline{D}}) : \underline{\underline{\tilde{\sigma}}}$
Conjugate force associated to damage	
$Y = -\rho\frac{\partial\Psi}{\partial D} = \frac{1}{2}\underline{\underline{\varepsilon}}^e : \underline{\underline{\underline{\underline{E}}}} : \underline{\underline{\varepsilon}}^e$	$\underline{\underline{Y}} = -\rho\frac{\partial\Psi}{\partial \underline{\underline{D}}}$
	$\Leftrightarrow \underline{\underline{Y}} = \frac{1}{4}\left[\underline{\underline{\varepsilon}}^e\left(\underline{\underline{\underline{\underline{E}}}} : \underline{\underline{\varepsilon}}^e\right) + \left(\underline{\underline{\underline{\underline{E}}}} : \underline{\underline{\varepsilon}}^e\right)\underline{\underline{\varepsilon}}^e\right]$
Potential of dissipation associated to irreversible damage process	
$\Phi_D = \frac{1}{2}\frac{Y^2}{S}\frac{1}{1-D}$	$\Phi_D = \frac{1}{2}\left(\underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T\right) : \underline{\underline{Y}}a(\underline{\underline{D}})$
	$a(\underline{\underline{D}}) = \left(\frac{(\underline{\underline{\tilde{s}}} - \underline{\underline{\tilde{X}}}) : \underline{\underline{\underline{\underline{M}}}}^{-1} : \underline{\underline{\underline{\underline{M}}}}^{-1} : (\underline{\underline{\tilde{s}}} - \underline{\underline{\tilde{X}}})}{(\underline{\underline{\tilde{s}}} - \underline{\underline{\tilde{X}}}) : (\underline{\underline{\tilde{s}}} - \underline{\underline{\tilde{X}}})}\right)^{\frac{1}{2}}$
Kinetic law of damage evolution	
$\dot{D} = \dot{\lambda}\frac{\partial\Phi_D}{\partial Y} = \frac{Y}{S}\dot{p}\Big\|_{p>p_D}$	$\underline{\underline{\dot{D}}} = \dot{\lambda}\frac{\partial\Phi_D}{\partial \underline{\underline{Y}}} = \underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T\dot{p}\Big\|_{p>p_D}$

Isotropic versus anisotropic model



$$\underline{\underline{\dot{D}}} = \underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T \dot{p} H(p - p_D)$$

$$\dot{D}_{ij} = C_{ik} Y_{kl} C_{jl} \dot{p} H(p - p_D)$$

$$\underline{\underline{C}} = \sum_{i=1,3} C_i \vec{n}_i \otimes \vec{n}_i$$

$$\underline{\underline{C}} = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix}_{(\vec{x}_1, \vec{x}_2)}$$

$$\underline{\underline{V}}_D = \left.\frac{d\underline{\underline{D}}}{dp}\right|_{p=p_D} = \underline{\underline{C}}\,\underline{\underline{Y}}\,\underline{\underline{C}}^T$$

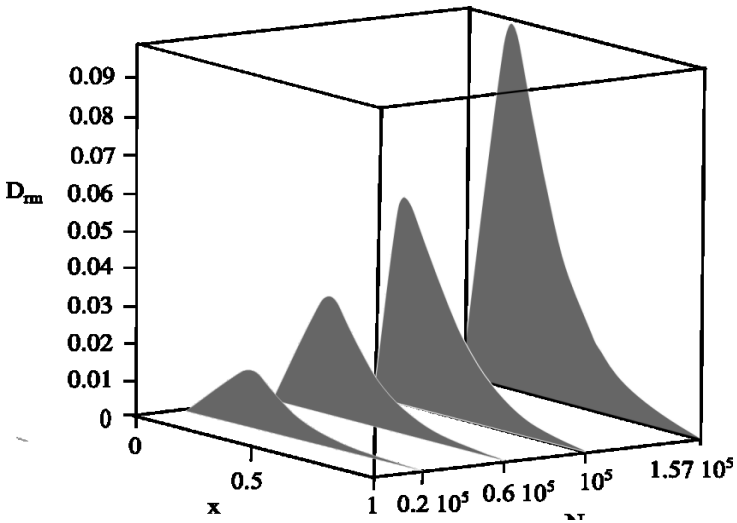
Texture directions:	*(1), (2)*
Principal directions of stress:	$(\vec{n}, \vec{m})$
Loading direction:	$(\vec{n})$
Principal direction of damage:	$(\vec{t})$

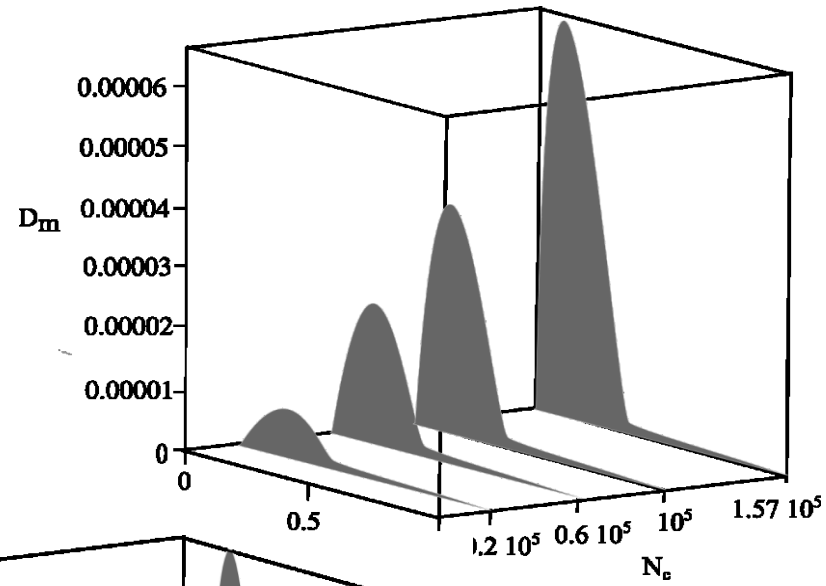
Evolution of damage parameter in the horn (magnetic lense)

radiation induced damage

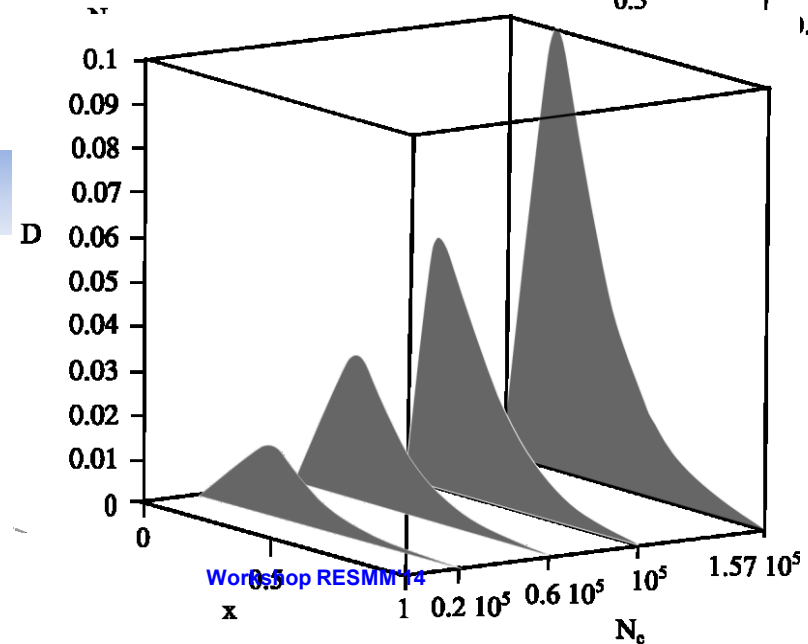
$D_{cr}=0.1$

mechanical damage

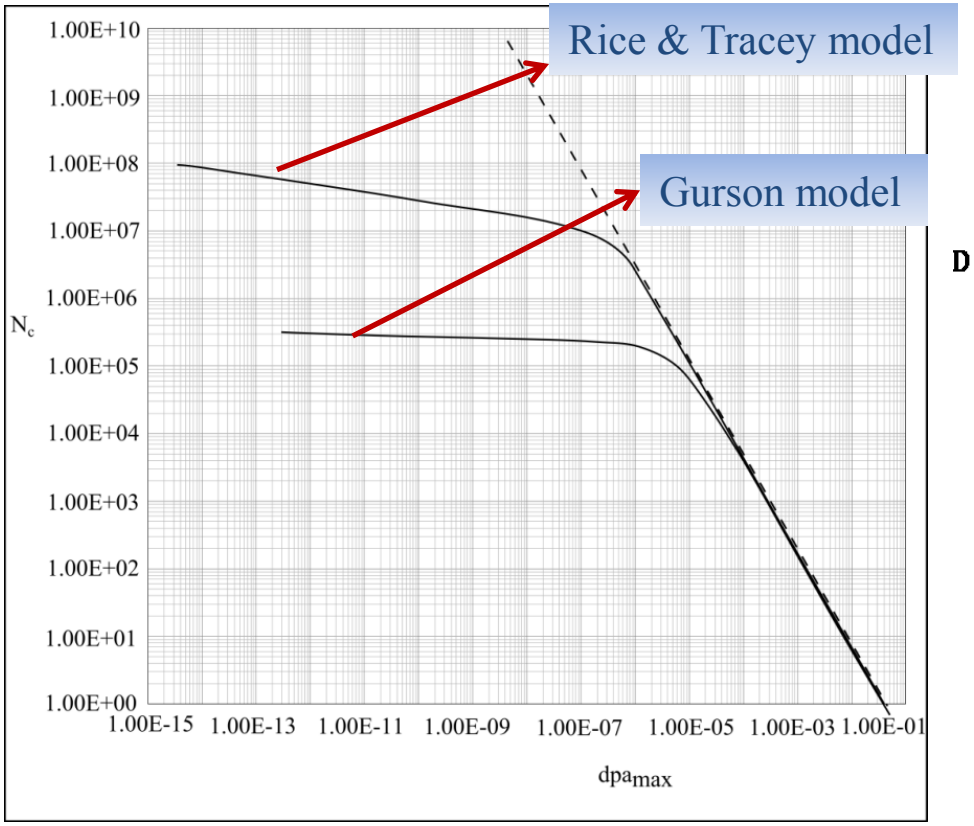


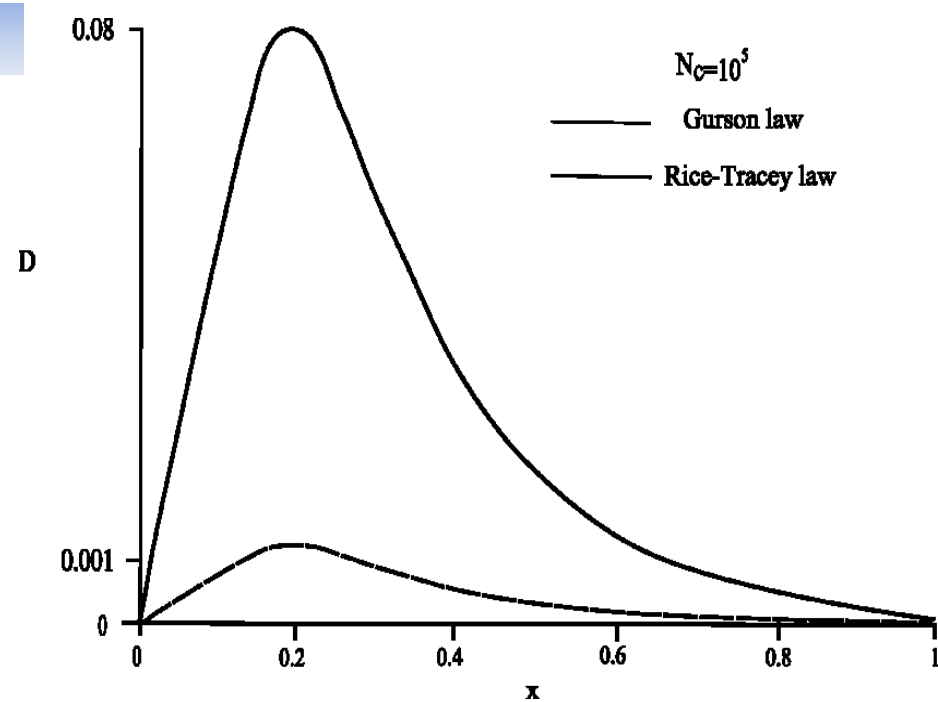


total damage parameter



Performance of Rice-Tracey and Gurson models (log-log)



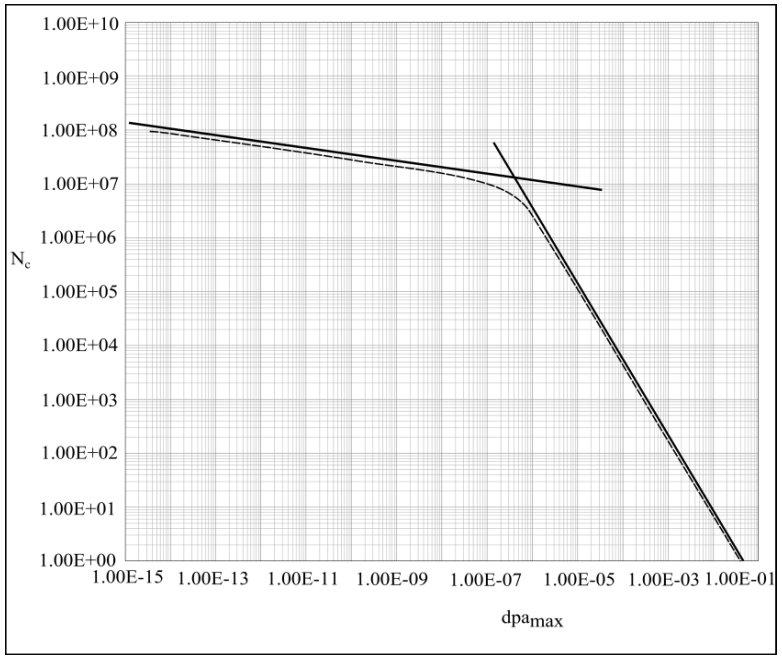


different sensitivity of both models

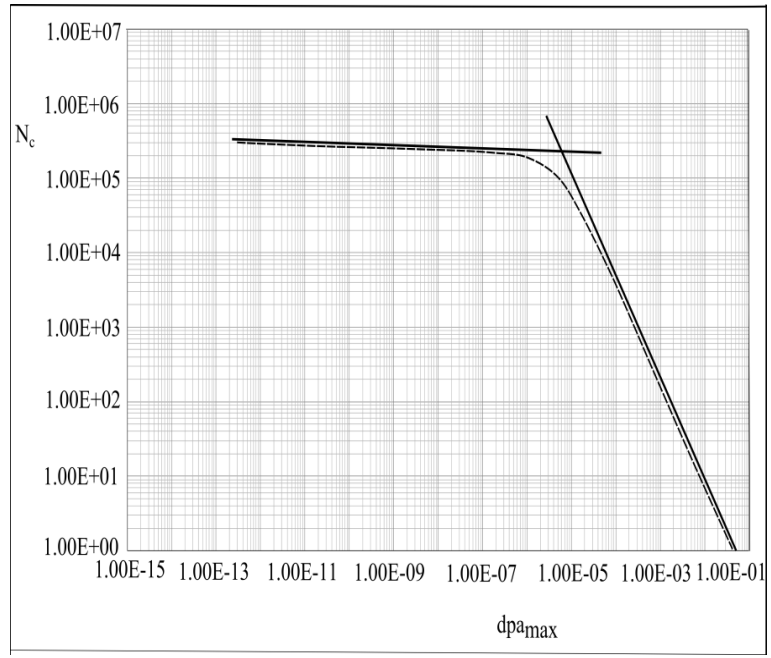
Rice & Tracey model predicts lower values of damage

Bilinear approximations for R-T and Gurson models

Rice & Tracey model



Gurson model



$$\log(N_c) = a + b\log(dpa_{\max})$$

Analytical formula - useful tool for estimation of number of cycles to failure

$$N_c = 10^a \, dpa_{\max}^b$$

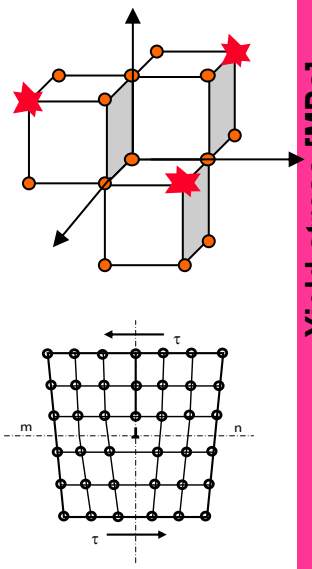
$$N_c = \begin{cases} 10^{-1.9} dpa_{\max}^{-1.4} & for \quad dpa_{\max} \geq 10^{-6} \\ 10^{6.1} dpa_{\max}^{-0.13} & for \quad dpa_{\max} < 10^{-6} \end{cases}$$

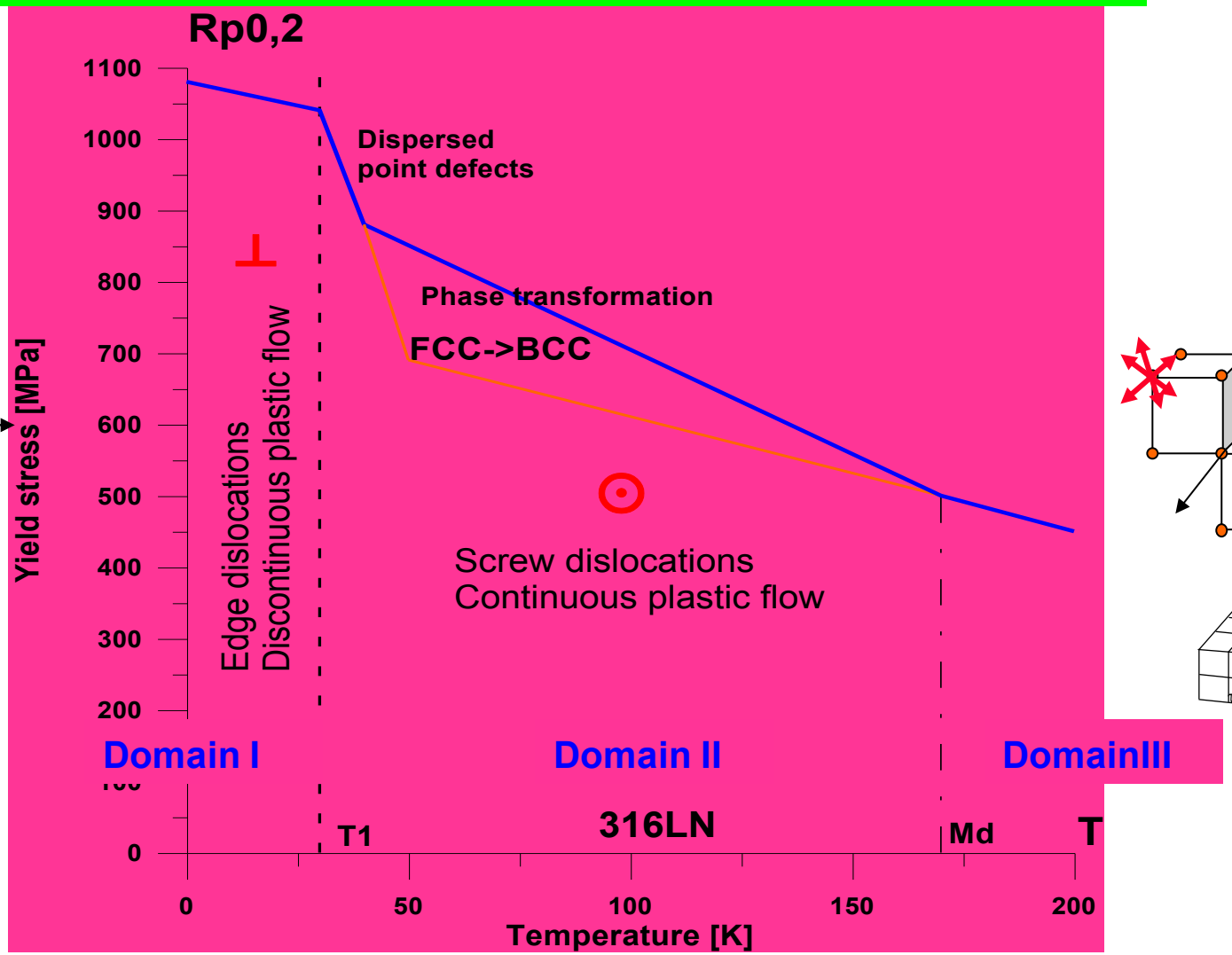
$$N_c = \begin{cases} 10^{-1.9} dpa_{\max}^{-1.4} & for \quad dpa_{\max} \geq 10^{-5} \\ 10^{5.43} dpa_{\max}^{-0.016} & for \quad dpa_{\max} < 10^{-5} \end{cases}$$

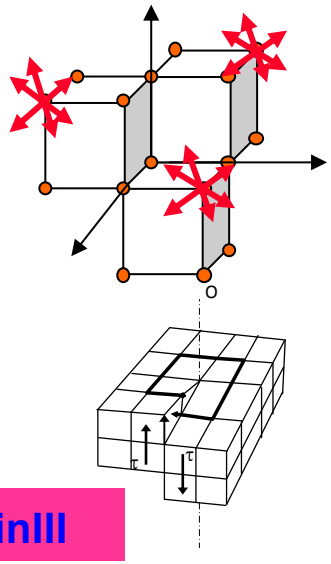
Specific coupled field problems

Coupled field problems

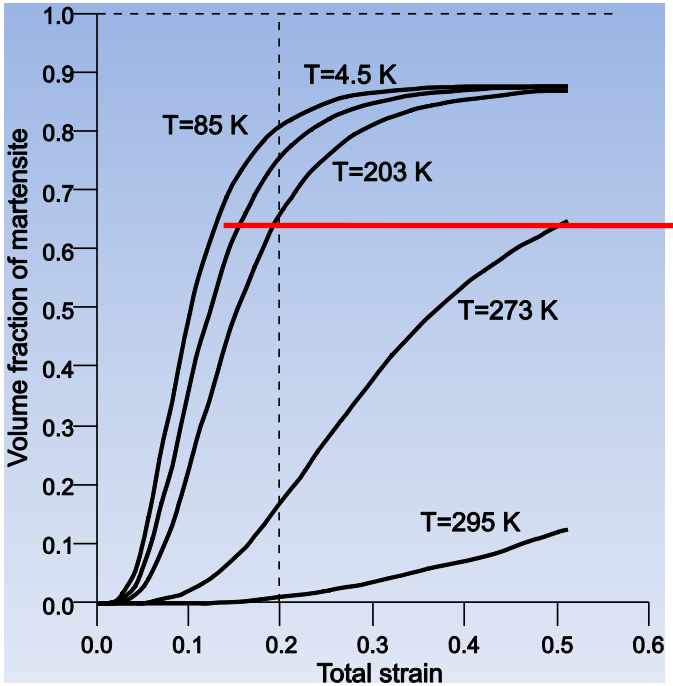
Mechanisms of plastic flow at cryogenic temperatures

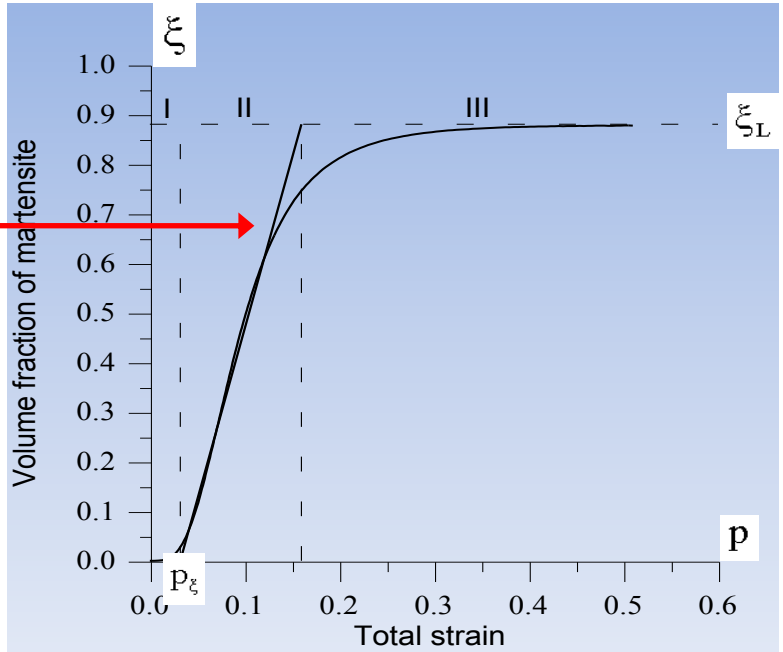




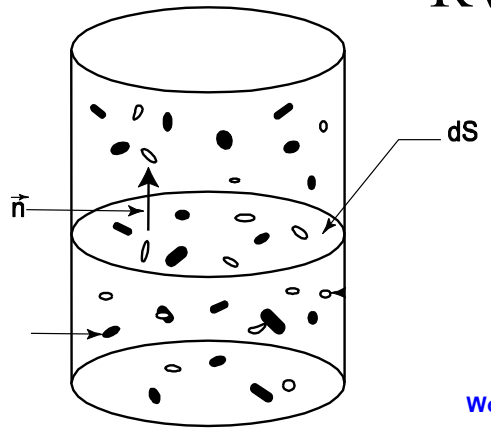


Kinetics of γ→α' phase transformation





RVE



Inclusions α'
(parameter ξ_α)

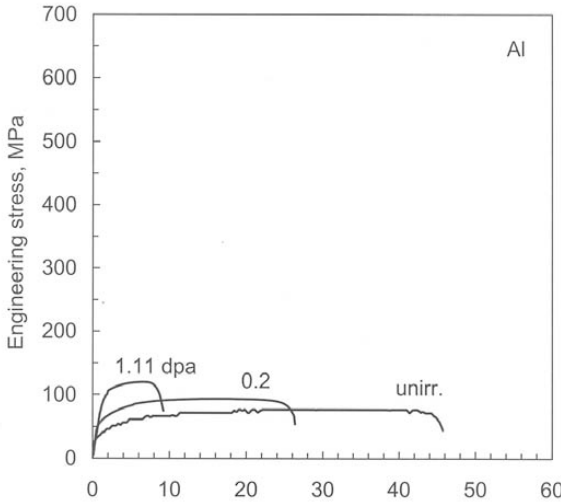
$$\xi_\alpha = \frac{dV_\xi}{dV} \quad ; \quad 0 \le \xi_\alpha \le 1$$

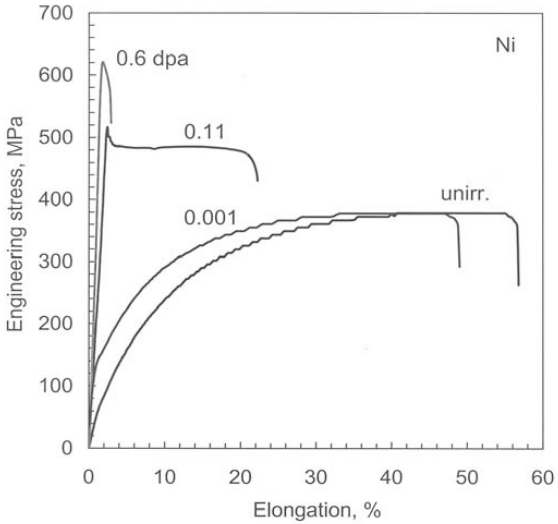
$$\dot{\xi}_\alpha = A\left(T, \underline{\underline{\dot{\varepsilon}}}^p, \underline{\underline{\sigma}}\right) \dot{p} H\left(\left(p - p_\xi\right)\left(\xi_L - \xi_\alpha\right)\right)$$

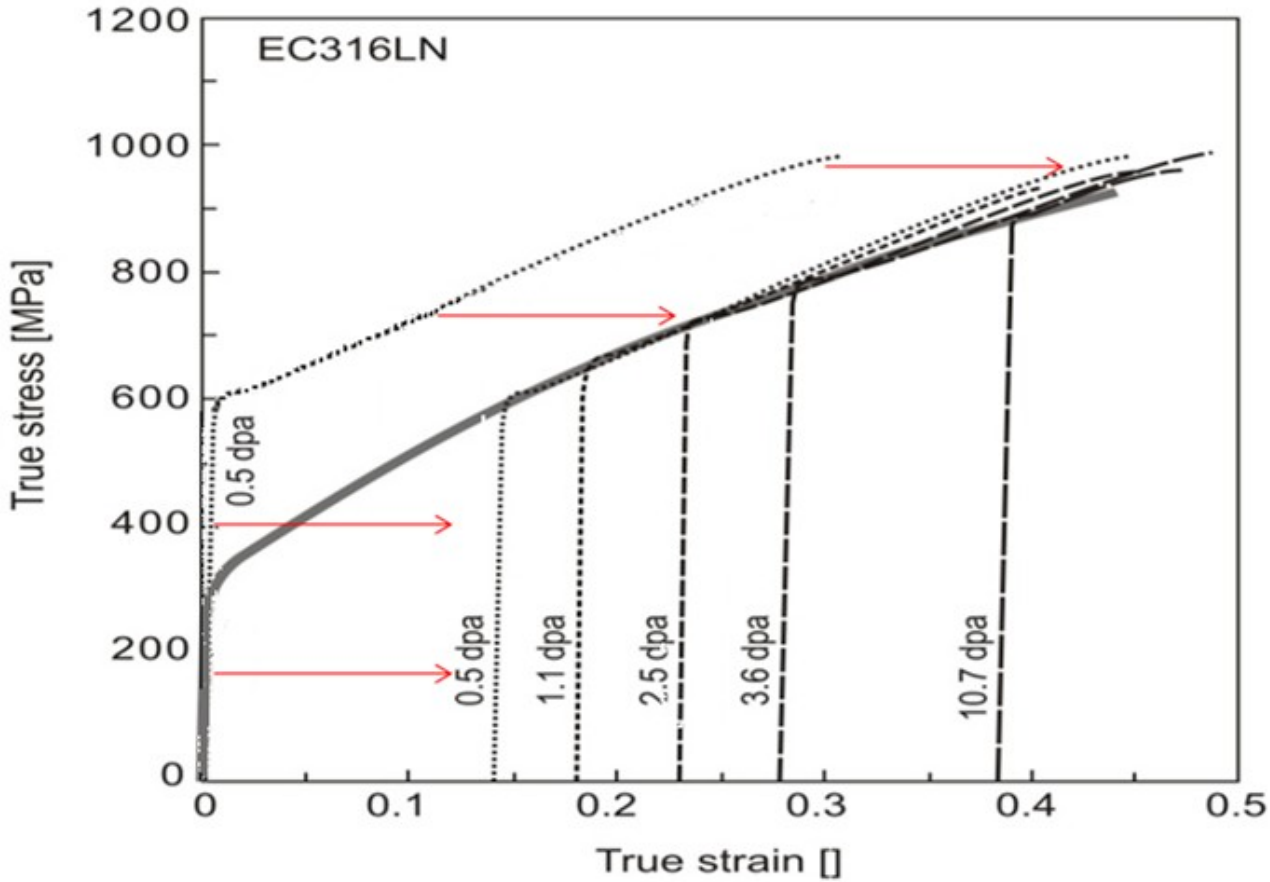
ξ_α – volume fraction of α' phase

Garion, Skoczeń; J. Appl. Mech., 2002

Stress-strain curves for irradiated samples



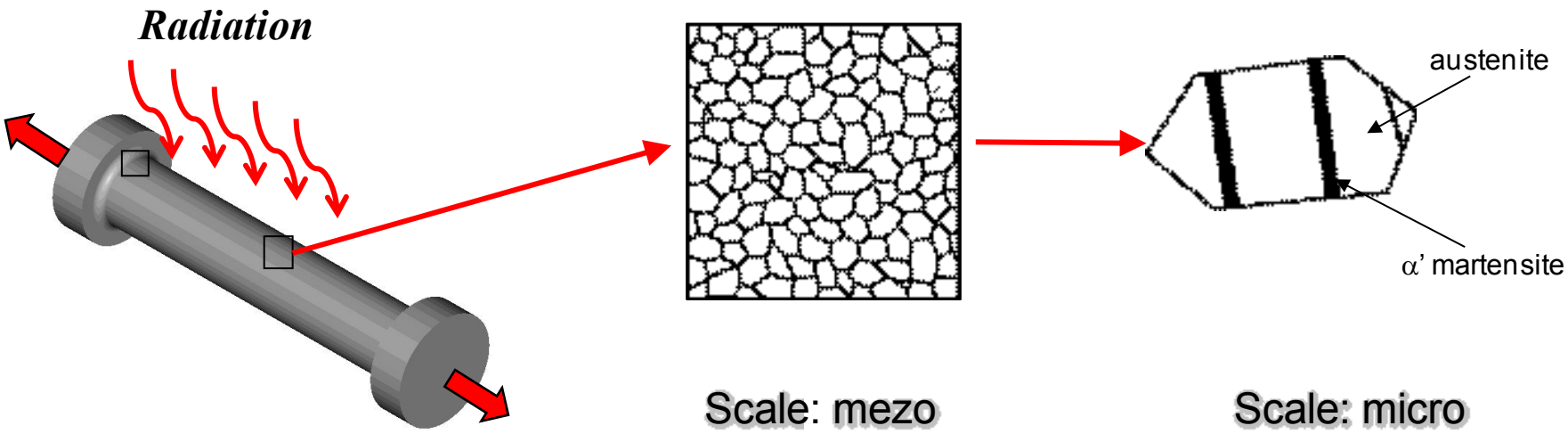




Currently available information is insufficient!

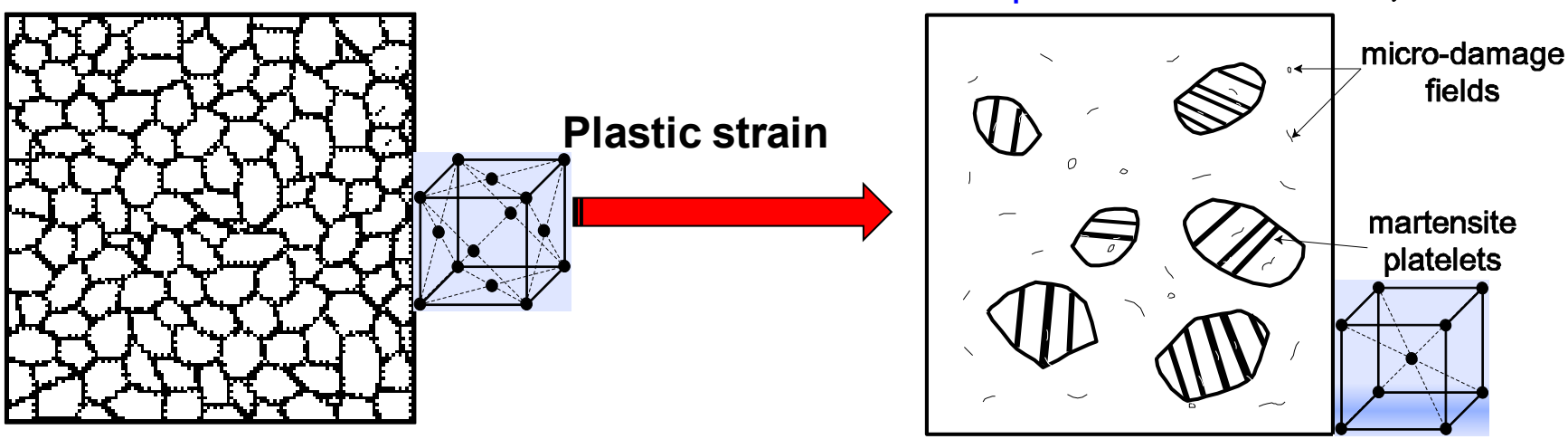
Source: S.J. Zinkle „Mechanical property changes in metals due to irradiation", Italy, 2004.

Plastic strain induced FCC-BCC phase transformation versus evolution of damage

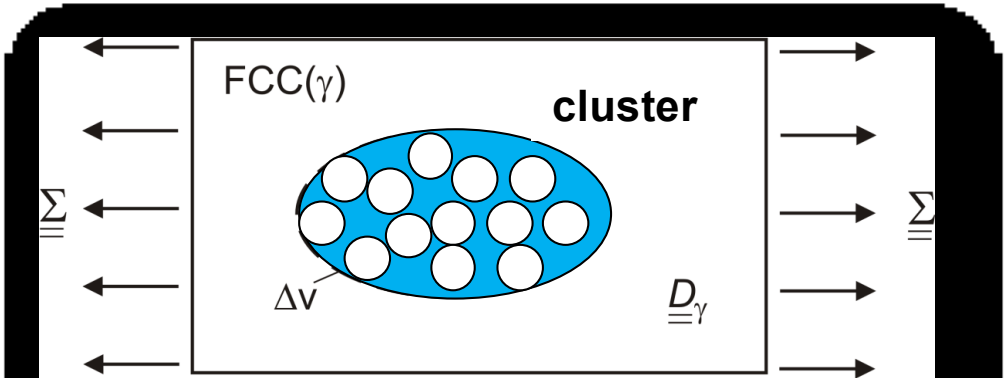


Single-phase continuum γ

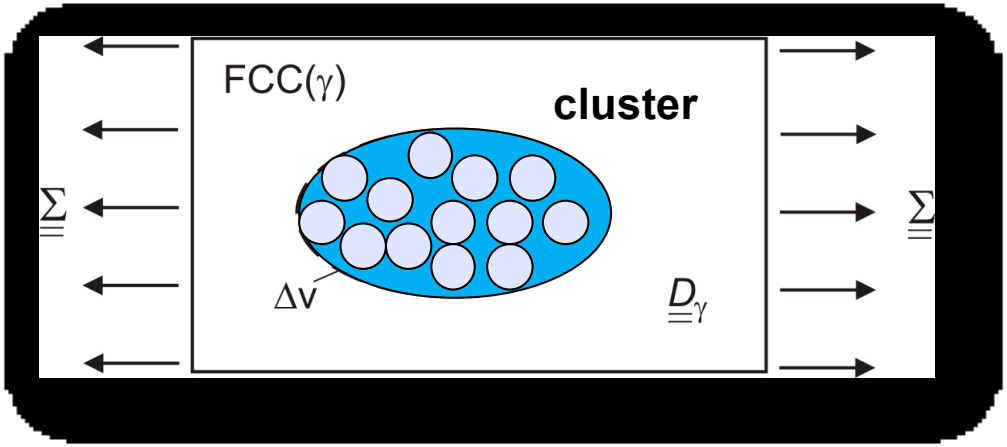
Two-phase continuum $\gamma + \alpha'$



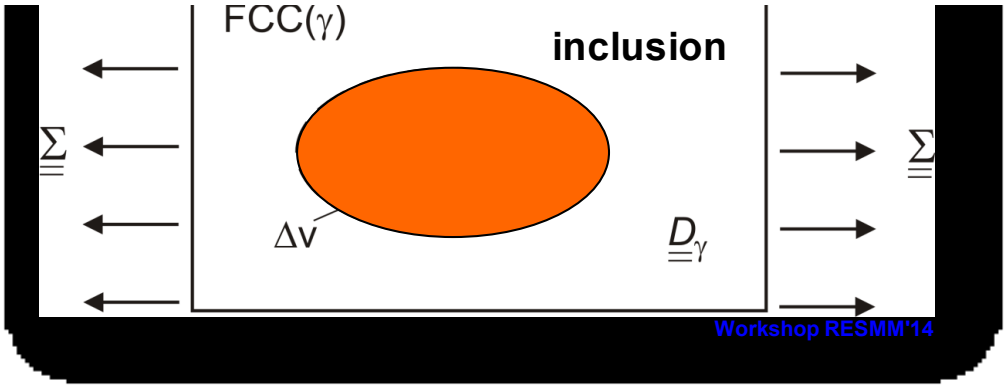
Type Eshelby entities: clusters of voids, α' inclusions



3D vacancy clusters: ξ_c



3D vacancy cluster with impurities (He): ξ_c

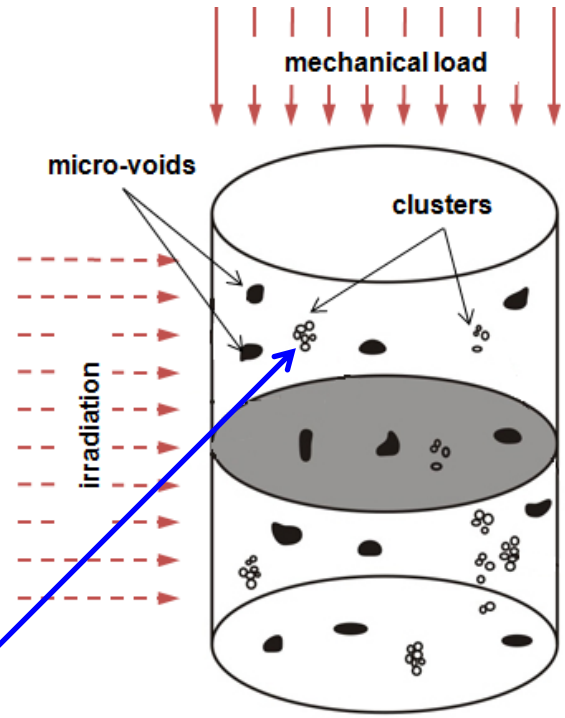


Inclusions of secondary phase: ξ_a

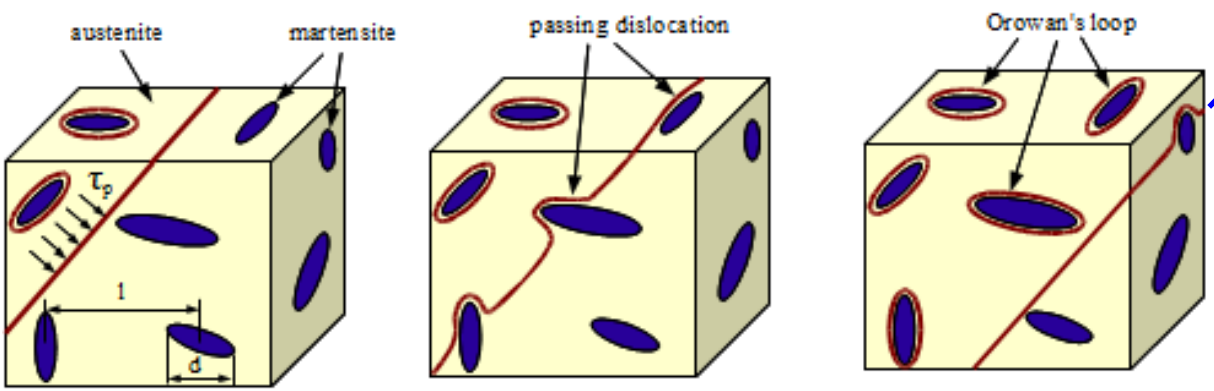
Hardening of irradiated metals and alloys

Defects due to irradiation:

1. **SFT – stacking fault tetrahedron**
2. **Faulted or perfect dislocation loops**
3. **Voids – 3D vacancy clusters**
4. **Cavities – 3D vacancy clusters with impurities (He)**



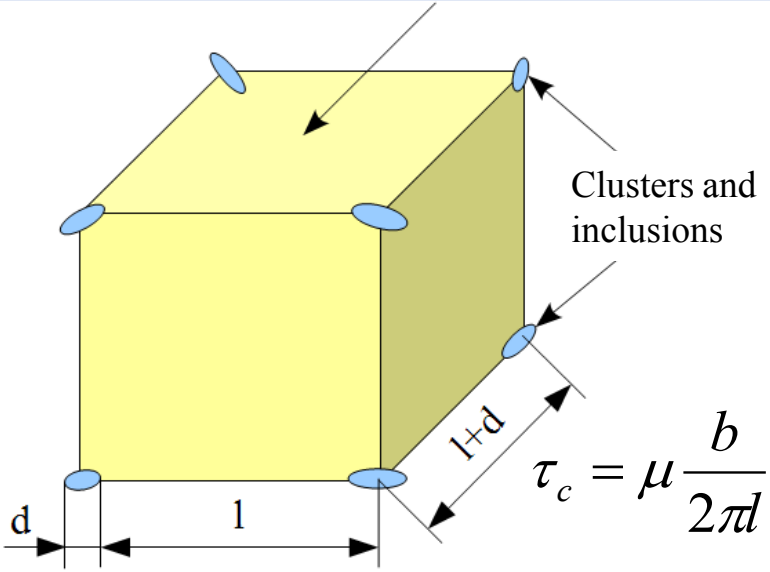
Interaction of dislocations with clusters of defects

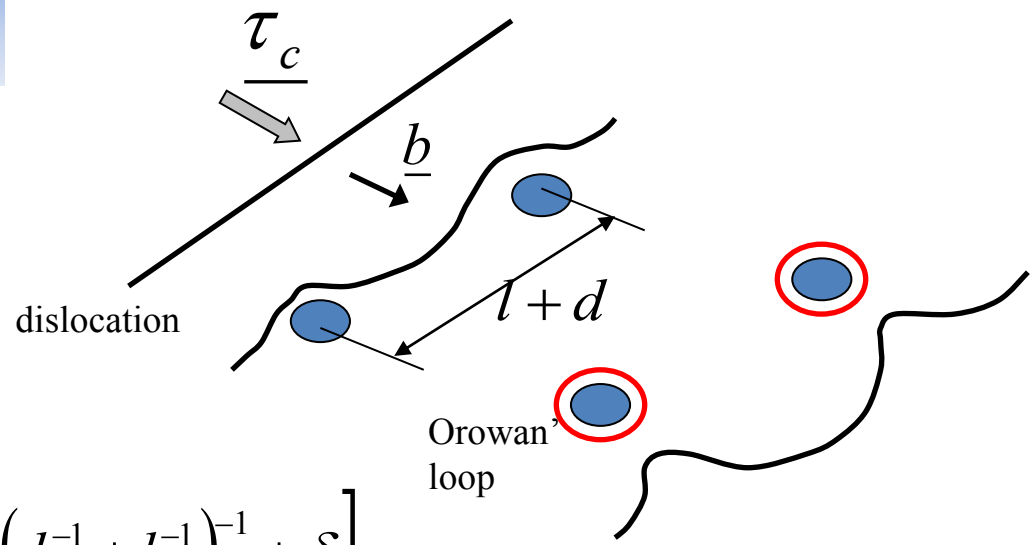


Type Eshelby inclusions (*J.D. Eshelby, Proc. Royal Soc. London, 1957*):

Micromechanics: Orowan mechanism (clusters + inclusions)

Interaction of dislocations with clusters and α' inclusions





$$\tau_c = \mu \frac{b}{2\pi d}\left[\ln\left(d^{-1}+l^{-1}\right)^{-1}+\delta\right]$$

$$\xi_c = q_c \frac{4}{3}\pi (r_c)^3$$

$$\xi_\alpha = \frac{dV_\xi}{dV}$$

$$\xi = \xi_c + \xi_\alpha$$

$$\tau_c = \frac{Gb}{d}\left(\frac{6\xi_0}{\pi}\right)^{\frac{1}{3}}\left(1+\frac{\xi-\xi_0}{3\xi_0}\right)$$

$$d\underline{\underline{\tilde{X}}}_a = \frac{2}{3}C_0(1+h\xi)d\underline{\underline{\varepsilon}}^p$$

Skoczeń; Int. J. Sol. Struct. 2007

Constitutive model including phase transformation and damage

Hardening caused by evolution of stiffness of two-phase continuum

Elastic-plastic γ lattice:

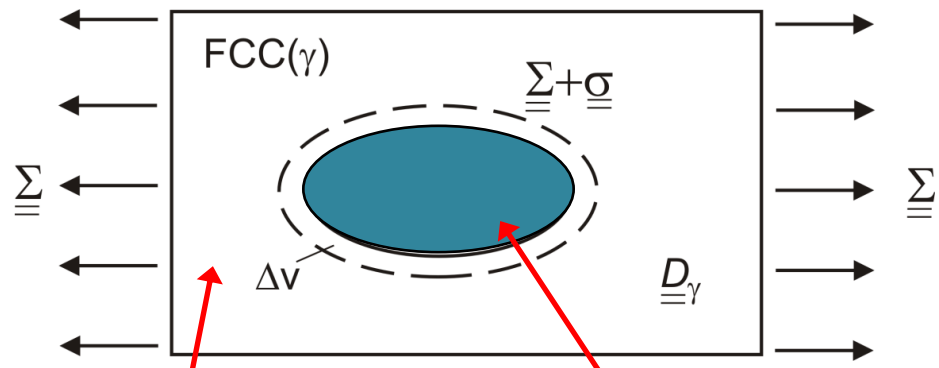
$$\underline{\underline{\underline{\underline{E}}}}_{ta} = 3k_a \underline{\underline{\underline{\underline{J}}}} + 2\mu_a \underline{\underline{\underline{\underline{K}}}} - 2\mu_a \frac{\underline{\underline{n}} \otimes \underline{\underline{n}}}{1 + \frac{C(\xi)}{3\mu_a}}$$

$$\boxed{\underline{\underline{\underline{\underline{E}}}}_{ta} = 3k_{ta} \underline{\underline{\underline{\underline{J}}}} + 2\mu_{ta} \underline{\underline{\underline{\underline{K}}}}}$$

$$\mu_{ta} = \frac{E_t}{2(1+\nu)} \qquad k_{ta} = \frac{E_t}{3(1-2\nu)} \qquad \boxed{E_t = \frac{EC}{E+C}}$$

α' elastic inclusions:

$$\boxed{\underline{\underline{\underline{\underline{E}}}}_{m} = 3k_m \underline{\underline{\underline{\underline{J}}}} + 2\mu_m \underline{\underline{\underline{\underline{K}}}}}$$

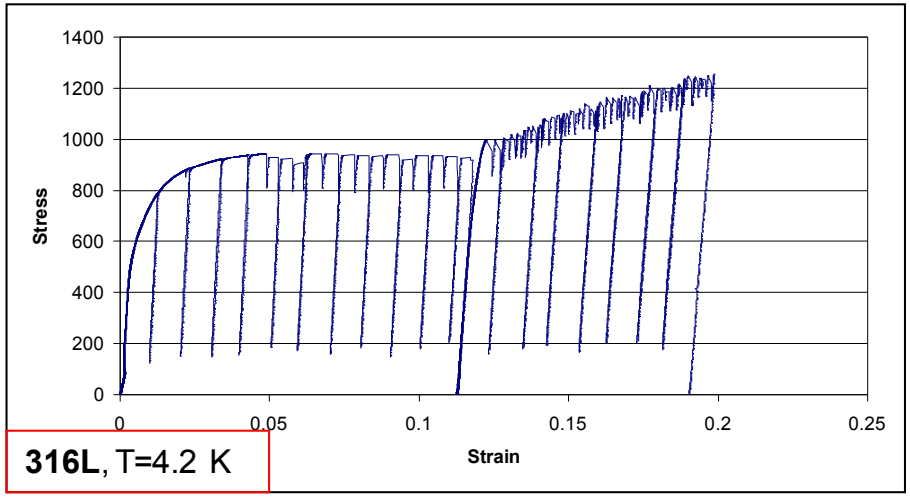


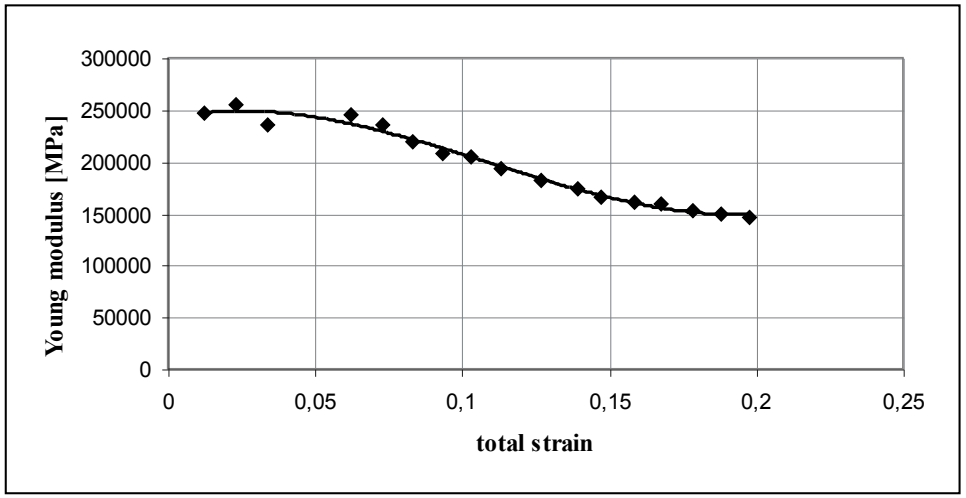
$$\boxed{\Delta\underline{\underline{\tilde{\sigma}}} = \underline{\underline{\underline{\underline{E}}}}_{ta} : \Delta\underline{\underline{\varepsilon}}} \qquad \boxed{\Delta\underline{\underline{\tilde{\sigma}}} = \underline{\underline{\underline{\underline{E}}}}_{m} : \Delta\underline{\underline{\varepsilon}}}$$

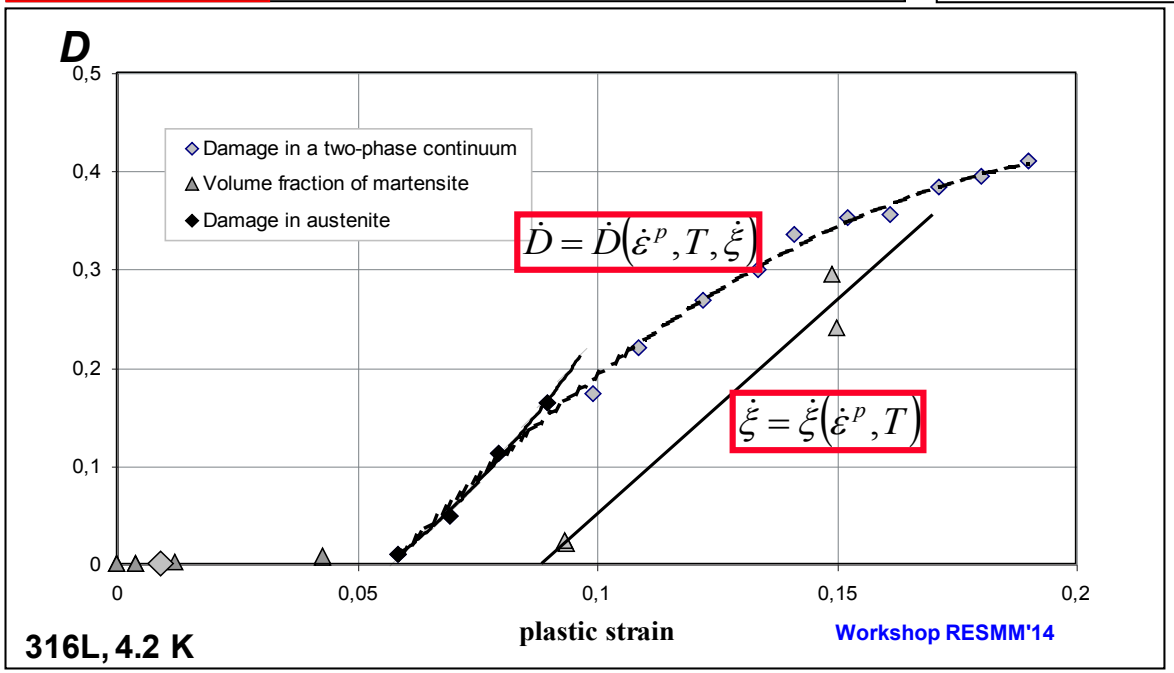
$$\boxed{\Delta\underline{\underline{\tilde{\sigma}}} = \underline{\underline{\underline{\underline{E}}}}_{H} : \Delta\underline{\underline{\varepsilon}}}$$

Linearization in the vicinity of current state (*R. Hill, J. Mech. Phys. Solids 1965*):

Coupling between the phase transformation and damage evolution in austenitic steels



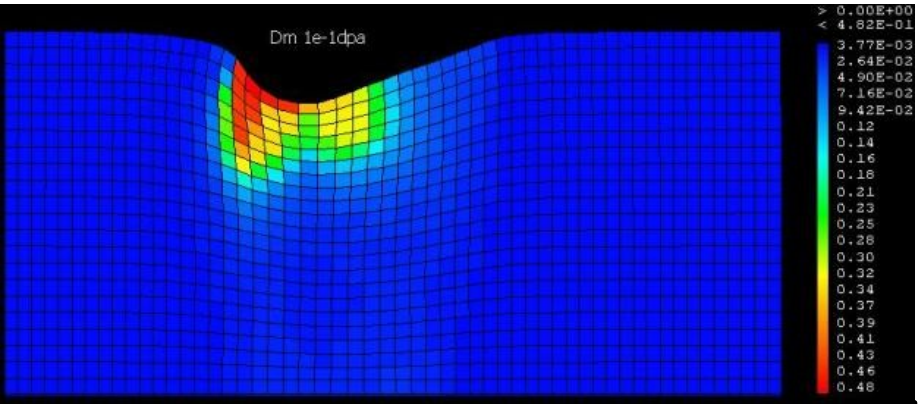




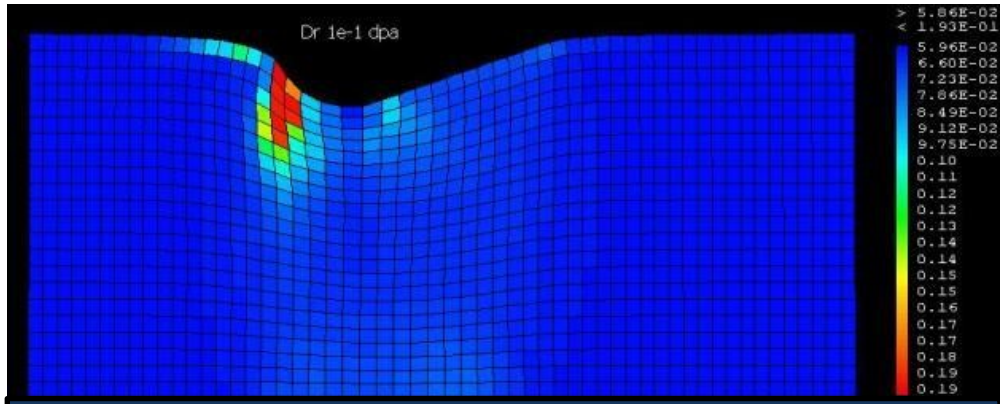
Phase transformation may substantially affect (slow down) evolution of micro-damage

H. Egner, B. Skoczeń, Int. J Plasticity 2010

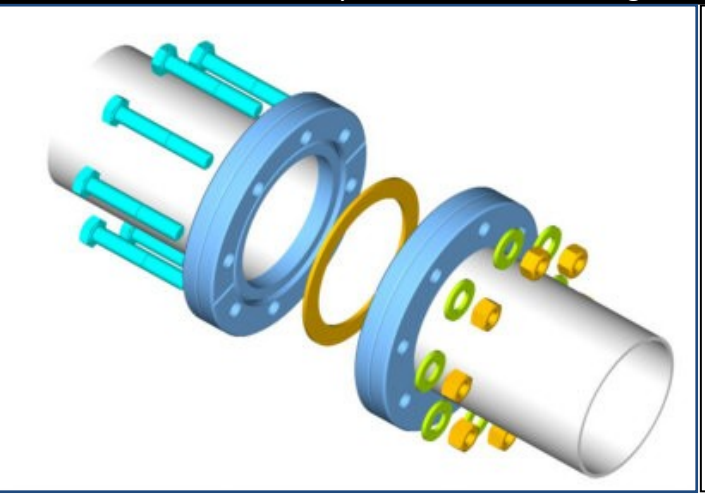
Application in UHV systems

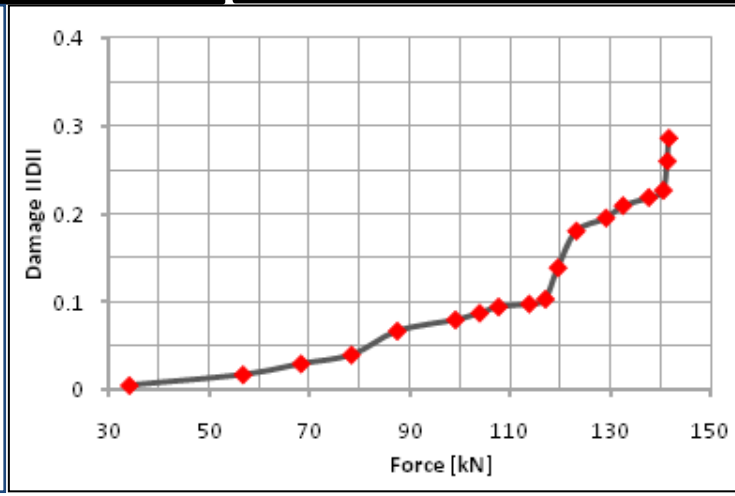


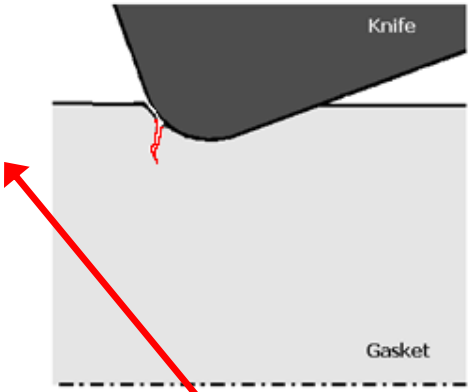
Mechanically induced micro-damage fields

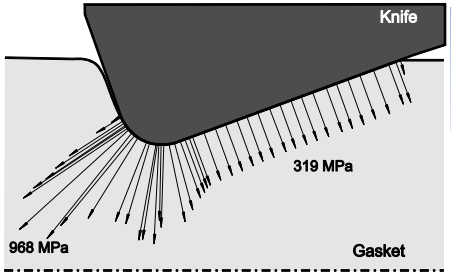


Irradiation induced micro-damage fields

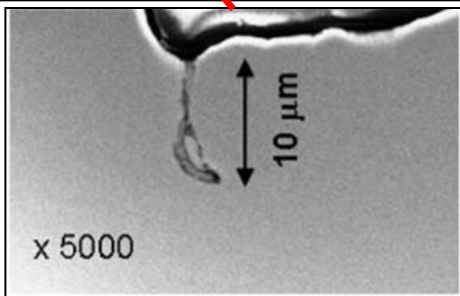


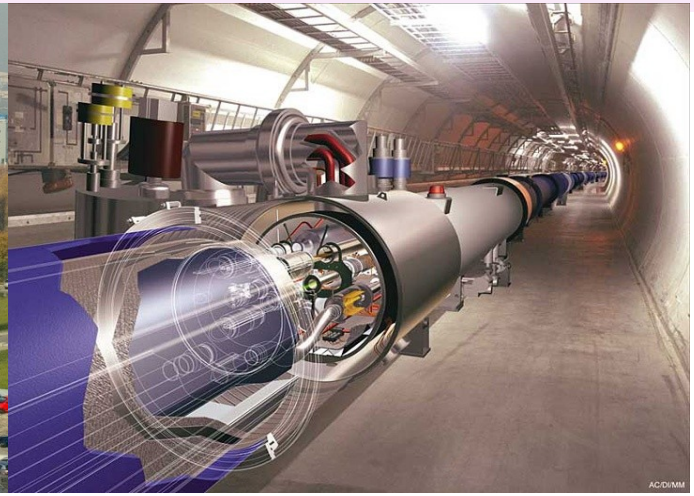






Macro-crack initiation



Conclusion

The constitutive model has to be calibrated in order to achieve correct performance and obtain reliable results in terms of number of cycles to failure as a function of dpa