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

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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, Nb₃Sn,
- NbAl, MgB₂,
- BSCCO2223,
- G10, G11
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

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EUROnu: High Intensity Neutrino Oscillation
Central Solenoid
\( \text{Nb}_3\text{Sn} \) 6 modules

Toroidal Field Coil
\( \text{Nb}_3\text{Sn} \) 18

Poloidal Field Coil
\( \text{NbTi} \) 6

Correction Coils
\( \text{NbTi} \) 18

Feeders
\( \text{NbTi} \) 31

Cable (\( \text{Nb}_3\text{Sn} \) strands)
Jacket (316LN or JK2LB)

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

\( ^2\text{H} \)
\( ^3\text{H} \)
\( ^4\text{He} + 3.5 \text{ MeV} \)
n + 14.1 \text{ MeV}

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Irradiation induced defects in the lattice

PKA primary knock-on atoms

Incident particle

Displacement cascade and formation of Frenkel pairs

Kinchin & Pease, 1955
Norgett, Robinson, Torrens, 1975

\[ N_{NRT} = \frac{0.8E_{dam}}{2E_d} \]
\[ E_{dam} = \text{NIEL} \]

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Irradiation induced defects in the lattice

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

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Irradiation induced micro-damage – types of defects

- SFT – stacking fault tetrahedron
- Faulted or perfect dislocation loops
- Voids – 3D vacancy clusters
- 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 Workshop RESMM'14
Defect concentration during irradiation - Aluminium

(for Al, after Verbiest and Pattyn, 1982)
Recombination ratio

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
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
Identification of damage evolution is based on analysis of unloading modulus

\[ \tilde{E} = E(1 - D) \]
Example of lifetime estimation for irradiated components

initial stress state

cyclic loading

beam

secondary particles flux

$\sigma$ vs $t$
Typical distribution of $dpa$ in the horn

Secondary particles flux: $\gamma$, $n$, $p^+$, $\pi^\pm$ and $e^\pm$

### 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

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

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

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

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

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

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

$q_c$ – number of clusters per unit volume

$r_c$ – average radius of clusters
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:

\[ d\xi = (1 - \xi) dp \]

\[ \dot{p} = \sqrt{\frac{2}{3} \dot{\varepsilon}^p \dot{\varepsilon}^p} \]
Mechanism of damage evolution under periodic irradiation

Description based on the Rice & Tracey law

\[ D_{i+1} = q_A \pi r_{i+1} \]
\[ D_i = q_A \pi r_i \]
\[ \Delta D_{i \rightarrow i+1} = q_A \pi (r_{i+1}^2 - r_i^2) \]

\[ \int \frac{dr_c}{r_c} = \alpha_r \exp \left( \frac{3\sigma_m}{2\sigma_{eq}} \right) \int_0^{\tilde{p}} dp \]

\[ r_{i+1} = r_i e^{A \tilde{p}} \]

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

\[ A := \alpha_r \exp \left( \frac{3\sigma_m}{2\sigma_{eq}} \right) \]
Analytical solution in the uniaxial stress state

\[ D_{r0} = q_A \pi r_c^2 \]

\[ D_{m1} = D_{r0} + \Delta D_{m(0 \rightarrow 1)} = D_{r0} + q_A \pi r_c^2 \left( e^{2A\bar{p}} - 1 \right) \]

\[ D_{m2} = D_{m1} + \Delta D_{m(1 \rightarrow 2)} + D_{r0} + \Delta D_{m(0 \rightarrow 1)} = 2D_{r0} + q_A \pi r_c^2 e^{2A\bar{p}} + q_A \pi r_c^2 e^{4A\bar{p}} - 2q_A \pi r_c^2 \]

\[ \vdots \]

\[ D_{m_{i+1}} = D_{m_i} + D_{r0} + \Delta D_{m(i \rightarrow i+1)} + \Delta D_{m(i-1 \rightarrow i)} + \ldots + \Delta D_{m(0 \rightarrow 1)} \]

\[ D_{rmN} = q_A \pi r_c^2 e^{2A\bar{p}} + q_A \pi r_c^2 e^{4A\bar{p}} + q_A \pi r_c^2 e^{6A\bar{p}} + \ldots + q_A \pi r_c^2 e^{2NA\bar{p}} \]

Geometric series

\[ D_{r0} = q_A \pi r_c^2 \sum_{n=1}^{N} e^{2nA\bar{p}} \]

\[ S_N = a_1 \frac{1 - q^N}{1 - q} \quad S_N = q_A \pi r_c^2 e^{2A\bar{p}} \frac{1 - e^{2A\bar{p}N}}{1 - e^{2A\bar{p}}} \]

\[ D_{rmN} = q_A \pi r_c^2 e^{2A\bar{p}} \frac{1 - e^{2A\bar{p}N}}{1 - e^{2A\bar{p}}} \]

Number of cycles to failure \( N_f \) based on the critical damage criterion

\[ D_{rm} = D_{cr} \]
Mechanism of damage evolution under periodic irradiation

Description based on the Gurson law

Evolution of porosity parameter $\xi$

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

$$\int_{\xi + \xi_0}^{\xi_{i+1}} \frac{d\xi}{1 - \xi} = \int_0^{\bar{\rho}} dp \quad K := e^{-\bar{\rho}}$$

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

Porosity parameter $\xi_i$ increases from cycle to cycle by $\xi_0$ due to emission of secondary particles flux.
Analytical solution for the uniaxial stress state

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

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

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Radiation and mechanical damage components: additive formulation

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

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

\[ D = D_m + D_r = D_m + \frac{1}{3} D_r I \]

- Identity tensor

anisotropic

isotropic

RVE

micro-voids
micro-cracks

clusters

n

A_s
Kinetics of mechanically induced micro-damage

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

$\dot{D} = \left( \frac{Y}{S} \right)^s \dot{p} H(p - p_D)$

$D = \sum_{i=1,3} D_i n_i \otimes n_i$

$\dot{D} = CYC^T \dot{p} H(p - p_D)$

Chaboche, 1988; Lemaitre, 1992

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

$316L, 4.2K$

$\varepsilon_{pD}$

RVE

Micro-cracks and micro-voids (parameter $D$)

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

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

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## Isotropic versus anisotropic model

<table>
<thead>
<tr>
<th>Isotropic model</th>
<th>Anisotropic model</th>
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<tr>
<td><strong>Helmholtz free energy</strong></td>
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</tr>
<tr>
<td>[ \Psi = \frac{1}{2} \rho \varepsilon: E(1-D): \varepsilon + \Psi_p ]</td>
<td>[ \Psi = \frac{1}{2} \rho \varepsilon: M(D): E: \varepsilon + \Psi_p ]</td>
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<tr>
<td><strong>Effective stress</strong></td>
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</tr>
<tr>
<td>[ \sigma = (1-D)\bar{\sigma} ]</td>
<td>[ \sigma = \frac{1}{2} ((I-D)\bar{\sigma} + \bar{\sigma}(I-D)) ]</td>
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<td>( \leftrightarrow \sigma = M(D): \bar{\sigma} )</td>
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<td><strong>Conjugate force associated to damage</strong></td>
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<td>[ Y = -\rho \frac{\partial \Psi}{\partial D} = \frac{1}{2} \varepsilon: E: \varepsilon ]</td>
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<td>( \leftrightarrow Y = \frac{1}{4} \left[ \varepsilon \left( E: \varepsilon \right) + \left( E: \varepsilon \right) \varepsilon \right] )</td>
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<td><strong>Potential of dissipation associated to irreversible damage process</strong></td>
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<td>[ \Phi_D = \frac{1}{2} \frac{Y^2}{S} \frac{1}{1-D} ]</td>
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</tr>
<tr>
<td>[ a(D) = \frac{\left( \bar{s} - \bar{X} \right): M^{-1} : M^{-1} : \left( \bar{s} - \bar{X} \right)}{\left( \bar{s} - \bar{X} \right) : \left( \bar{s} - \bar{X} \right)^{1/2}} ]</td>
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<td><strong>Kinetic law of damage evolution</strong></td>
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<td>[ \dot{D} = \dot{\lambda} \frac{\partial \Phi_D}{\partial Y} = \frac{Y}{S} \hat{p} \bigg</td>
<td>_{p&gt;p_D} ]</td>
</tr>
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</table>
Isotropic versus anisotropic model

\[
\dot{D} = CY C^T \dot{p}H(p - p_D)
\]

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

\[
C = \sum_{i=1,3} C_i \vec{n}_i \otimes \vec{n}_i
\]

\[
C = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix}_{(\bar{x}_1, \bar{x}_2)}
\]

\[
V_D = \left. \frac{d D}{dp} \right|_{p=p_D} = CY C^T
\]

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 lens)

- Radiation induced damage
  - $D_{cr} = 0.1$
- Mechanical damage
- Total damage parameter
Performance of Rice-Tracey and Gurson models (log-log)

Rice & Tracey model predicts lower values of damage

Gurson model

different sensitivity of both models
Bilinear approximations for R-T and Gurson models

Rice & Tracey model

Gurson model

\[ \log(N_c) = a + b \log(dpa_{\text{max}}) \]

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

\[ N_c = 10^a dpa_{\text{max}}^b \]

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

\[ N_c = \begin{cases} 10^{-1.9} dpa_{\text{max}}^{-1.4} & \text{for } dpa_{\text{max}} \geq 10^{-5} \\ 10^{5.43} dpa_{\text{max}}^{-0.016} & \text{for } dpa_{\text{max}} < 10^{-5} \end{cases} \]
Specific coupled field problems
Coupled field problems

Mechanisms of plastic flow at cryogenic temperatures

Temperature [K]

Yield stress [MPa]

Domain I

Domain II

Domain III

FCC->BCC

Screw dislocations

Continuous plastic flow

Dispersed point defects

Phase transformation

Edge dislocations

Discontinuous plastic flow

Rp0,2

T1

316LN

Md

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Kinetics of $\gamma \to \alpha'$ phase transformation

Inclusions $\alpha'$ (parameter $\xi_{\alpha}$)

\[ \xi_{\alpha} = \frac{dV_{\xi}}{dV}; \quad 0 \leq \xi_{\alpha} \leq 1 \]

\[ \dot{\xi}_{\alpha} = A(T, \dot{\varepsilon}^p, \sigma) \dot{p}H((p - p_{\xi})(\xi_L - \xi_{\alpha})) \]

$\dot{\xi}_{\alpha}$ – volume fraction of $\alpha'$ phase

Garion, Skoczeń; J. Appl. Mech., 2002

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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.
Type Eshelby entities: clusters of voids, $\alpha'$ inclusions

- 3D vacancy clusters: $\xi_c$
- 3D vacancy cluster with impurities (He): $\xi_c$
- Inclusions of secondary phase: $\xi_\alpha$
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

Micromechanics: Orowan mechanism (clusters + inclusions)

Interaction of dislocations with clusters and $\alpha'$ inclusions

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

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

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

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

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

$$
\frac{d \tilde{X}}{da} = \frac{2}{3} C_0 \left( 1 + h\xi \right) d\varepsilon^p
$$
Constitutive model including phase transformation and damage

Hardening caused by evolution of stiffness of two-phase continuum

Elastic-plastic $\gamma$ lattice:

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

$$E_{ta} = 3k_{ta} J + 2 \mu_{ta} K$$

$$\mu_{ta} = \frac{E_t}{2(1+v)} \quad k_{ta} = \frac{E_t}{3(1-2v)}$$

$\alpha'$ elastic inclusions:

$$E_m = 3k_m J + 2 \mu_m K$$


$$\Delta \tilde{\sigma} = E_{ta} : \Delta \varepsilon$$

$$\Delta \tilde{\sigma} = E_m : \Delta \varepsilon$$

$$\Delta \tilde{\sigma} = E_H : \Delta \varepsilon$$
Coupling between the phase transformation and damage evolution in austenitic steels

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

316L, T=4.2 K

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

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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.