Kinetics of evolution of radiation induced damage

Aneta Ustrzycka¹, Błażej Skoczeń^{2*}

^{1,2}Institute of Applied Mechanics, Cracow University of Technology Warszawska 24, 31-155 Kraków, Poland e-mail: anetaustrzycka@mech.pk.edu.pl¹,blazej.skoczen@pk.edu.pl²

Abstract

The problem investigated in the work concerns the physical processes involved in radiation damage and the way they affect the mechanical properties of ductile materials. Multiscale modeling of evolution of radiation induced micro-damage in ductile materials subjected to periodic stress states in the inelastic range is presented. The resulting micro-structural and damage evolution causes profound changes of the macroscopic properties and severely degrades the lifetime of the components subjected to irradiation. The evolution of radiation induced damage is combined with the evolution of classical micro-damage of mechanical origin (micro-cracks and micro-voids), within the common framework of Continuum Damage Mechanics (CDM). Two kinetic laws: the Rice and Tracey model and the Gurson model may be conveniently applied to describe the evolution of radiation induced damage in the form of clusters of voids embedded in the metallic matrix. Closed form analytical solutions for the problem of periodic irradiation combined with cyclic axial loads was obtained.

Keywords: radiation induced damage, Frenkel pairs, vacancies, interstitial atoms, displacement per atom, evolution of clusters of voids, Continuum Damage Mechanics (CDM) framework

1. Introduction

Exposure to high energy radiation degrades the microstructure of materials. Energetic particles penetrating a solid displace the lattice atoms from their original positions. In the elastic collisions (initiated when a given atom is struck by a high energy particle), incident particles transfer recoil energy to the lattice atoms. The initial primary knock-on atoms recoil with a given amount of kinetic energy that is dissipated in a sequence of collisions with the other lattice atoms. As a result of cascade process, atoms in the solid can be displaced from their equilibrium lattice positions, creating vacancies and interstitials. These vacancy-interstitial pairs are called Frenkel pairs. The vacancies of the Frenkel pairs often form clusters by means of diffusion.

As an example of typical problem related to evolution of radiation induced damage, degradation of material properties in a thin-walled irradiated cylindrical part of detector of particles has been investigated. The coaxial target - detector configuration is shown in Fig. 1. The target is hit by highenergy particles beam. The process of beam absorption is associated with emission of secondary particles flux in the radial direction. The secondary particles induce micro-damage in the thin-walled cylinder surrounding the target. As the cylinder is simultaneously subjected to mechanical loads, the fields of radiation and mechanically induced damage occur in the same lattice. This problem is used as an illustration of different nature of both damage types. Thus, the ultimate goal is lifetime prediction expressed in terms of the number of beam cycles for components of particle detectors [1,2].

Two kinetic laws of damage evolution were taken into account: the Rice and Tracey model and the Gurson model. Both of them address the evolution of porosity in the form of spherical or ellipsoidal voids in a different way.



Figure 1: Coaxial target - detector configuration

The Rice & Tracey model predicts the growth of an initially spherical void in an infinite, rigid - perfectly plastic material subjected to a uniform remote strain field.

$$dr_c = r_c \alpha_r \exp\left(\frac{3\sigma_m}{2\sigma_{eq}}\right) dp \,. \tag{1}$$

The radius increment dr_c is derived as a function of the equivalent plastic strain dp, the stress triaxiality factor $(3\sigma_m/2\sigma_{eq})$, the current radius r_c and a scalar multiplier α_r .

On the other hand, the Gurson model is based on the definition of the porosity parameter ξ :

$$\dot{\xi} = (1 - \xi) \dot{\varepsilon}_{kk}^p \,, \tag{2}$$

where $\dot{\varepsilon}_{kk}^{p}$ denotes trace of the plastic strain rate tensor.

The mechanically induced damage is calculated following the Lemaitre-Chaboche model.

Both Rice & Tracey and Gurson kinetics may conveniently be applied to describe the evolution of radiation induced

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damage in the form of clusters of voids embedded in the metallic matrix.

2. Analytical solutions for the problem of periodic irradiation combined with cyclic axial loads

Based on the known *dpa* in the *RVE*, the density of defects q_A (clusters of voids) caused by irradiation is computed [3]:

$$q_{c} = \begin{cases} C_{qI}(dpa)^{n_{qI}} & for \quad dpa < D_{S} \\ C_{qII}(dpa)^{n_{qII}} & for \quad dpa \ge D_{S} \end{cases}$$
(3)

The mechanism of damage evolution for multiple irradiation cycles is shown in Fig. 2.



Figure 2: The mechanism of damage evolution

Single cycle is composed of emission of the particles flux, production of radiation induced damage expressed by the porosity parameter ξ_0 and further mechanical loading. The porosity parameter ξ_i increases from cycle to cycle by ξ_0 . The porosity parameter ξ , used by Gurson, can be directly recalculated to obtain the classical damage parameter *D*.

To find a closed-form analytical solution for one dimensional problem presented in Fig. 2 the recurrence relations are postulated. Integrating the post-irradiation damage evolution equation:

$$\int_{D_{i}}^{D_{i+1}} dD = q_{A} 2\pi \int_{r_{i}}^{r_{i+1}} r \, dr \,, \tag{4}$$

one obtains the following recurrence relation for damage parameter:

$$\Delta D_{i \to i+1} = q_A \pi \left(r_{i+1}^2 - r_i^2 \right) \,. \tag{5}$$

Integrating the Rice & Tracey law, the increase of cluster of voids radius reads:

$$r_{i+1} = r_i e^{A\widetilde{p}} \tag{6}$$

Finding the *N*-*th* term in the sequence indicates that all terms create a geometric series:

$$D_{rmN} = ND_{r0} - Nq_A \pi r_{c0}^2 + q_A \pi r_{c0}^2 e^{4A\tilde{p}} + q_A \pi r_{c0}^2 e^{6A\tilde{p}} + \dots + q_A \pi r_{c0}^2 e^{2NA\tilde{p}}, \quad (7)$$

$$\frac{q_A \pi r_{c0}^2 e^{2A\tilde{p}} + q_A \pi r_{c0}^2 e^{4A\tilde{p}} + q_A \pi r_{c0}^2 e^{6A\tilde{p}} + \dots + q_A \pi r_{c0}^2 e^{2NA\tilde{p}}}{Geometric \ series}, \quad (7)$$

The following criterion has been used:

$$D_{rmN_f} = q_A \pi r_{c0}^2 e^{2A\tilde{p}} \frac{1 - e^{2A\tilde{p}N_f}}{1 - e^{2A\tilde{p}}} = D_{cr}, \qquad (8)$$

where D_{cr} denotes a critical value of damage parameter, corresponding to lattice failure.

The relation between the number of cycles to failure N_f as a function of dpa on single cycle is presented in Fig. 3.



Figure 3: Number of cycles to failure N_f as a function of dpa

The solid line represents the performance of Rice & Tracey model. For comparison the dashed line represents the number of cycles to failure as a function of dpa corresponding to irradiation of the material not subjected to mechanical stress.

3. Concluding remarks

Finally, the results contained in the present paper can be summarized in the following way:

1) formulation of the problem of radiation induced damage evolution under mechanical loads, including the effect of partial recombination of Frenkel pairs,

2) application of Rice & Tracey and Gurson kinetic laws to the evolution of post-irradiation damage,

3) additive formulation for total damage including both radiation induced and mechanical components,

4) closed form analytical solutions for the problem of periodic irradiation combined with cyclic axial load, and corresponding to Rice & Tracey and Gurson models.

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