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Effect of self-interstitial diffusion anisotropy in electron-irradiated zirconium: A cluster dynamics modeling

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Abstract

A model based on the cluster dynamics approach was proposed in [A. Hardouin Duparc, C. Moingeon, N. Smetniansky-de-Grande, A. Barbu, J. Nucl. Mater. 302 (2002) 143] to describe point defect agglomeration in metals under irradiation. This model is restricted to materials where point defect diffusion is isotropic and is thus not applicable to anisotropic metals such as zirconium. Following the approach proposed by Woo [C.H. Woo, J. Nucl. Mater. 159 (1988) 237], we extended in this work the model to the case where self-interstitial atoms (SIA) diffusion is anisotropic. The model was then applied to the loop microstructure evolution of a zirconium thin foil irradiated with electrons in a high-voltage microscope. First, the inputs were validated by comparing the numerical results with Hellio et al. experimental results [C. Hellio, C.H. de Novion, L. Boulanger, J. Nucl. Mater. 159 (1988) 368]. Further calculations were made to evidence the effect of the thin foil orientation on the dislocation loop microstructure under irradiation. The result is that it is possible to reproduce for certain orientations the 'unexpected' *vacancy* loop growth experimentally observed in electron-irradiated zirconium [M. Griffiths, M.H. Loretto, R.E. Sallmann, J. Nucl. Mater. 115 (1983) 313; J. Nucl. Mater. 115 (1983) 323; Philos. Mag. A 49 (1984) 613]. This effect is directly linked to SIA diffusion anisotropy.
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1. Introduction

Zirconium alloys are used for fuel cladding in the nuclear industry and are subject to 'irradiation growth', which represents an anisotropic deformation of the material without any applied stress (see for example [7]). This irradiation growth is related to the elimination of point defects on the different sinks (dislocations lines, surfaces, grain boundaries) and also to their agglomeration in the form of dislocation loops. But in zirconium and its alloys, some aspects of dislocation loop microstructure evolution under irradiation are rather unusual compared to cubic metals, such as the growth of vacancy loops [4–6,8]. Some authors proposed that this kind of unexpected behavior could be accounted for by diffusion anisotropy of self-interstitial atoms (SIA) [2].

Concerning the modeling of the loop microstructure evolution under irradiation, a model based on the cluster dynamics approach was proposed in [1]. Nevertheless, as

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far as zirconium is concerned, this model is not applicable because it is based on the assumption that point defects diffuse isotropically, which is not true for zirconium. Indeed, diffusion of point defects in zirconium is known to be anisotropic, specially for SIA [9–11].

This papers aims at extending the cluster model presented in [1] to the case where point defect diffusion is anisotropic, using the approach proposed by Woo [2]. After reminding the reader of the main equations of the cluster model, we will show how it is possible to extend the model to anisotropic diffusion. It will then be applied to describe the evolution of the dislocation loop microstructure in an electron-irradiated zirconium thin foil.

2. The cluster dynamics model

Equations: We will first set the basic equations of the model for a medium where point defect diffusion is supposed to be isotropic [1]. The evolution of the loop size distribution under electron irradiation is obtained by resolving the following differential equations system:

$$\begin{aligned}
\frac{dC_{ni}}{dt} &= [\beta^i_{(n-1)i}C_{1i}]C_{(n-1)i} + [\beta^v_{(n+1)i}C_{1v} + \alpha^i_{(n+1)i}]C_{(n+1)i} \\
&\quad - [\alpha^i_{ni} + \beta^v_{ni}C_{1v} + \beta^i_{ni}C_{1i}]C_{ni}, \\
\frac{dC_{nv}}{dt} &= [\beta^v_{(n-1)v}C_{1v}]C_{(n-1)v} + [\beta^i_{(n+1)v}C_{1i} + \alpha^v_{(n+1)v}]C_{(n+1)v} \\
&\quad - [\alpha^v_{nv} + \beta^i_{nv}C_{1i} + \beta^v_{nv}C_{1v}]C_{nv}, \\
\frac{dC_{1i}}{dt} &= G - R_{iv}C_{1i}C_{1v} - K^i_dC_{1i} - K^i_sC_{1i} \\
&\quad - 2\beta^i_{1i}C_{1i}C_{1i} + 2\alpha^i_{2i}C_{2i} + \beta^v_{2i}C_{1v}C_{2i} \\
&\quad - C_{1i}\sum_{n=2}^{\infty}\beta^i_{ni}C_{ni} - C_{1i}\sum_{n=2}^{\infty}\beta^i_{nv}C_{nv} + \sum_{n=3}^{\infty}\alpha^i_{ni}C_{ni}, \qquad (1) \\
\frac{dC_{1v}}{dt} &= G - R_{iv}C_{1i}C_{1v} - K^v_dC_{1v} - K^v_sC_{1v} \\
&\quad - 2\beta^v_{1v}C_{1v}C_{1v} + 2\alpha^v_{2v}C_{2v} + \beta^i_{2v}C_{1i}C_{2v} - C_{1v}\sum_{n=2}^{\infty}\beta^v_{nv}C_{nv} \\
&\quad - C_{1v}\sum_{n=2}^{\infty}\beta^v_{ni}C_{ni} + \sum_{n=3}^{\infty}\alpha^v_{nv}C_{nv}, \\
\frac{dC_{2i}}{dt} &= \beta^i_{1i}C_{1i}C_{1i} - \alpha^i_{2i}C_{2i} - \beta^i_{2i}C_{1i}C_{2i} \\
&\quad + \alpha^i_{3i}C_{3i} - \beta^v_{2i}C_{1v}C_{2i} + \beta^v_{3i}C_{1v}C_{3i}, \\
\frac{dC_{2v}}{dt} &= \beta^v_{1v}C_{1v}C_{1v} - \alpha^v_{2v}C_{2v} - \beta^v_{2v}C_{1v}C_{2v} \\
&\quad + \alpha^v_{3v}C_{3v} - \beta^i_{2v}C_{1i}C_{2v} + \beta^i_{3v}C_{1i}C_{3v}.
\end{aligned}$$

n is the number of monomers (vacancies or SIA) included in a cluster (loop) of size n, $C_{n\theta}$ is the concentration of the clusters of size n per unit volume (with $\theta = i$ for interstitials (SIA) and $\theta = v$ for vacancies), $\beta^{\theta'}_{n\theta}C_{1\theta'}$ is the frequency at which a cluster of type θ absorbs a defect of type θ', $\alpha^{\theta}_{n\theta}$ is the frequency at which a cluster of type θ emits a defect of type θ, R_{iv} is the vacancy-SIA recombination rate, $K^{\theta}_dC_{1\theta}$ is the absorption rate of the defects of type θ by the dislocation lines, $K^{\theta}_sC_{1\theta}$ is the absorption rate of the defects of type θ by the surfaces. G is the point defect creation rate, i.e. the number of Frenkel pairs (1 Frenkel pair = 1 vacancy + 1 SIA) created under electron irradiation per second and per cm^3. G is also often expressed in dpa s^{-1} (dpa = displacement per atom). The differential equation system (1) is based on the assumptions that only monomers (vacancies and SIA) are mobile and that a cluster of type θ can emit point defects of the same type only. It can be shown that the latter assumption is realistic provided that the point defect supersaturation is large, which will be the case here since the point defect production rate is high ($G = 1.5 \times 10^{-4}$ dpa s^{-1}, see Table 1).

Rate coefficients: The expressions of the rate coefficients appearing in the differential equations system (1) are presented below.

2.1. SIA-vacancy recombination

The recombination rate R_{iv} is given by

$$R_{iv} = 4\pi r_{iv}(D_i + D_v). \qquad (2)$$

r_{iv} is the recombination radius, D_i and D_v are the SIA and vacancy diffusion coefficients respectively.

2.2. Absorption of point defects by dislocation lines

The absorption rate $K^{\theta}_dC_{1\theta}$ of the defects of type θ by the dislocation lines is

$$K^{\theta}_dC_{1\theta} = \rho Z^{\theta}_dD_{\theta}C_{1\theta}. \qquad (3)$$

ρ is the dislocation density in the material, D_θ is the diffusion coefficient of the defect of type θ and Z^{θ}_d is a dimensionless factor which represents the absorption efficiency of point defects by the dislocation lines. This factor makes it possible to take the elastic interaction between point defects and dislocations into account. Z^{θ}_d is usually taken equal to 1 for vacancies (no elastic interaction) and about 1.1–1.2 for SIA.

2.3. Absorption of point defects by dislocation loops

The absorption frequency $\beta^{\theta'}_{n\theta}C_{1\theta'}$ of a defect of type θ' by a loop of type θ is

$$\beta^{\theta'}_{n\theta}C_{1\theta'} = 2\pi r_nZ^{\theta'}_{n\theta}D_{\theta'}C_{1\theta'}. \qquad (4)$$

r_n is the cluster radius. If we make the assumption that the point defects agglomerate to form dislocation loops, r_n can be written as follows:

$$r_n = \sqrt{\frac{nV_{at}}{\pi b}}. \qquad (5)$$

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