Rate Theory Modeling of Helium-Induced Swelling in Fe-Cr-Ni Austenitic Model Alloy

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1. Introduction

Austenitic stainless steels such as Type 316 stainless steel are widely used as structural materials in nuclear systems. During neutron irradiation, displacement damage continuously produces vacancies and self-interstitial atoms. In addition, helium can be generated through nuclear transmutation reactions. These irradiation-induced defects migrate through the material and interact with dislocations, grain boundaries, solute atoms, and defect clusters. In particular, the accumulation of vacancies and helium can promote the nucleation and growth of cavities, which eventually results in irradiation-induced volumetric swelling.

In this study, a rate-theory model is developed to describe helium-assisted irradiation swelling in austenitic stainless steel. The major alloying elements of Type 316 stainless steel are represented using an Fe-Cr-Ni-Mo alternative model alloy. The model describes the production, migration, recombination, and sink absorption of vacancies, interstitials, and helium, followed by the nucleation and growth of He-vacancy cavities.

2. Rate Theory Model for Helium-Induced Swelling

2.1 Point-defect evolution

Under irradiation, the concentrations of vacancies and self-interstitial atoms are calculated using coupled rate equations. The general form of the governing equations is

$$\frac{dC_v}{dt} = G_v - K_{iv}C_iC_v - K_v^2D_vC_v - J_{v,cav} \quad (1)$$

$$\frac{dC_i}{dt} = G_i - K_{iv}C_iC_v - K_i^2D_iC_i - J_{i,cav} \quad (2)$$

Where C_v and C_i are the concentrations of vacancies and interstitials, respectively. G_v and G_v represent the irradiation-induced defect production rates, and K_{iv} represents vacancy-interstitial recombination. D_v and D_i are the diffusion coefficients of vacancies and inter-stitials, while K_v^2 and K_i^2 represent the effective sink strengths associated with dislocations, grain boundaries, and other microstructural sinks. $J_{v,cav}$ and $J_{i,cav}$ represent the defect fluxes absorbed by cavities.

The diffusion coefficient of each mobile defect is described using an Arrhenius relation,

$$D_x = D_{0,x}exp\left(-\frac{E_{m,x}}{k_BT}\right) \quad (3)$$

Where $D_{0,x}$ is the diffusion pre-factor, $E_{m,x}$ is the migration energy, k_B is the Boltzmann constant, and T is the absolute temperature. Equation (3) provides the principal connection between irradiation temperature and defect transport.

2.2 Cavity growth and swelling

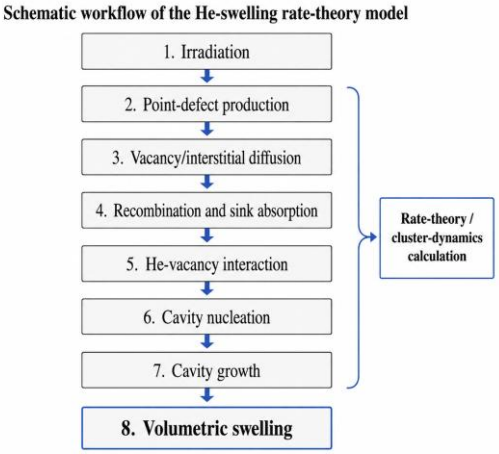
Once a stable cavity population is formed, its size evolves according to the net vacancy and interstitial fluxes arriving at the cavity surface. A simplified cavity growth relation can be expressed as

$$\frac{dR}{dt} = \frac{\Omega}{4\pi R^2} \cdot (J_v - J_i) \quad (4)$$

Where R is the cavity radius, Ω is the atomic volume, and J_v and J_i are the vacancy and interstitial absorption rates of the cavity. For helium-containing cavities, the internal helium population additionally affects cavity stability and vacancy emission. The total volumetric swelling is calculated from the volume occupied by the cavity population,

$$Swelling(\%) = 100 \cdot \frac{4\pi}{3}\sum N_c(R) \cdot R^3 \quad (5)$$

Where $N_c(R)$ represents the number density of cavities having radius R. Therefore, the present calculation follows the sequence.



<Figure 1.> Schematic of He-induced swelling

3. Conclusions

A rate-theory framework is being developed to predict helium-assisted irradiation swelling in austenitic stainless steel. The model describes the coupled evolution of vacancies, self-interstitial atoms, helium, and He-vacancy cavities under irradiation. Point-defect production, recombination, migration, sink absorption, cavity nucleation, and cavity growth are treated within a continuous temperature-dependent kinetic framework.

The principal objective of the model is to calculate cavity number density, cavity size, and volumetric swelling as functions of irradiation temperature and dose. Material-dependent defect energetics for the Fe-Cr-Ni-Mo model alloy are being obtained through DFT calculations and will be used as input parameters for the kinetic model.

After completion of rate theory concentration calculations, the predicted irradiation temperature-dependent swelling behavior will be compared with available irradiation swelling data for Type 316 stainless steel. The final model is expected to provide a physics-based description of the effects of helium generation and alloy-dependent defect kinetics on irradiation swelling.

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