Dimensional instability analysis of iron base alloy by rate theory

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1. Introduction

Iron based alloys are one of the most promising candidate materials for fast breeder reactor since iron based alloy could maintain reasonable mechanical strength in harsh environment condition. However, recently there are two group i.e., UNIST or Tera-power, try to establish the long cycle fuel design. hence more high radiation, temperature, and pressure condition is avoidable. In this situation, there is no experiment and theoretical evidence that iron based alloy can be sustainable over 200 dpa. The preliminary result of this study could be theoretical base for safety analysis.

Therefore, in this study, the aim of this study is understanding of radiation effect on the dimensional instability of iron base materials with stress applied condition. The originality of this study is consideration of self-interstitial clusters (SIAs) behavior in stress condition i.e., modification of SIAs cluster absorption rate is calculated in rate theory. Specifically, from the mean field assumption, nucleation and growth behavior of dislocation loops and void was calculated by 3D and 1D reaction kinetics in rate theory. Finally, irradiation swelling and creep were analyzed by sink behavior.

2. Methodology

After the first observation of irradiation degradation [1], various experimental and theoretical approach have been carried out to understand dimensional instability by analysis of microstructure characteristic. Among the various method, MD simulation and TEM analysis have been used to demonstrate the radiation effect on microstructure. From those experimental and simulation result, it was confirmed that various sinks are developed after radiation damage with high number density and large size change. Therefor to simulate sink development, analytical model was firstly suggested from the basis of chemical reaction kinetics, which is call standard rate theory (SRT).

Once in a time, SRT was only method to simulate the sink development in microstructure. However, there was limitation to explain various experimental results such as void lattice ordering, swelling saturation, and different swelling behavior of bcc and fcc.

This limitation is caused by simplified assumed of SRT i.e., only 3-D mobile Frenkel pair was considered. However, after 2 decades later, production bias method (PBM) was suggested in cluster dynamic method (CDM) to consider cascade induced SIAs cluster effect on materials.

Therefore, in paper, irradiation swelling and creep model was developed by CDM. Moreover, stress effect on defect migration was considered to explain preferential loop nucleation and growth in hoop stress condition. The fundamentals of rate theory are well-explained in previous works [2, 3]. In this paper, it will be simply summarized. The bellow equation is about simple CDM master equation. In this equation SIAs cluster effect was ignored, hence, only point defect generation, agglomeration, and emission were considered.

$$\frac{dC_i}{dt} = K_o - K_{iv}C_iC_v - \sum_n \rho_n Z_n^i C_i D_i + \left(E_i^2 + \beta_v^2\right)C_{2i} + E_i^3 C_3 + E_i^4 C_{4i} \tag{1}$$

$$\frac{dC_{2i}}{dt} = \eta G_{dpa}\frac{f_{icl}^2}{2} + \beta_i^1 C_i/2 + \left(\beta_v^3 + E_i^3\right)C_{3i} - \left(\beta_v^2 + \beta_i^1 + E_i^1\right)C_{2i} \tag{2}$$

$$\frac{dC_{3i}}{dt} = \eta G_{dpa}\frac{f_{icl}^3}{3} + \beta_i^2 C_2 + \left(\beta_v^4 + E_i^4\right)C_{4i} - \left(\beta_v^3 + \beta_i^3 + E_i^3\right)C_{3i} \tag{3}$$

$$\frac{dC_{4i}}{dt} = \eta G_{dpa}\frac{f_{icl}^4}{4} + \beta_i^3 C_{3i} - \left(\beta_v^4 + \beta_i^4 + E_i^4\right)C_{4i} \tag{4}$$

Where $C_{v\,or\,i}$ is vacancy or interstitial concentration in the iron matrix (cm^{-3}), $C_{xv\,or\,\mathrm{x}i}$ is vacancy or interstitial cluster concentration in the iron matrix (cm^{-3}), K_0 is the defect generation rate ($\mathrm{cm}^{-3}s^{-1}$), which means vacancy and interstitial are combined to be a perfect lattice atom. G_{dpa} is the cluster defect generation rate ($cm^{-3}s^{-1}$), f_{cl}^{x} is the fraction of cluster, η is the cascade efficiency, K_{iv} is the recombination rate (cm^3s^{-1}), ρ_n is the density of sink of n type in the iron matrix (cm^{-2}), $Z_n^{v\ or\ i}$ is the vacancy or interstitial bias factor of sink on n type in the iron matrix, which is a dimensionless number, and $D_{v\ or\ i}$ is the diffusion coefficient of vacancy or interstitial in the matrix (cm^2s^{-1}). β is the point defect absorption constant, E is the point defect emission constant, ρ_n is the density of a specific sink such as dislocation line, dislocation loop, void, and precipitation in the iron matrix (cm^{-2}).

The key idea of PBM is the mobile interstitial cluster is generated and reacted with other sinks. Hence modified master equation of simple CDM is necessary. The most important of SIAs diffusivity is 1 dimensional diffusivity. Hence, by adopting the theoretical basis of one dimensional approach, which is described in Borodin's work approach. Master equation could be fully described. The noticeable point in this study, Singh's approach was adopted in master equations i.e., mean size approximation was adopted in SIAs cluster. Specifically, mean size of SIAs cluster was considered rather than considering each SIAs cluster. Hence SIAs cluster number density is expressed simply bellow.

$$\frac{dC_g}{dt} = K_g(t) - D_g C_g k_g^2 \tag{5}$$

Here C_g is the MIC number density concentration, K_g is the generation rate of SIAs cluster, D_g SIAs cluster diffusion coefficient, and K_g^2 sink strength. The equation about sink strength is

$$k_g = \frac{\pi\rho d_{abs}}{4} + \sigma_v N_v \tag{6}$$

Here d_{abs} is effective interaction diameter, R_g is grain radius, σ_v are the cross-section clusters with size. Master equation is modified to consider negative or positive effect of SIAs cluster on cluster number density.

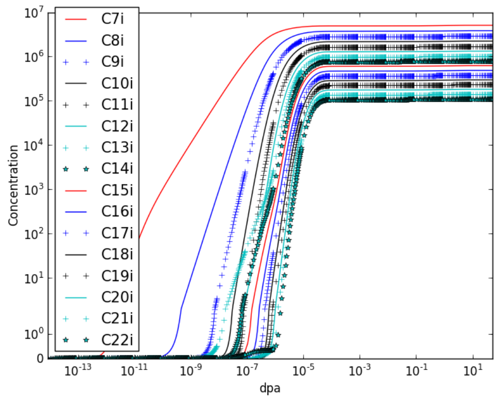
$$\begin{aligned}\frac{dC_x}{dt} &= K + \beta_i^{x-1}C_{x-1i} - \left(\beta_v^x + \beta_i^x + E_i^x\right)C_{xi} \\ &- \beta_{SIA}^x C_{xi} + \beta_{SIA}^{x-x_g} C_{(x-x_g)i}\left(x > x_g\right)\end{aligned} \tag{7}$$

$$\begin{aligned}\frac{dC_x}{dt} &= K + \beta_i^{x-1}C_{x-1i} - \left(\beta_v^x + \beta_i^x + E_i^x\right)C_{xi} \\ &+ \beta_{MIT}^{x-x_g} C_{(x-x_g)i}\left(x > x_g\right)\end{aligned} \tag{8}$$

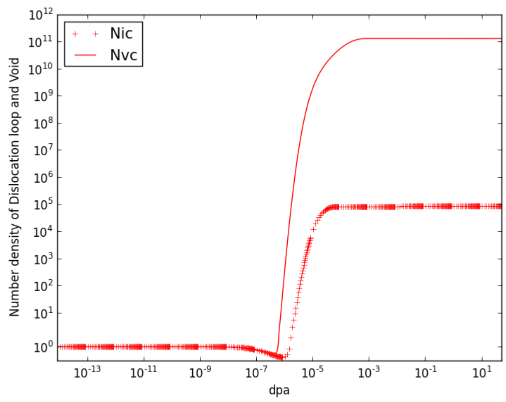
3. Irradiation creep model.

Radiation induced dimensional change is mainly caused by reaction with defect and sink. In case of irradiation growth, in which non-stress applied condition, normal defect flux behavior could fully explain dimensional instability given diffusivity. However, in case of irradiation creep, reaction mechanism is somewhat different with normal condition. Brailsford considered stress effect on reaction by using modification of vacancy emitting rate of dislocation loop. However, this approach does not account diffusivity change in defect in free matirx. Therefore, in this paper, MD simulation results was accounted to accurate calculation of dimensional instability.

4. Result & Discussion



(a)



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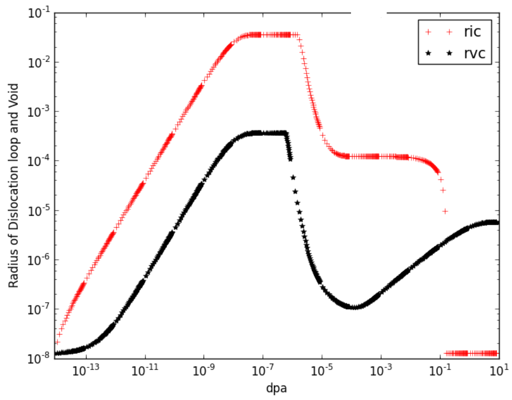
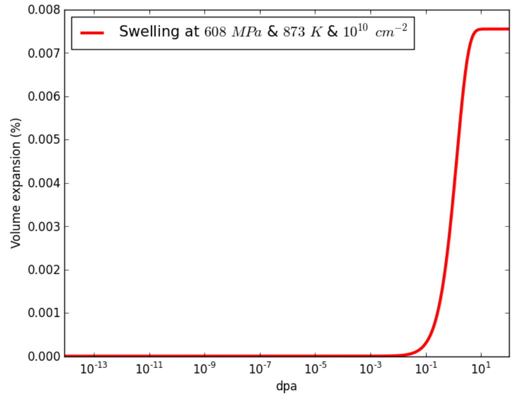


(c)



(d)

Fig.1. (a) defect concentration of point defect in iron matrix; (b) dislocation loop and void number density; (c) dislocation loop and void average radius; (d) irradiation creep elongation

Point defect, cluster number density, and radius was calculated to calculate irradiation creep. Both point defect and cluster defect are saturated 10^{-3} dpa. The radius behavior of dislocation loop show dissolution in high temp region. However, in case of void show saturation at 10^{-4} cm. Therefore, irradiation swelling also show saturation.

5. Summary

The aim of this study is understanding of stress and radiation effect on irradiation swelling and creep. From the PBM approximation, sink behavior was calculated. It was confirmed that SIAs significant effect on swelling saturation. location loop number density, cluster behavior will be more specifically demonstrated by microstructural analysis in next research step.

Acknowledgement

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