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Effect of elastic stress field near grain boundaries on the radiation induced segregation in binary alloys

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Abstract

An important problem of radiation resistance of structural materials for reactors (different types of steels, including steels doping by low radio-active elements) is their phase stability under neutron irradiation which is associated with the formation of solute radiation induced segregation (RIS) near grain boundaries. The diffusion of alloying elements under irradiation due to interstitial and vacancy diffusion mechanisms towards grain boundaries, which are perfect sinks for point defects results in the RIS formation near grain boundaries. Each grain boundary has the effective elastic stress field produced by the microstructure of grain boundaries. This elastic field can affect the formation of RIS in the dependence on an irradiation dose due to accumulation of impurity elements, gas atoms (helium), formation on grain boundary helium bubbles and precipitates especially at high doses of irradiation. The precipitates and overpressurised helium bubbles are the sources of internal stress fields too and they can dramatically change the effective stress field near grain boundaries. It will result in the redistribution of alloying elements near grain boundaries due to the additional diffusion driving force which is determined by the interaction energy of point defects with effective stress field near grain boundary.

1. Introduction

The formation of RIS near grain boundaries under neutron irradiation in reactor structural materials is one of the serious physical problems which affects the radiation resistance of these materials. Such physical phenomena as radiation embrittlement and intergranular fracture are caused by a redistribution of alloy components and segregation formation near grain boundaries. RIS and precipitate formation on grain boundaries can significantly change alloy composition and currents of point defects to defect clusters in matrix (voids, dislocation loop, precipitates) that can change the behavior of such very important phenomenon as radiation swelling in these materials. The investigations of RIS formation are based on analytical models taking into account inverse-Kirkendall effect [1–4]. Many papers [5–8] have been published concerning the description of this phenomenon under irradiation.

The width of distribution of RIS near grain boundary is located usually in the interval 10–100 nm. It is well known that the grain boundaries

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and interfaces can be modeled by discretely distributed array of grain boundary dislocation wall [9]. Each grain boundary dislocation interacts with point defects and impurity atoms due to produced elastic stress field near it. The interaction energy of grain boundary with point defects results in the additional driving force for point defects and impurity atoms in the currents of them to grain boundary. The characteristic distance where grain boundary (dislocation wall) can interact with point defects and can effect on diffusion processes is equal 3–20 nm [9]. So it is very interesting to investigate how the interaction energy of grain boundary with point defects and additional driving force can change the distribution of RIS near grain boundaries.

In this paper we investigate the effect of elastic stress fields near grain boundary on the formation of RIS in an irradiated binary alloy. For this aim we consider a two-component alloy as an ideal solution with random distribution of A- and B-types of atoms. These atoms can occupy both the lattice sites: substitution and interstitial positions. We will consider here a semi-infinite irradiated binary alloy with a flat surface and assume that dislocations and voids constitute the volume sinks for point defects in the matrix. Near the grain boundary we will take into account the effect of elastic stress field on point defect motion due to acting of an additional driving force on diffusion process which is determined by the interaction of point defects with the elastic stress field near grain boundary.

2. Governing equations of the model

The spatial profiles of the point defects near grain boundary are determined by the following steady-state system of diffusion equations for point defects:

$$-\omega\nabla\overrightarrow{j_{\mathrm{v}}} + G_{\mathrm{v}} - k_{\mathrm{v}}^2 D_{\mathrm{v}}(C_{\mathrm{v}} - \overline{C}_{\mathrm{v}}^{\mathrm{eq}}) = 0 \tag{1}$$

$$-\omega\nabla\overrightarrow{j_{\mathrm{Yi}}} + G_{\mathrm{Y}} - (k_{\mathrm{Yi}})^2 d_{\mathrm{i}}(C_{\mathrm{Yi}} - \overline{C}_{\mathrm{Yi}}^{\mathrm{eq}}) = 0; \quad \mathrm{Y} = \mathrm{A,B} \tag{2}$$

Here C_{v} and C_{Yi} are the atomic concentrations of vacancies and interstitials of Y-type, respectively; $\overrightarrow{j_{\mathrm{v}}}$ and $\overrightarrow{j_{\mathrm{Yi}}}$ are the point defects currents; ω is the atomic volume. D_β is the diffusion coefficient of the β-type of point defects ($\beta = \mathrm{v}$, Ai, Bi); $d_{\mathrm{Y}\beta} = (1/6)\lambda_\beta^2 z_\beta \nu_{\mathrm{Y}\beta}$ is the partial diffusion coefficient [3]; λ_β, z_β are the diffusion jump length and the number of nearest neighbors for β-type of point defect, respectively; $\nu_{\mathrm{Y}\beta} = \nu_{\mathrm{Y}\beta}^0 \exp(-\Phi_{\mathrm{Y}\beta}^m/T)$, $\nu_{\mathrm{Y}\beta}^0$ is the attempt frequency of atomic jumps; $\Phi_{\mathrm{Y}\beta}^m$ is the Gibbs free enthalpy of the Y-atom migration via the β-type of point defect.

$$D_{\mathrm{v}} = d_{\mathrm{Av}} C_{\mathrm{A}} + d_{\mathrm{Bv}} C_{\mathrm{B}} \tag{3}$$

Here C_{Y} (Y = A,B) is the atomic concentration of Y-atoms occupying the substitutional positions.

For simplicity the equal partial diffusion coefficients of the different alloy species via interstitials ($D_{\mathrm{Yi}} = d_{\mathrm{Yi}} = d_{\mathrm{i}}$) are suggested below. $\overline{C}_\beta^{\mathrm{eq}}$ is the equilibrium defect concentration at the surfaces of volume sinks averaged over the ensemble of the volume sinks.

The sink strengths in the bulk are given by:

$$k_\beta^2 = Z_\beta^d \rho_{\mathrm{d}} + 2\pi N_{\mathrm{V}} \left\langle Z_\beta^V R_{\mathrm{V}} \right\rangle, \quad x \geqslant \Lambda \tag{4}$$

Here Z_β^d are the bias factors for the absorption of β-type of point defect at the dislocations; N_{V}, R_{V}, and Z_β^{V} are the void volume density, radius and bias factor, respectively; $\langle\rangle$ denotes the average over the ensemble of the volume sinks; ρ_{d} is the dislocation density. Λ is the width of defect-free zone near the surface or the grain boundary [10–12], $k_\beta^2 = 0$ for $x < \Lambda$. In the following numerical calculations we will use $\Lambda = 100\lambda$, where λ is the lattice spacing.

Defect accumulations during irradiation are described by generation rates, both for vacancies and interstitials, $G_{\mathrm{v}} = G_{\mathrm{i}} = G_{\mathrm{A}} + G_{\mathrm{B}}$ (where G_{Y} are the partial generation rates describing displacements of Y-atoms from lattice sites). These generation rates are considered as input parameters. We suppose that the partial damage rates G_{Y} are given by the following relations [7]:

$$G_{\mathrm{Y}} = \frac{\eta_{\mathrm{Y}} C_{\mathrm{Y}} G_{\mathrm{v}}}{\eta_{\mathrm{A}} C_{\mathrm{A}} + \eta_{\mathrm{B}} C_{\mathrm{B}}} = \eta_{\mathrm{Y}} C_{\mathrm{Y}} G, \tag{5}$$

where η_{Y} is the partial damage efficiency, and the effective generation rate G is defined as:

$$G = \frac{G_{\mathrm{v}}}{\eta_{\mathrm{A}} C_{\mathrm{A}} + \eta_{\mathrm{B}} C_{\mathrm{B}}} \tag{6}$$

At the surface or grain boundary ($x = 0$) we suppose the equilibrium concentrations of point defects adjusted on elastic field energy:

$$C_\beta(0) = \overline{C}_\beta^{\mathrm{eq}} \exp\left(-\frac{U_\beta}{T}\right)$$
$$\overline{C}_\beta^{\mathrm{eq}} = \exp\left(\frac{S_\beta^{\mathrm{f}}}{k}\right) \exp\left(-\frac{H_\beta^{\mathrm{f}}}{kT}\right) \tag{7}$$

Here S_β^{f} and H_β^{f} are the defect formation entropy and enthalpy, respectively, U_β is the interaction energy of point defects with the grain boundary.