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The governing quantitative characteristics of radiation-induced segregation in Fe-Cr-Ni alloy

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A profound consequence of irradiation (neutron, proton, electron and heavy ion) of metal alloys is the spatial redistribution of alloy components. As a result, there are enrichment or depletion of the main, solute and impurity components of the alloy near the defect sinks. This phenomenon is called radiation-induced segregation (RIS) and leads to degradation of mechanical and physicochemical properties of materials.

The spatial and temporal evolution of the concentrations of alloy components C_k ($k = \mathrm{Fe, Cr, Ni}$) and point defects (PD) (vacancies C_v and interstitials C_i) in the ternary concentrated Fe-Cr-Ni alloys under irradiation is described by the system of five coupled nonlinear partial differential equations [1-3]:

$$\begin{cases} \frac{\partial C_k}{\partial t} = -\nabla \mathbf{J}_k, \\ \frac{\partial C_v}{\partial t} = -\nabla \mathbf{J}_v + K_0 - R_{iv} C_v C_i - k_v^2 D_v \left(C_v - C_v^{eq}\right), \quad (1) \\ \frac{\partial C_i}{\partial t} = -\nabla \mathbf{J}_i + K_0 - R_{iv} C_v C_i - k_i^2 D_i \left(C_i - C_i^{eq}\right). \end{cases}$$

where the fluxes of atoms species k is $\mathbf{J}_k$, vacancies $\mathbf{J}_v$ and interstitial $\mathbf{J}_i$ defined as:

$$\mathbf{J}_k = -\left(\sum_{d=v,i} d_{k,d} C_d\right) \nabla C_k + C_k \left(d_{k,v} \nabla C_v - d_{k,i} \nabla C_i\right), (2)$$

$$\mathbf{J}_v = -\sum_{k=\mathrm{Fe,\,Cr,\,Ni}} d_{k,v} C_k \nabla C_v + \alpha C_v \left(\sum_{k=\mathrm{Fe,\,Cr,\,Ni}} d_{k,v} \nabla C_k\right), \quad (3)$$

$$\mathbf{J}_i = -\sum_{k=\mathrm{Fe,\,Cr,\,Ni}} d_{k,i} C_k \nabla C_i - \alpha C_i \left(\sum_{k=\mathrm{Fe,\,Cr,\,Ni}} d_{k,i} \nabla C_k\right), \quad (4)$$

K_0 is the production rate of radiation PD, R_{iv} is the recombination rate of PD, k_v^2 and k_i^2 are the sink strengths for vacancies and interstitials respectively, C_v^{eq} and C_i^{eq} are the equilibrium vacancy and interstitial concentrations, D_v and D_i are the diffusion coefficients of vacancies and interstitial, $d_{k,v}$ and $d_{k,i}$ are the diffusivity coefficients of vacancies and interstitial. The system with the corresponding initial and boundary conditions is solved numerically (a detailed solution algorithm is given in [2]).
The aim of the present paper is to calculate the governing quantitative characteristics of RIS for Fe-20%Cr-8%Ni alloy under the irradiation. That are: concentration profiles of atoms species k $C_k(x)$ and PD $C_{v(i)}(x)$, surface concentration of atoms species k C_k^{Surf}, the value of surface enrichment (depletion) of atoms species k ΔC_k, the full width of the concentration profile of atoms species k at half maximum enrichment (depletion) FWHM_k, segregation area of atoms species k S_k and discriminant of RIS of atoms species k in a steady state $\mathfrak{D}_k$. For example, production rate dependence of surface depletion, FWHM and segregation area for Cr and Ni are shown in Fig. 1.

Fig. 1. Production rate dependence of surface Cr depletion ΔC_{Cr} and Ni enrichment ΔC_{Ni} (solid line), $\mathrm{FWHM}_{\mathrm{Cr}}$ and $\mathrm{FWHM}_{\mathrm{Ni}}$ (dashed line) and segregation area of Cr S_{Cr} and Ni S_{Ni} (dash-dotted line). Calculations were performed at temperature$T = 400\tilde{}^\circ$C, dose $D = 10\tilde{}$dpa (displacement per atom).

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