**EFFECT OF INTERNAL SINK STRENGTH ON DIFFUSION MASS TRANSPORT IN ALLOYS UNDER HIGH DOSE ION IRRADIATION**

V.A. Pechenkin, A.D. Chernova, and V. L. Molodtsov  
SSC RF The Institute for Physics and Power Engineering,  
Obninsk, 249033, Russia  
vap@ippe.ru  
F.A. Garner  
National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)  
Moscow, Russia

**ABSTRACT**

Accelerators are used for simulation of neutron radiation effects in structural materials for advanced fission and fusion reactors. However, some specific neutron-atypical features of ion irradiation should be accounted for in analysis of ion irradiated alloys. These features include surface sinking, non-uniformity of point defect (PD) generation rate with depth, radiation-induced segregation (RIS) along the ion path, and local accumulation and diffusion of implanted ions, especially at very high damage levels of 200-1000 dpa.

We have developed a model of non-steady-state RIS in four-component substitutional alloys along the ion range during self ion irradiation, accounting for these features, and most recently have incorporated the effects of internal sink strength. The model also allows calculation of RIS near individual PD sinks under both ion and neutron irradiation. Predictive modeling of RIS is performed in model fcc Fe-Cr-Ni and bcc Fe-Cr-Si-Ni alloys under irradiation with 7 MeV Ni$^{2+}$ and 1.8 MeV Cr$^{3+}$ ions currently used in Russia and Ukraine, respectively. The model is then evaluated against published data on Ni distribution in F82H ferritic-martensitic steel irradiated with 4 MeV Ni$^{3+}$ ions, as well as on data of Ni accumulation near void surfaces in Fe-15Cr-30Ni irradiated in the EBR-II reactor. It is seen that higher radiation-induced sink strengths slow down the diffusion overall, but are especially important to slow down the redistribution of continuously injected ions.

**KEY WORDS**  
Ion irradiation, neutron irradiation, radiation-induced segregation, fcc Fe-Cr-Ni alloys, bcc Fe-Cr-Si-Ni alloys

1. **INTRODUCTION**

Under spatially uniform irradiation characteristic of neutron reactors RIS leads to significant changes in alloy composition near microstructural features such as grain boundaries, specimen surfaces, dislocations, precipitates and voids. As a consequence RIS strongly affects precipitate phase content, void swelling, corrosion, embrittlement and other radiation-induced degradation phenomena. (see e.g. [1-6]). The RIS phenomenon also reveals itself in regions of high spatial non-uniformity of PD generation rate that is characteristic of ion irradiation. Moreover, accumulation of implanted ions, especially at very high damage levels of 200-1000 dpa, can change the composition and therefore cannot be ignored.
Recently we developed a model for non-steady-state RIS in four-component substitutional alloys along the projected range under self ion irradiation, accounting for these various features [7]. In this paper we have extended this model to account for the influence of internal sink strength. Predictive modeling of RIS is performed in fcc Fe-19Cr-16Ni and bcc Fe-12Cr-2Si alloys under ion irradiation. The alloys are simple model analogues for EK-164 austenitic steel, a promising cladding material for fast reactors using sodium coolant, and EP-823 ferritic-martensitic steel, a promising cladding material for fast reactors using Pb or PbBi coolant. The self-ion choices are 7 MeV Ni$^{++}$ ions [7,8] and 1.8 MeV Cr$^{++}$ ions [9], both currently used in swelling and RIS studies in Russia and Ukraine, respectively.

Doses up to 300 displacements per atom (dpa) are explored, with the dpa assignment corresponding to the peak damage rate for the chosen ion. The peak dpa rates chosen were 3·10$^3$ dpa/s and 2·10$^2$ dpa/s for the 7 and 1.8 MeV ions, respectively. Both standard (NRT) and effective (accounting for cascade efficiency) dpa rates are employed.

This model is then evaluated against published data on Ni distribution in F82H ferritic-martensitic steel irradiated with 4 MeV Ni$^{++}$ ions [10]. The model is also evaluated against data on Ni accumulation near void surfaces in Fe-15Cr-30Ni irradiated in the EBR-II reactor [11].

2. MODEL DESCRIPTION

Considering a four-component alloy with species notations A, B, C, D we have the following diffusion equations for the concentrations of alloy elements and point defects (see [7]):

$$\frac{\partial C_m}{\partial t} = -\nabla J_m - K_B C_m, \quad m = A, C, D, \quad \frac{\partial C_B}{\partial t} = -\nabla J_B + K_B (1-C_B),$$

$$\frac{\partial C_v}{\partial t} = -\nabla J_v + K + \delta_{\alpha_1} K_B - RC_v C_i - k_2 D_v (C_A - C_B), \quad n = v, i$$

where $K_B$ is the spatially non-uniform implantation rate of B-component ions (atoms per second per lattice site); $K$ is the spatially non-uniform PD generation rate (dpa/s); $\delta_{\alpha_1} = 1, \quad \delta_i = 0, \quad R$ is the PD recombination factor; $k_2^2, C_v, D_v$ are PD sink strengths, thermal equilibrium concentrations and diffusion coefficients ($D_v = d_v^A C_A + d_v^B C_B + d_v^C C_C + d_v^D C_D$, where $d_v^m$ are the m-species diffusivities via vacancy ($n = v$) and interstitial ($n = i$) mechanisms). Component and PD fluxes $J$ are taken from [12]; $\delta_{\alpha_1} K_B$ term in the equation above accounts for an additional source of interstitials due to the ion implantation. Note that implantation of bombarding B-species affects the concentrations of all components.

Diffusivity coefficients were chosen and discussed earlier in [7]. In simulations smooth approximations of the depth profiles of radiation damage $K$ and implanted ions $K_n$ rates along the projected range of metal ions were used. The original profiles were calculated with TRIM-98 code. “Standard” (NRT dpa [13]) PD generation rates were estimated with TRIM code using the Kinchin and Pease option [14]. For the “effective” dpa rates a cascade efficiency of 0.3 was used [14,15].

The model also allows calculation of RIS near individual PD sinks. In this case the last term in the equations for PD concentrations is omitted. The system of diffusion equations is then solved in the cell surrounding the PD sink, voids under neutron irradiation in this case.
3. RESULTS AND DISCUSSION

3.1 Predictive modeling

Earlier in [7], RIS simulations were carried out at 675°C for Fe–19Ni–16Cr (base components of EK-164 steel) and at 500°C for Fe–12Cr–2Si with and without 0.5% Ni (base components of EP-823 steel) for doses up to 300 dpa. Due to high PD generation rates under ion irradiation, only PD recombination was found to be important in the simulations. An analysis has revealed that this is correct at PD sink strengths up to $10^{14}$ m$^{-2}$. At lower PD sink strengths the kinetics of mass transport are similar to those considered in [7]. Effects of higher PD sink strengths are demonstrated on Figures 1-2 for highest doses of 300 dpa. The positions of peak damage rate and peak ion injection rate are marked by $R_d$ and $R_i$ accordingly.

![Figure 1](image1.png)

**Figure 1.** Calculated profiles of Si and Cr along the projected range of 1.8 MeV Cr$^{+3}$ ions in Fe–2Si–12Cr at 15 000 s (300 dpa). Parameters of sink strength are: $k_0^2 = 0$, $k_0^2 = 10^{14}$ m$^{-2}$, $k_0^2 = 10^{15}$ m$^{-2}$, $k_0^2 = 10^{16}$ m$^{-2}$

![Figure 2](image2.png)

**Figure 2.** Calculated profiles of Ni and Cr along the projected range of 7 MeV Ni$^{++}$ ions in Fe–19Ni–16Cr at 15 000 s (300 dpa). Parameters of sink strength are: $k_0^2 = 0$, $k_0^2 = 10^{14}$ m$^{-2}$, $k_0^2 = 10^{15}$ m$^{-2}$, $k_0^2 = 10^{16}$ m$^{-2}$. 
First of all, it is obvious that surface-affected segregation occurs very early in response to inverse-Kirkendall and solute-drag effects, tending to saturate. More importantly, the injected ions continue to cause substantial changes in local composition, although diffusion is constantly working to minimize the magnitude of injected peak. Deeper penetrating ions (7.5 MeV) cause less changes in local composition overall compared to shallower-penetrating ions (1.8 MeV).

It is seen that increasing the PD sink strength slows down mass transport in general, delaying diffusion of implanted ions out of injected region. While slower-diffusing Cr and Ni tend not to exhibit a significant shift in peak concentration positions with increasing sink strength, faster-diffusing Si does exhibit a shift with increasing sink strength.

If we invoke a decrease of cascade efficiency to 30% a delay in mass transfer kinetics is observed as shown in Figure 3. However, the observed influence is second-order in magnitude compared to the effects of surface, dpa gradients and ion injection.

![Figure 3. Calculated profiles of Si and Cr along the projected range of 1.8 MeV Cr$^{+3}$ ions in Fe–2Si–12Cr at 15 000 s (300 dpa): ——— cascade efficiency 0.3, - - - - cascade efficiency 1.0.](image)

### 3.2 Evaluation of published implantation and segregation data

In ref. [10] data are published on the Ni distribution in F82H ferritic-martensitic steel irradiated simultaneously with 1 MeV He$^+$ and 4 MeV Ni$^{3+}$ ions at 450°C to peak 100 dpa. The depth dependence of swelling, cavity number density and radius, dislocation density were also presented in that paper. RIS simulations were carried out for the Fe–8Cr analogue of F82H with and without accounting for dislocation sink strength. For RIS simulation along the projected range of 4 MeV Ni$^{3+}$ ions smooth approximations of the depth profiles of radiation damage and implanted ions were used. The original profiles were calculated using the TRIM-98 code. Figure 4 presents calculated Ni and Cr profiles in comparison with experimental data on Ni content.
Figure 4. Calculated and experimental profiles of Ni content along the projected range of 4 MeV Ni\(^{3+}\) ions in Fe–8Cr at 100 dpa: \(- \cdots - k_a^2 = 0, \quad k_a^2 = 1.5 \times 10^{15} \text{m}^2\), \(- \cdots -\) implanted ions profile with no account of RIS and radiation-enhanced diffusion, filled squares denote experimental data of [10].

Without diffusion the calculated implant profile is much narrower and taller than that indicated by the measurement. Diffusion in the absence of internal sinks provides a better fit, but incorporating a sink strength of \(k_a^2 = 1.5 \times 10^{15} \text{m}^2\) marginally improves the fitting to the experimental data.

In [11] the microstructural and microchemical evolution of Fe–XNi–15Cr alloys irradiated in the EBR-II reactor was investigated. Data on swelling, void size distribution, dislocation and loop number density and also on Ni segregation near void surfaces were obtained at four fast neutron fluences. Experimental data on swelling in Fe-15Cr-30Ni and on the Ni content both near the void surfaces and in the bulk are presented in Figure 5.

Figure 5. Experimental data on swelling and Ni content near void surfaces and in the bulk of Fe-15Cr-30Ni alloy under neutron irradiation [11], R is the void radius.
For modeling of Ni segregation near void surfaces the system of equations (1), (2) was modified. Homogeneous irradiation was modeled with damage rate $K = 10^{-6}$ dpa/s typical for EBR-II ($\sim$5 dpa per $10^{20}$ n/m²) [16]. The terms with $K_B$ and the last term in (2) were omitted. The size of cell surrounding the void with the cell size was determined by the distance between PD sinks estimated from [11]. Calculations of Ni accumulation near surfaces of two void sizes ($R = 15$ nm and $R = 65$ nm) are presented in Figure 6.

As observed in the cited experiment, Ni concentrations at void surfaces quickly exceed 40% for both void sizes and the Ni content at the cell boundary at 37 dpa is noticeably lower than the initial matrix content.

4. CONCLUSIONS

During ion irradiation the effect of RIS on compositional distribution is seen at the sample surface, as well as in regions with large gradients in dpa rate. Steady state profiles near the surface establish during early at doses of only several dpa, whereas alloy contents in the region of ion implantation change continuously during the irradiation. Changes in composition can be rather large in some regions, but are most important at regions where microstructural data are usually extracted.

At high doses, the impact of continuous ion implantation cannot be ignored. Deeper penetrating ions (7.5 vs. 1.8 MeV) cause less change in alloy content along the projected range than do shallower penetrating ions. Increasing the sink strength slows down mass transport kinetics in general and therefore mass transfer of implanted ions out of injected region in particular.

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