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# An analysis of void swelling dose dependence in ion irradiated V–Fe alloys

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**Abstract**

The microstructure of V–*X*Fe alloys ($X = 0$, 2, 5 and 7 at.%) irradiated as thin foils at 625°C with 50 KeV $V^+$ ions to damage doses ranging from 2.5 to 40 dpa at averaged dose rate of $5 \times 10^{-3}$ dpa/s has been investigated. Data on mean void diameter, void number density, void volume fraction ($\Delta V/V$) and total dislocation length per unit volume have been obtained. From these data the sink strengths for voids and dislocations were found and the void swelling bias factor (SBF) as a function of iron content was determined. Both $\Delta V/V$ and SBF reveal maxima at about 5 at.% Fe. For an interpretation of a decrease in $\Delta V/V$ and SBF at iron contents above 5 at.%, in the present work, the model developed previously is generalized to account for the diffusivity dependence on alloy composition. 

## 1. Introduction

Vanadium alloys are now considered as candidate fusion reactor materials. Some of them seem to be of interest for revealing the physical reasons of a high sensitivity of void swelling to alloy composition. Matsui et al. [1] have observed exceptionally large swelling of ~100% in a V-5 at.% Fe alloy after irradiation in FFTF to 34 dpa at 600°C in contrast to the swelling in pure vanadium of ~1.4% under similar irradiation conditions [2]. In the previous work, [3] we have studied the swelling in V–Fe alloys for iron content up to 5 at.% irradiated with $V^+$ ions at several temperatures and doses. It was shown that a strong increase in swelling with an increase in the iron content can be related to the radiation-induced segregation (RIS) of iron near void surfaces.

The objective of the present work is to investigate the void swelling in V–Fe alloys irradiated with $V^+$ ions for iron contents up to 7 at.%. An attempt is made to interpret the observations in terms of RIS, taking into account the dependence of alloy component diffusivities via vacancy and interstitial mechanisms on alloy composition.

## 2. Experimental results

Thin foils of pure V and V–2 at.% Fe, V–5 at.% Fe and V–7 at.% Fe alloys were irradiated with 50 keV $^{51}V^+$ ions at 625°C to an average dose rate over the foil thickness of $5 \times 10^{-3}$ dpa/s to damage doses of 2.5, 10, 20 and 40 dpa. TEM-data on the microstructure are shown in the Table 1. From the microstructural data, sink strengths of voids and dislocations as well as void volume fraction rates were determined at 20 dpa and then the void swelling bias factor was calculated using the approach and parameters of Ref. [3]. The values of SBF calculated are 1.1%, 1.9%, 6% and 3% for iron contents 0, 2, 5 and 7 at.% respectively. Both $\Delta V/V$ and SBF have maximum at about 5 at.% Fe.

## 3. Discussion

### 3.1. Effect of radiation-induced segregation on swelling

As was shown by Wolfer [4], radiation-induced segregation around point defect sinks such as voids, dislocations and others produces new drift forces on both interstitials and vacancies including Kirkendall forces as well as drift forces caused by gradients of point defect formation and migration energies. The latter can be of

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Table 1
Data on the microstructure in ion irradiated V–Fe alloys, $T_{irr} = 625°C$, dose rate $K = 5 \times 10^{-3}$ dpa/s

| Material | Microstructural feature | Dose (dpa) | | | |
|---|---|---|---|---|---|
| | | 2.5 | 10 | 20 | 40 |
| V | Mean void diameter $d_v$, nm | 4 | 7.8 | 10.9 | 15 |
| V–2Fe | | 6 | 11.5 | 16 | 23 |
| V–5Fe | | 15 | 29 | 40 | 57 |
| V–7Fe | | 10 | 19 | 24 | 31 |
| V | Void concentration $N_v$, $10^{20}$ m$^{-3}$ | 100 | 190 | 200 | 180 |
| V–2Fe | | 60 | 80 | 90 | 80 |
| V–5Fe | | 5 | 17 | 24 | 18 |
| V–7Fe | | 9 | 35 | 42 | 39 |
| V | Void volume fraction $\Delta V/V$, % | 0.05 | 0.7 | 1.5 | 4.6 |
| V–2Fe | | 0.10 | 0.9 | 2.8 | 7.2 |
| V–5Fe | | 0.13 | 3.1 | 11.5 | 25 |
| V–7Fe | | 0.08 | 2.2 | 5.6 | 10.8 |
| V | Dislocation density, $\rho_d$, $10^{14}$ m$^{-2}$ | 2.0 | 8.7 | 14 | 14 |
| V–2Fe | | 10 | 23 | 19 | 17 |
| V–5Fe | | 20 | 24 | 23 | 30 |
| V–7Fe | | 10 | 22 | 26 | 30 |

the same order of magnitude as the stress-induced drift forces produced by edge dislocations in an uniform alloy. Hence, RIS can result in a significant modification of SBF.

In the earlier work, [3] we have used the well known 'method of constant boundary concentration' [5–7] to calculate point defect sink strengths and SBF taking into account both the elastic point defect-sink interaction and RIS. The following assumptions have been made for the SBF calculation: (1) At high swelling rates, RIS around rapidly climbing dislocations is much weaker than that around motionless dislocations [8] and can be neglected (the case of segregation-free dislocation), (2) The ratio of vanadium to iron diffusivities via vacancy mechanism $\lambda = d_{V,v}/d_{Fe,v}$ was assumed to be independent of alloy composition and was taken as $\lambda_{v1} = 0.22$ in accordance with the experimental data by Coleman et al. [9] for self-diffusion and tracer diffusion of $^{59}$Fe in vanadium, (3) The unknown ratio of component diffusivities via an interstitial mechanism $\lambda_i = d_{V,i}/d_{Fe,i}$ was considered as a fitting parameter being independent of the alloy composition and satisfying an additional condition $\lambda_i < \lambda_v$ in order to ensure an enrichment of iron around sinks in accordance with observations [10].

At $\lambda_i = 0.1$ a satisfactory agreement between calculated and 'experimental' SBFs for iron contents up to 5 at.% was achieved. However, the model, under the assumptions made, predicts an increase of the SBF with increase in the iron content up to 30 at.% and then a slow decrease of the SBF at higher contents that is in contrast to 'experimental' data on SBF.

In order to correct the model, we revise the assumptions given above and take into account the dependence of $\lambda_v$ and $\lambda_i$ on alloy composition. As was discussed earlier in Ref. [3], experimental data on impurity diffusion of vanadium and self-diffusion in iron [11] show that the value of $\lambda_v$ can increase with increasing iron content reaching $\lambda_v = \lambda_{v2} = 2.85$ in nearly pure iron. Because the dependence of $\lambda_v$ on alloy composition is unknown, we will use the following linear approximation: $\lambda_v = \lambda_{v1} + C_{Fe}(\lambda_{v2} - \lambda_{v1})$. In order to ensure an enrichment of iron around sinks at low iron contents, a relatively small value of $\lambda_i$ ($\lambda_i < \lambda_{v1}$) independent of alloy composition was used in the earlier model from Ref. [3]. Such a small value of $\lambda_i$ was based on the concept of mixed dumbbells consisting of an vanadium atom and undersized iron atom. This concept is probably valid only at low iron contents, whereas at higher iron contents, $\lambda_i$ can be of the order of unity. For a phenomenological account for this possibility we will use below a linear approximation: $\lambda_i = \lambda_{i1} + C_{Fe}(\lambda_{i2} - \lambda_{i1})$. As was discussed in Ref. [3], at relatively low swelling rates, RIS around slowly climbing dislocations can be significant and should be accounted for in the calculations. So, in addition to the assumption (1) we consider another limiting case, RIS is independent of dislocation velocity.

### 3.2. Steady-state component profiles around point defect sinks

The method for deriving the analytical expressions for alloy component profiles around sinks has been developed in Refs. [12–14]. Using the linear approximations for $\lambda_v$ and $\lambda_i$, one can obtain the following expression for A-component profiles around sinks in a binary substitutinal alloy:

$$\frac{C_A}{(1 - C_A)^{v_1}}(1 + \beta_1 C_A)^{v_2} \exp(\beta_2 C_A) = \text{const } C_{v0}^{\theta}, \qquad (1)$$

where

$$v_1 = \frac{\lambda_{i1} - \lambda_{v1}}{\lambda_{v1}\lambda_{i1}(\lambda_{i2} - \lambda_{v2})} \frac{\lambda_{v0}/R_v + \lambda_{i0}/R_i}{1/R_v + 1/R_i},$$

$$v_2 = v_1 - \frac{(\lambda_{v1}\lambda_{i2} - \lambda_{v2}\lambda_{i1})^2}{\lambda_{v1}\lambda_{v2}((\lambda_{i2} - \lambda_{i1}) - (\lambda_{v2} - \lambda_{v1}))^2},$$

$$\beta_1 = \frac{\lambda_{v2} - \lambda_{i2}}{\lambda_{v1} - \lambda_{i1}} - 1,$$

$$\beta_2 = \frac{(\lambda_{v1} - \lambda_{i1})(\lambda_{v2} - \lambda_{v1})(\lambda_{i2} - \lambda_{i1})}{\lambda_{v1}\lambda_{i1}((\lambda_{v2} - \lambda_{v1}) - (\lambda_{i2} - \lambda_{i1}))},$$

$$\theta = \frac{\lambda_{i1} - \lambda_{v1}}{\alpha\lambda_{i1}\lambda_{v1}} \frac{1}{1/R_v + 1/R_i},\ R_n = C_{A0} + \lambda_{n0}(1 - C_{A0}),$$

$$\lambda_{n0} = \lambda_{n1} + C_{A0}(\lambda_{n2} - \lambda_{n1}),$$

$C_{A0}$ is the uniform A-component concentration in an unirradiated alloy, $n$ represents $v$ and $i$ for vacancies and interstitials, respectively, $C_{v0}$ is the vacancy concentration profile around the sink in segregation-free alloy, the normalization constant must be obtained from the condition of equality of mean $C_A$ value to $C_{A0}$ in a cell, and $\alpha$ is the thermodynamical factor.

It should be noted, that in the case when $\lambda_{v1} = \lambda_{v2} = \lambda_v$ and $\lambda_{i1} = \lambda_{i2} = \lambda_i$ Eq. (1) reduces to that used earlier in Ref. [3] for $\lambda_v$ and $\lambda_i$ independent of alloy composition.

### 3.3. Calculation of the swelling bias factor

The method of the SBF calculation has been developed earlier in Ref. [3]. Using this method, the point defect fluxes $J_n$ ($n = i,v$) should be written as

$$J_n = -\nabla D_n C_n + D_n C_n \nabla F_n(r), \tag{2}$$

where $r$ is the distance from the sink surface. $F_n(r)$ functions were obtained in Ref. [3] for composition independent $\lambda_n$ and must now be changed. For SBF calculations, only the differences $W_n = F_n(\infty) - F_n(r)$ are needed, and have the following form for the above-mentioned linear $\lambda_n$ approximation:

$$W_n = \frac{E_n^f(r) - \delta_n \alpha E_n^m(r)}{kT} - \frac{E_n^f(\infty) - \delta_n \alpha E_n^m(\infty)}{kT} + (1 + \delta_n\alpha)\ln\frac{D_{n0}}{D_n} + \delta_n\alpha(\lambda_{n2} - \lambda_{n1}) \int_{C_{A0}}^{C_A} \frac{(1-x)\,dx}{x + (\lambda_{n1} + x(\lambda_{n2} - \lambda_{n1}))(1-x)}, \tag{3}$$

where $\delta_n = 1$ for vacancies and $\delta_n = -1$ for interstitials, $E_n^f$ and $E_n^m$ are the point defect formation and migration energies, $D_{n0}$ and $D_n$ are the point defect diffusion coefficients in unirradiated and irradiated alloys respectively. When deriving Eq. (3), it was assumed that diffusivities of vanadium, $d_{Vv}$ and $d_{Vi}$ , are independent of alloy composition, but diffusivities $d_{Fev}$ and $d_{Fei}$ are linear functions of iron content.

In the present work, the calculations of SBF were made by this method with the profiles given by Eq. (1) and $W_n$ from Eq. (3). Results of the model SBF calculations are shown in Figs. 1 and 2 together with $B_{exp}$ values determined from ion irradiation data (present work) and from neutron irradiation data by Matsui et al. [15]. Since the data on dose dependence of swelling and sink strengths for voids and dislocations were not reported in Ref. [15], only crude estimations of $B_{exp}$ were made for the case of neutron irradiation, assuming the swelling V–Fe alloys is a linear function of dpa and the ratio of sink strengths for voids and dislocations is unity (see Ref. [3]). The letter estimations should be corrected accounting for the microstructural data for neutron irradiated V–Fe alloys.

In Fig. 1, the results of calculating the SBFs are shown for the case of segregation-free dislocations. Curve 1 was obtained using the composition independent values of $\lambda_v$ ($\lambda_{v1} = \lambda_{v2} = 0.22$) and $\lambda_i$ ($\lambda_{i1} = \lambda_{i2} = 0.1$). Curve 2 corresponds to the case when $\lambda_v$ is the linear function of iron concentration ($\lambda_{v1} = 0.22,\ \lambda_{v2} = 2.85$), but $\lambda_i$ is constant ($\lambda_{i1} = \lambda_{i2} = 0.1$). Curve 3 shows the SBF behavior when both $\lambda_v$ and $\lambda_i$ are linear functions of composition ($\lambda_{v1} = 0.22,\ \lambda_{v2} = 2.85,\ \lambda_{i1} = 0.1,\ \lambda_{i2} = 0.8$). Curve 4 was obtained when taking into account that the point defect formation and migration energies (in eV) depend on iron content parabolically: $E_v^f = 2.2\text{-}0.2\ C_{Fe}^2$, $E_v^m = 1.1 - 0.5\ C_{Fe}^2$, $E_i^f = 4.2 - 1.2\ C_{Fe}^2$, $E_i^m = 0.1 + 0.2\ C_{Fe}^2$ (see Ref. [3]) for constant values of $\lambda_v$ and $\lambda_i$ ($\lambda_{v1} = \lambda_{v2} = 0.22,\ \lambda_{i1} = \lambda_{i2} = 0.1$). It can be shown from Fig. 1 that the results of calculations are extremely sensitive to the compositional dependence of both the

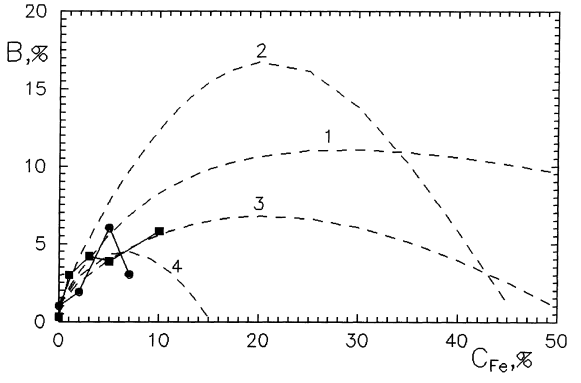


Fig. 1. Experimental (circles-this work, squares-from Ref. [15]) and predicted dependencies of SBF on iron concentration in V–Fe alloys in the case of segregation-free dislocations: (1) $\lambda_{v1} = \lambda_{v2} = 0.22,\ \lambda_{i1} = \lambda_{i2} = 0.1$; (2) $\lambda_{v1} = 0.22,\ \lambda_{v2} = 2.85,\ \lambda_{i1} = \lambda_{i2} = 0.1$; (3) $\lambda_{v1} = 0.22,\ \lambda_{v2} = 2.85,\ \lambda_{i1} = 0.1,\ \lambda_{i2} = 0.8$; (4) $\lambda_{v1} = \lambda_{v2} = 0.22,\ \lambda_{i1} = \lambda_{i2} = 0.1$, parabolic dependence of point defect activation energies on iron content.

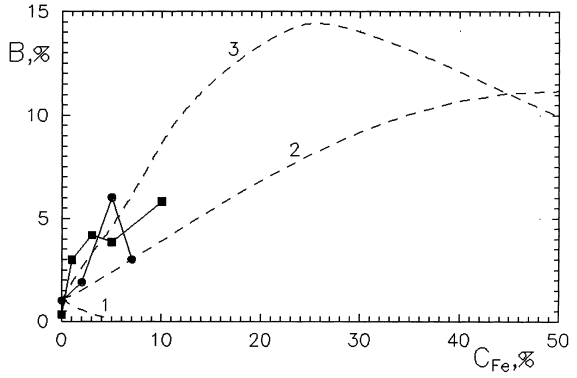


Fig. 2. Experimental (circles-this work, squares-from Ref. [15]) and predicted dependencies of SBF on iron concentration in V–Fe alloys for constant $\lambda_v$ and $\lambda_i$ in the case of velocity independent RIS around dislocations: (1) point defect activation energies independent of alloy composition, (2) linear dependence and (3) parabolic dependence of point defect activation energies on iron content.

point defect activation energies and alloy component diffusivities.

In Fig. 2, the results of calculating the SBFs are shown for another case when RIS around dislocations does not depend on climb velocity. All curves in Fig. 2 correspond to the case of both $\lambda_v$ and $\lambda_i$ being independent of alloy composition. Curve 1 shows the SBF in the case when point defect formation and migration energies do not depend on iron content. Curve 2 corresponds to the point defect activation energies being linear functions of iron content as follows: $E = E_V - (E_V - E_{Fe})C_{Fe}$, where $E_V$ and $E_{Fe}$ are the activation energies in pure V and Fe, respectively. Curve 3 was found assuming the following dependence of the activation energies on alloy composition: $E = E_V - 2(E_V - E_{Fe})C_{Fe} + (E_V - E_{Fe})C_{Fe}^2$. As seen from Fig. 2, it is possible to fit the SBF to $B_{exp}$ by an appropriate choice of point defect activation energy dependencies on alloy composition. Unfortunately, such dependencies are not available for the present.

From the calculations made, one can conclude that experimental data on void swelling and SBF dependence on iron content in V–Fe alloys can be explained within the framework of the RIS theory in both of the extreme cases considered: when RIS occurs or does not occur around dislocations.

## 4. Conclusions

In V–Fe alloys irradiated at 625°C with 50 keV $V^+$ ions to several doses up to 40 dpa, both the void swelling and bias factor reveal maxima at about 5 at.% Fe.

Analytical expressions for steady state component profiles around point defect sinks in irradiated binary alloys have been derived in the case when both the ratios of component diffusivities via vacancy and interstitial mechanisms are linear functions of alloy composition.

The method of 'constant boundary concentration' for the calculation of SBF has been generalized with an objective to take into account the dependence of component diffusivities as well as point defect formation and migration energies on alloy composition.

Experimental data on the dependence of void swelling and SBF on alloy composition in V–Fe alloys irradiated with vanadium ions can be described within the framework of the RIS theory if appropriate dependences of point defect formation and migration energies on iron content are chosen.

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