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The voids kinetics during diffusion process

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HIGHLIGHTS

- Voids growth due to the drift velocity and vacancy migration.
- Experimental results in Fe–Pd and β-NiAl–Cu systems are shown.
- Radius of the void is estimated.
- Two-dimensional approach is proposed.

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ABSTRACT

In this paper it is shown that the small voids, cracks or inclusions may act as sinks for vacancies or sources for interstitial atoms if the density is very close to equilibrium by numerical simulations. The two dimensional model is presented based on the generalized Darken concept. The void radius is estimated and compared with experimental results in Fe–Pd and β-NiAl–Cu systems. During the studies the following question arises: where is the most favorable place of the void formation. This question will be discussed.

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1. Introduction

The Kirkendall experiment [1] has focused new attention on the mechanism of diffusion in metallic systems. After his experiment there is no longer doubt that a marker shift occurs in diffusion couples and indicates the vacancy mechanism of the diffusion [2]. The first purely macroscopic formalism to explain the Kirkendall phenomena was presented by Darken [3]. He suggested that each component, say A and B, in a couple must be given its own characteristic diffusion coefficient. This formalism leads to the Kirkendall shift when the diffusion coefficients differ. The porosity plays no role in Darken formalism, since it is assumed that the lattice will swell or shrink in such a way as to maintain the equilibrium density [2]. Bardeen [4] demonstrated that Darken's equation can be derived with the use of the vacancy theory if one assumes that there is a sufficient density of source and sinks of vacancies. The first detailed analysis of the porosity formation was presented by Seitz [2]. The porosity has been observed in diffusion couples demonstrating the Kirkendall effect. It was shown, that the holes were formed by the precipitation of supersaturated vacancies produced by unequal diffusion currents of the Kirkendall effect. Seitz calculated the number of the vacancy jumps during their lifetime (about 10^{11}). The first experimental evidence that the holes form from a supersaturated solution by a process of heterogeneous nucleation was presented by Balluffi [5].

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He has shown, that required relative excess vacancy concentration for hole formation in most specimens is probably <0.01. Balluffi suggested that the holes will form in all systems when vacancies are pumped into any small region of the diffusion zone at the rate of about 10^{16} /s/cc.

In our last papers we have shown the model which allows to calculate the average void's growth [6,7]. In this paper, after Seitz, we will show (by 2 dimensional calculations) that the small voids, cracks or inclusions may act as sinks for vacancies or sources for interstitial atoms if the density is very close to equilibrium. We will present, that Darken's theory can be applied for void's growth calculation in 2 dimensional calculations when the initial small voids (cracks) are introduced. Moreover in this paper the analytical expression of the void's radius will be presented. The simulation results are compared with experiments in Fe–Pd system and the radius of the voids in βNiAl–Cu system is estimated.

2. Voids' growth and its radius

The mathematical description of the voids' growth during multi-component diffusion process will lie on the generalized Darken approach. The core of the model is the mass conservation law for each component:

$$\frac{\partial N_i}{\partial t} + \nabla \cdot J_i = 0 \tag{1}$$

where N_i is the molar ratio of the ith component, J_i denotes its overall flux. The overall flux, after Darken, is a sum of the diffusion and drift fluxes:

$$J_i = j_i + N_i \upsilon^{drift} \tag{2}$$

the diffusion flux, j_i can be determined by e.g. Fick's first law:

$$j_i = -D_i^I \nabla N_i \tag{3}$$

where D_i^I is the intrinsic diffusion coefficient. The equation for the change in the vacancy concentration over time is defined as:

$$\frac{\partial N_v}{\partial t} + \nabla \cdot j_v + \frac{N_v - N_v^{eq}}{\tau_v} = 0 \tag{4}$$

where N_v is the vacancy molar fraction, j_v is the vacancy flux. N_v^{eq} and τ_v denote the vacancy equilibrium molar fraction and relaxation time, respectively. The strength of sinks can be characterized by the mean free path of vacancies $L_V \approx \sqrt{D_V \tau_V}$ [8]. In Eq. (4) term $N_V \upsilon^{drift}$ is small, since the vacancy ratio is small. Thus, we can neglect this term. The vacancy flux is a sum of the fluxes of the components, mainly:

$$\sum_{i=1}^{r} j_i + j_v = 0 \;\Rightarrow\; j_v = \sum_{i=1}^{r} D_i^I \nabla N_i. \tag{5}$$

The drift velocity, υ^{drift}, introduced in Eq. (2) can be determined by volume continuity equation (after summation of Eqs. (1) for all components and assuming that the vacancy concentration does not influence the drift velocity) by solving the Poisson equation:

$$\nabla \cdot \left(\sum_{i=1}^{r} j_i + \upsilon^{drift} \right) = 0. \tag{6}$$

The void's radius depends on the concentration of the vacancies and its diffusion coefficient. In this paragraph we have shown the analytical expression for the void's radius. We will start our analysis basing on the expression derived by Gusak and Storozhuk [8] generalized for multicomponent mixtures:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = D_V \left(N_V - N_V^{eq}\right) \left(\frac{1}{L_V} + \frac{1}{R}\right) \tag{7}$$

where: L_V denotes the mean free path of vacancies, N_V and N_V^{eq} are the vacancy concentration and equilibrium vacancy concentration ($N_V^{eq} = 0.0002$), respectively. The vacancy diffusion coefficient is $D_V = \frac{\sum_{j,i=1}^{r} D_i^I D_j^I}{N_V \sum_{\substack{i,j=1 \\ i \neq j}}^{r} D_i^I N_j}$ (for binary systems the vacancy diffusion coefficient is reduced to the following form: $D_V = \frac{D_1^I D_2^I}{N_V \left(D_1^I N_2^+ D_2^I N_1\right)}$). Above expression can be solved numerically to determine the radius of the void (note, that when the initial stage for void formation is neglected this equation can be reduced to the following form $\mathrm{d}R/\mathrm{d}t = D_V \left(N_V - N_V^{eq}\right) 1/L_V$ and solved by simple Euler schema $R = D_V \left(N_V - N_V^{eq}\right) 1/L_V \, t + R^{\min}$. The $R^{\min}$ denotes the minimal void's radius ($R^{\min} = 10^{-8}$ m) and t is the experimental time in seconds). Finally for the binary A–B system the following set of the equations should be solved:

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