



The interdiffusion in copper-nickel alloys

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ABSTRACT

In this paper the interdiffusion process and Frenkel effect (Kirkendall porosity) are studied in Ni-Cu and NiAl-Cu systems at 1273 K. The generalized Boltzmann-Matano method is used for calculation of the intrinsic diffusion coefficients as a polynomial function in the whole composition range. The calculated interdiffusion coefficient in Cu-Ni diffusion couple decrease with increasing Ni content. The total decrease of interdiffusion coefficient exceeds two orders of magnitude. The equation for the void growth rate is obtained. The experimental results of diffusion and voids formation are analyzed. The voids radii is estimated and compared with experiments.

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1. Introduction

High oxidation resistance, mechanical properties, low density and high melting temperature of the NiAl intermetallic compound have attracted scientific attention to this material [1]. The B2 type offers potential as a highservice-temperature material, for example, in aero gas turbine engines [2,3]. However, many application of NiAl would require access to suitable joining technologies [3]. The pure Cu can be used for interlayer during diffusional bonding process [2]. The copper shows extensive solid solubility in both NiAl and nickel [4].

The essential is the knowledge about high temperature diffusion for better understanding of the mechanical properties. The scientists nowadays debate about the diffusion mechanism in B2 compounds. From Rabkin works, we know, that the usual mechanism involving jump to the nearest neighbor vacancy is improbable in B2 compounds as that migration may locally destroy the chemical order [1]. Recent data of Herzig and co-workers on Ni tracer diffusion in NiAl support the triple defect mechanism of Ni diffusion [5].

The main kinetic parameter describing the diffusion in multi-component system is the intrinsic diffusion coefficient. In binary systems the Boltzmann-Matano (B-M) analysis [6] can be used for determination of this parameter. However in ternary and higher

order systems the B-M method is invalid. In our previous paper we have shown the generalization of B-M analysis [7,8]. The key idea is the knowledge about the position of Kirkendall plane. This additional data allows for determination of the intrinsic diffusion coefficient at the position of the markers. Then, assuming, that the logarithm of diffusivities are determined by polynomial function (at least of order 2) the diffusion coefficients for each component in multicomponent diffusion couple can be approximated [7].

During the interdiffusion process, due to the differences in diffusion coefficients numerous phenomena occur: the lattice shift, the stress generation and relaxation, the nonequilibrium distribution of vacancies and voiding [9–13]. Voiding is a result of relaxation of pure material or alloy supersaturated with vacancies. The relaxation of vacancy subsystem can proceed by joining of vacancies into voids [14,15].

In this work the interdiffusion in Cu-Ni and Cu-NiAl at the temperature 1273 K will be investigated. Thus, the objective of this work is to determine the kinetic parameters - intrinsic diffusion coefficients. Moreover the voids radii - the Frenkel and Kirkendall effects will be investigated in both experimental and numerical analysis.

2. Voids growth and its radius

The void radius depends on the concentration of the vacancies and its diffusion coefficient. The analysis bases on the expression derived by Gusek and Storozhuk [16]:

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$$\frac{dR}{dt} = D_V (N_V - N_V^{eq}) \left(\frac{1}{L_V} + \frac{1}{R} \right) \quad (1)$$

where: L_V denote the mean free path of vacancies, N_V and N_V^{eq} are the vacancy molar fraction and equilibrium vacancy molar fraction ($N_V^{eq} = 0.0002$), respectively. The generalized vacancy diffusion

coefficient $D_V = \frac{\sum_{j=1}^r D_i^j}{N_V \sum_{i=1}^r D_i^j N_i}$ where D_i^j denotes the intrinsic diffusion coefficient of the i -th component.

The equation for the time evolution of the vacancy concentration is defined as:

$$\frac{\partial N_V}{\partial t} + \text{div} j_V + \frac{N_V - N_V^{eq}}{\tau_V} = 0 \quad (2)$$

where N_V is the vacancy molar fraction, j_V is the vacancy flux. The 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 $L_V \approx D_V \tau_V$ [16]. The vacancy flux is defined as a sum of the diffusion and drift parts:

$$j_V = j_V^d + N_V v^{\text{drift}} \quad (3)$$

In Equation (3) term $N_V v^{\text{drift}}$ is small ($N_V v^{\text{drift}} \approx 0$), since the vacancy ratio is small ($N_V \ll N_i$) and can be neglected.

Already from Darken analysis, we know that the overall sum of the fluxes should equal zero. Thus the vacancy flux is a sum of the fluxes of the components, mainly:

$$j_V = \sum_{i=1}^r D_i^j \text{grad } N_i \quad (4)$$

where N_i is the molar ratio and D_i^j is intrinsic diffusion coefficient of the component.

Moreover, voids growth during multi-component diffusion process will lay on the generalized Darken approach. The core of the model is the mass conservation law for each component:

$$\frac{\partial N_i}{\partial t} + \text{div} \left(-D_i^j \nabla N_i + N_i \sum_{i=1}^r D_i^j \nabla N_i \right) = 0 \quad (5)$$

2.1. Solution - numerical method

The numerical treatment of the method comes down to solving

$$D_i^j (N_i^* = N_i^*(t, x_K)) = -\frac{1}{2t} \left(\frac{\partial x}{\partial N_i} \right)_{N_i^*} \left[x_K (N_i^* - N_i^{-\infty}) - \int_{-\infty}^{x_K} (N_i - N_i^{-\infty}) dx + (N_i^* - N_i^{-\infty}) \frac{x_K}{2t^{1/2}} \right], \quad i = 1, 2, \dots, r \quad (9)$$

a set of ordinary differential equations $dy/dt = f(y, t)$. Thus, the explicit Euler method can be used - the passage from time t_k to $t_{k+1} = t_k + \Delta t$ was carried out by one-step evaluation. Moreover, the advancement $t_k \rightarrow t_{k+1}$ was executed in which $y_{k+1} = y_k + \Delta t \cdot f(y_k, t_k)$ with $f(y, t)$ evaluated for $t = t_k$ and $y = y_k$.

The method of lines to solve numerically the ODEs system

resulting from the space discretization was used [17]. The uniform grid, contained 100 mesh points, was used and the concentrations were defined at points x_k . The space derivatives in the equations were approximated by two point (first derivative) and three point (second derivative) uniform finite differences:

$$\frac{\partial \Phi}{\partial x}(x_k, t) \approx \frac{x_{k+1} \Phi - x_{k-1} \Phi}{x_{k+1} - x_{k-1}} \quad (6)$$

and

$$\frac{\partial^2 \Phi}{\partial x^2}(x_k, t) \approx \frac{x_{k+1}^2 \Phi(x_k - x_{k-1}) + x_{k-1}^2 \Phi(x_{k+1} - x_k) - x_k^2 \Phi(x_{k+1} - x_{k-1})}{0.5(x_{k+1} - x_{k-1})(x_{k+1} - x_k)(x_k - x_{k-1})} \quad (7)$$

Both were calculated from Taylor expansion.

The time integrator, used in the present computations to solve the ODEs, was based on the adaptive step size Runge-Kutta-Fehlberg method. The six evaluations of the functions from the fifth-order Runge-Kutta algorithm were used to make the another combinations implemented in the fourth-order Runge-Kutta method. A difference between these two estimates served as an estimate of the truncation error. Hence, the step size was adjusted [18].

2.2. The initial and boundary conditions

The remaining initial data necessary in the calculations include: terminal composition of the diffusion couple (representing the terminal points of the diffusion path), diffusion coefficients of the components in all phases, processing time and temperature - results section.

The boundary conditions in presented model should be applied for the fluxes of the components in each phase. Mainly, the closed system is assumed, thus the diffusion fluxes at the boundary equals zero:

$$j_i^d = -D_i^j \nabla N_i = 0 \text{ at the boundary} \quad (8)$$

the two-phase zone formation is not introduced into the model.

The above set of equations allows calculating the voids and concentration time evolution in the system where diffusion coefficients are known. In this paper the intrinsic diffusion coefficients were determined from the Ni-Cu experimental results with Generalized Boltzmann-Matano analysis. This method allows determination of the diffusivities in multicomponent systems where the Kirkendall position is known. In this method the intrinsic diffusion coefficient can be estimated at the Kirkendall plane position as [8]:

where x_K denotes the Kirkendall plane position, hence position for which intrinsic diffusivity is calculated.

Thus, the unique logarithm of intrinsic diffusivity as a polynomial (parabolic) function of molar ratio can be approximated. The comparison of the original BM and GBM method in Ni-Cu system is presented in results section.

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