Physica A 509 (2018) 265–274

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

The diffusion path model in a ternary multiphase system

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HIGHLIGHTS

- The Diffusion Path (DP) method.
- Diffusion path in open systems.
- Sequence of intermetallic phases generation.

ARTICLE INFO

Article history:
Received 26 February 2018
Received in revised form 6 June 2018
Available online xxxx

Keywords:
Diffusion
Intermetallic compounds
Entropy production
Phase competition

ABSTRACT

In this paper the Diffusion Path (DP) method is presented. The method allows for the determination of the diffusion path during a reactive diffusion process. The initial conditions of the method are the phase diagram, diffusion coefficients in the phases and initial composition of the diffusion couple. The method allows for the determination of the diffusion path—the intermetallic phases generated during the diffusion process and the order of their generation. The results of the DP method are compared with the experimental results obtained for the Ti-NiCu diffusion couples with various Ni to Cu content ratio.

1. Introduction

The exposure of metallic elements to high temperature results in a number of processes. First of all, the diffusion of the alloying elements is accelerated. The latter causes formation of new intermetallic phases, which most likely possess different mechanical and physical properties; therefore, their formation can substantially alter the overall compound properties. The numerical characteristic of the physical process is a critical field. It allows for modeling the physical parameters at high temperature. Therefore, also the modeling of the lifetime for the real components is possible.

The diffusion in two- and multiphase zones differs substantially from the diffusion in the single phase and can lead to the effects such as zig-zag diffusion, horns at the diffusion path, and jumps of the concentrations without a typical interface boundary [1–3]. Such diffusion processes were demonstrated in the Ni–Cr–Al system. There were many theoretical as well as experimental studies describing the phase diagrams for the latter system [4–19]. However most of the research is confined to Ni-rich corner at high temperatures, i.e., above 1273 K. Most of the numerical investigations were made by the DICTRA software [20]. The software was applied to calculate the interdiffusion in the two-phase zone where the zig-zag diffusion path was generated. However, none of the manuscripts solves the more general problem of the uniqueness of the diffusion path during the process.

In this paper the progress in the calculation of the diffusion process is presented. For the first time the Diffusion Path method is formulated and used for the determination of the diffusion path during the ternary reactive diffusion process.

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https://doi.org/10.1016/j.physa.2018.06.020
0378-4371/

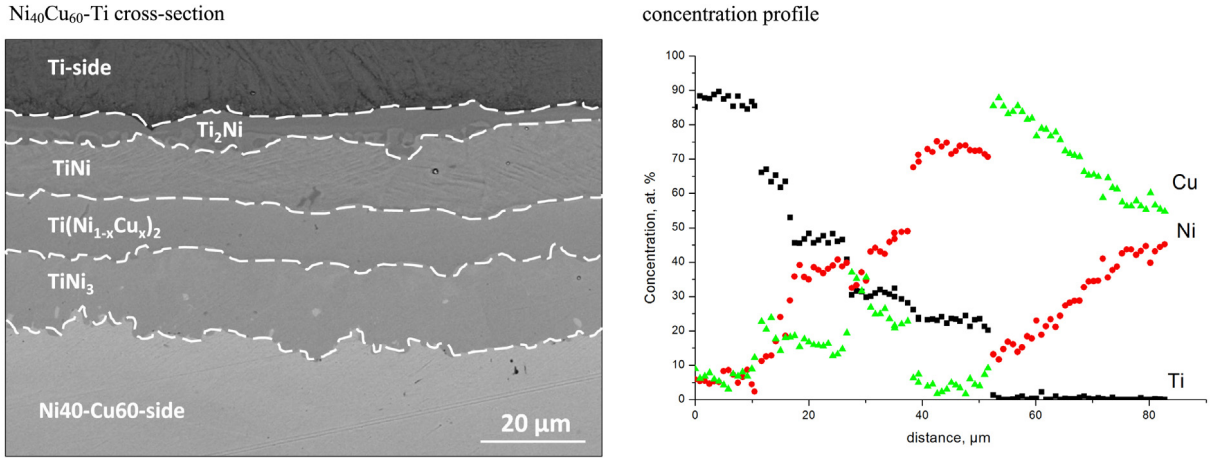

Fig. 1. The cross-section and concentration profile of $Ni_{40}Cu_{60}$-Ti sample after diffusion at 1123 K for 160 h.

Moreover, the competition problem is also described, namely the order of the phase generation during the mass transport. The results of the approximation method are compared with experimental results obtained for Ti-NiCu diffusion couples. The Ti-NiCu system was chosen due to its ability to generate many intermetallic phases during the process. It is shown that the method determines the order of formation of all phases properly. However, at the moment, the method cannot determine the concentration profiles and generation of two-phase zones. To determine the concentration profile the additional equations should be introduced, namely the mass conservation law at the boundaries of each phase [21].

2. Results

In this section the results of the calculations will be presented. The diffusion path will be determined from mathematical lemmas. Moreover, the experimental results will be presented to verify the computations in the NiCu-Ti system.

2.1. Experiments

The rods of CuNi high purity model alloys (99.9% purity) with nominal compositions of 40 at.% Ni + 60 at.% Cu and 60 at.% Ni + 40 at.% Cu, respectively, were provided by the company Goodfellow from England. The disk-shaped samples were cut from the ingot by spark erosion. The surfaces of the disks were ground and polished to mirror finish using SiC papers and diamond pastes up to 0.25 µm particle size. The high purity Ti disks (99.9% purity) were also cut from the rod and polished according to the procedure mentioned above. Such prepared disks were connected in molybdenum holder to form the diffusion couple. The diffusion couples were annealed in a tube furnace in a protective argon atmosphere at 1123 K for 160 h. After annealing, the disks were cut in the middle and then metallographic cross-sections were prepared from one half. No Kirkendall–Frenkel effect was observed on the microphotographs. The samples were then analyzed to obtain the concentration profiles in the bulk interdiffusion zone by the SEM equipped with EDS. The experimental results of the diffusion are shown in Figs. 1 and 2.

The concentration profiles allowed for the determination of the diffusion paths on the isothermal ternary phase diagram, Fig. 3.

The diffusion paths in both samples started in γ phase (Ni-Cu phase), then the atoms jump to the $TiNi_3$ phase. After that, both diffusion paths cross the τ_1 ($Ti(Ni_xCu_{1-x})_2$) and finally jump to the TiNi phase. Then, in the case of $Ni_{40}Cu_{60}$, the diffusion path goes through Ti_2Cu while in case of $Ni_{60}Cu_{40}$, the sample jumps to the Ti_2Ni phase.

Thus, the question is **why do diffusion paths connected at the beginning in pure Ti and at the end in $Ni_{40}Cu_{60}$ and $Ni_{40}Cu_{60}$ (small difference) differ?**

2.2. Calculations

The diffusion path (DP) method allows for the determination of the diffusion path in the multiphase ternary system (at present the concentration profile is not approximated). The following assumptions hold:

1. The diffusion does not form the two-phase zones—thus the neighboring phases are in thermodynamic equilibrium.
2. The initial composition of the diffusion couple is known.
3. The conodes are evenly distributed between phase boundaries.