



Fundamentals of interdiffusion microstructure maps for dual-alloy systems

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Abstract

Interdiffusion microstructure maps (IMMs) are drawn on isothermal phase diagrams. They predict how the interdiffusion microstructure varies in a dual alloy when one alloy composition is fixed while the other is varied across a region of the phase diagram. The microstructure is defined in terms of its layers and the velocity direction of boundaries between layers. Previous work involved maps based on experimental, calculated and simulated interdiffusion microstructures. In the current work IMMs for four model systems were obtained from phase field simulations. The IMMs in this study differ from previous work in that one contains a more complicated IMM with seven areas separated by seven lines that meet at a seven-line node and one contains a less complicated IMM with only one area. Also, it was found that the microstructures at all nodes investigated to date are similar by having the microstructure of the initial dual alloy. During interdiffusion treatments the initial interface is stationary and only the amounts of phases on either side of the interface will vary with time. A list of fundamental properties of IMMs is given that combines findings from the current and previous work. In the list are three mechanisms by which microstructures change. One of these had not been seen before. In this mechanism an inversion of the microstructure occurs as the composition crosses from one side to the other of a two-phase region. These fundamentals are the foundation on which IMMs are constructed and can be a guide for their interpretation.

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1. Introduction

When two alloys are in contact they become a dual alloy. At elevated temperatures dual alloys can interdiffuse and react to form new phases and new microstructures in the vicinity of the contact interface. The affected volume is called the “interdiffusion zone” and the new microstructure formed is called the “interdiffusion microstructure”. One of the salient features of an interdiffusion microstructure is its division

into microstructurally distinctive layers in terms of the phases present. The interdiffusion microstructure can be different from the starting microstructure, thus changing the properties of the dual alloy system. It follows that the microstructure and how it varies with the dual alloy composition have importance to multi-alloy system design.

An interdiffusion microstructure map (IMM) is a graphical representation drawn on a two-dimensional (2-D) isothermal phase diagram. It shows how the interdiffusion microstructure changes when one dual-alloy composition varies while the other dual-alloy composition is fixed. As such it has relevance to a number of obvious applications such as high temperature coatings and metal joining, as well as to solar panels [1–3] and multi-layer composites

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[4,5]. Accordingly, the objective of this work is to describe the fundamental features of such diagrams, drawing on the current and previous work, in order for IMM to be more readily constructed and interpreted.

There can be different types of interdiffusion microstructures on an IMM. The types are characterized by phases in the layers and the movement direction of the layer boundaries. The types can be described by a short-hand notation introduced in Ref. [6]. For example, an interdiffusion microstructure described by the notation $\gamma + \beta | \gamma + \beta > \gamma' > \gamma + \gamma'$ indicates four distinctive layers within the interdiffusion zone (i.e., $\gamma + \beta$, $\gamma + \beta$, γ' and $\gamma + \gamma'$ layers). The caret dividing two adjacent layers in the short-hand notation indicates the moving direction of the boundary relative to the initial interface of the dual alloy, while a vertical line “|” indicates a stationary boundary at the initial interface. When the interdiffusion zone is much smaller than the dual alloys and interdiffusion is diffusion-controlled, then the boundaries always move away from the initial interface.

Previous work has shown that a particular type of interdiffusion microstructure can be found over an area of compositions on a 2-D phase diagram section. The areas for different types are contiguous, meeting along a line. The lines can be straight or curved and form nodes where three or more lines meet. Special microstructures are associated with both the lines and the nodes.

Meisenkothen and Morral [7] found five interdiffusion microstructures on their experimental IMM for Ni–Cr–Al dual alloys in which the fixed alloy contained $\gamma + \gamma'$ phases and the varied alloy contained $\gamma + \beta$ phases. The five microstructures occurred in five areas of the $\gamma + \beta$ region of an isothermal section of the phase diagram. The areas were separated by five lines that met at a node. It was shown that the lines had to meet at the node in order to satisfy the fundamentals of IMM.

Boettinger et al. [8] found three interdiffusion microstructures on a model three-component IMM in which the fixed alloy contained $\alpha + \beta$ phases and the varied alloy contained just the α phase. The IMM was derived using a simplified phase diagram and ternary kinetic equations for velocities between layers. The three areas were separated by three lines that met at a node.

How one interdiffusion microstructure changes to another was analyzed in both papers. Both found that there are two mechanisms for microstructures changing from one type to another. In one mechanism a boundary velocity changes from positive to negative. In the other, velocities of interfaces on either side of a layer become equal [7,8]. In this case, the thickness of the layer will become zero due to the equal velocities of the two interfaces and thus the microstructure will change to a new type which does not form such a layer. Note that the above findings on model systems as well as the conclusions made in this paper are based on the assumption of local equilibrium and infinite dual alloys.

Following Ref. [7], the line separating area I and II on the IMM will be referred to as line I/II in accord with

the areas on either side of the line. And the boundary velocity will be denoted by v with the boundary type indicated on the superscripts. For example, the velocity of boundary $\alpha > \beta$ will be denoted by $v^{\alpha > \beta}$.

2. Theory and simulation

Model thermodynamic and kinetic properties were used in a phase field model to simulate interdiffusion microstructures in four model systems, S1–S4. These microstructures were the basis for drawing IMM and analyzing the mechanisms by which one microstructure changed to another.

2.1. The thermodynamic model

In all four systems, elements A, B and C were assumed to form regular solutions. Therefore the free energy function of each system was:

$$G_m = RT(X_A \ln X_A + X_B \ln X_B + X_C \ln X_C) + I_{AB}X_A X_B + I_{BC}X_B X_C + I_{AC}X_A X_C + I_{ABC}X_A X_B X_C \quad (1)$$

where G_m is the molar free energy, R is the gas constant, T is the temperature, I_{AB} , I_{AC} , I_{BC} and I_{ABC} are regular solution interaction parameters and X_A , X_B and X_C are mole fractions of A, B and C.

2.2. The phase field model

In the phase field approach, any microstructure in a ternary system can be characterized by two composition fields X_B and X_C , which are spatially continuous and time-dependent. The temporal evolutions of the concentration of Elements B and C are obtained by solving the generalized Cahn–Hilliard diffusion equations under the assumption of constant molar volume V_m [9–11]:

$$\frac{1}{V_m} \frac{\partial X_B}{\partial t} = \nabla [M_{BB} \nabla (\mu_B - \mu_A - 2\kappa_{BB} \nabla^2 X_B - 2\kappa_{BC} \nabla^2 X_C)] + \nabla [M_{BC} \nabla (\mu_C - \mu_A - 2\kappa_{BC} \nabla^2 X_B - 2\kappa_{CC} \nabla^2 X_C)] \quad (2)$$

$$\frac{1}{V_m} \frac{\partial X_C}{\partial t} = \nabla [M_{CB} \nabla (\mu_B - \mu_A - 2\kappa_{BB} \nabla^2 X_B - 2\kappa_{BC} \nabla^2 X_C)] + \nabla [M_{CC} \nabla (\mu_C - \mu_A - 2\kappa_{BC} \nabla^2 X_B - 2\kappa_{CC} \nabla^2 X_C)] \quad (3)$$

in which t is time; μ_A , μ_B and μ_C are the chemical potentials of elements A, B and C, respectively (obtained from Eq. (1)); κ_{BB} , κ_{CC} and κ_{BC} are the gradient energy coefficients; and M_{BB} , M_{BC} , M_{CB} and M_{CC} are the chemical mobilities defined in the laboratory reference frame, which are related to the atomic mobilities β_k by the following equations [12,13]:

$$M_{ij} = \frac{1}{V_m} \sum_{k=1}^n (\delta_{ik} - X_i)(\delta_{jk} - X_j) X_k \beta_k \quad (4)$$

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