

Predicting Interdiffusion in High Temperature Coatings*

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Abstract: Interdiffusion can be a major cause of failure in coated parts that see service at elevated temperatures. Ways to measure the extent of interdiffusion and mathematical equations for predicting these measures are given. The equations are based on the error function solution to the diffusion equation and do not take into account variations of the diffusivity with composition. Also, when the substrate of the coating is multiphase, the equations do not take into account the precipitate morphology, but do take into account that precipitates can act as sinks or sources of solute as the average composition of the substrate varies. The equations are meant to be alloy design tools that indicate how changing substrate or coating chemistry will reduce the extent of interdiffusion.

Key words: interdiffusion; high temperature coatings; multicomponent diffusion; multiphase diffusion; coating design

Introduction

When high temperature coatings interdiffuse with their underlying substrate, the changes in composition can reduce the life of a part either by reducing the oxidation resistance of the coating or by compromising the mechanical properties of the coating and/or substrate. In such cases, interdiffusion predictions can be equated to life-time predictions.

Interdiffusion can be predicted using various methods depending on the accuracy needed and the databases available. Of these, the phase field method^[1] is the most accurate. It can predict microstructure morphology and phase constitution with remarkable accuracy, but requires the use of highly trained personnel and extensive computer time. A finite difference program, DICTRA^[2], requires less training and runs on a PC, but cannot take precipitate morphology into account. A third option is to estimate interdiffusion

using mathematical equations. That is the option to be discussed herein. The equations are less precise because they normally must assume that all kinetic parameters are constant across the interdiffusion zone and that precipitates can only act as point sources or sinks of solute. However, their simplicity can make them a valuable tool for alloy and coating design.

In the following discussion, three measures of interdiffusion will be defined: the diffusion distance, the amount of interdiffusion, and the composition of the coating surface. Regardless of the number of phases or components in the coating/substrate system, there are various approximations that can predict these measures. Therefore, even in the case of a two-phase, $\gamma+\beta$ MCrAlY coating on a $\gamma+\gamma'$ nickelbase superalloy that may contain five or more components, one could still use the single-phase equation to obtain a first approximation.

1 Diffusion Equation

The fundamental equation used to model diffusion is the well known differential equation^[3] for the variation of concentration, C , with distance, x , and time, t :

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$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial C}{\partial x} \quad (1)$$

When dealing with coating problems, it is helpful to normalize Eq. (1) by multiplying both sides by the initial coating thickness squared to create normalized variables^[4]. These are useful when plotting data that are obtained from samples having coatings with different initial thicknesses, x_0 . However, in the present work, there is no advantage to normalizing the variables. Therefore, solutions will be written explicitly in terms of x , x_0 , and t . Also Eq. (1) will be simplified to:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2)$$

by assuming that the diffusivity, D , is constant. Equation (2) is Fick's Second Law^[3].

For an n -component system, the same equation applies except that the concentration, C , is an $(n-1)$ -dimensional column vector and the diffusivity, D , is an $(n-1) \times (n-1)$ property matrix. In what follows the "rounded bracket notation"^[5] will be used with column vectors written as $[C]$ and square matrices as $[D]$. Rows and columns of square matrices will be written as (D_i) and $[D_i]$, respectively. The subscript i is a number which indicates which row or column is involved.

2 Measures of Interdiffusion

Three measures of interdiffusion can be calculated based on error function solutions to Eq. (2). One is the diffusion distance, x_D , which for tracer atoms is related to the root-mean-squared distance traveled by a tracer atom in time t . In terms of the error function solution, x_D can be equated to the distance where the error function argument, $x/(2\sqrt{Dt})$, is one, i.e., when $\text{erf}(1)=0.84$. Considering that the error function varies between 0 at the origin and 1 at infinity, it follows that the diffusion distance gives an estimate of where the majority of interdiffusion has occurred. The diffusion distance is illustrated in Fig. 1 on a schematic concentration profile.

A second measure of interdiffusion is the amount of solute that has crossed the coating/substrate interface in the diffusion time, t_D . It is illustrated in Fig. 1 by the cross-hatched area, S . A separate value is obtained for each solute and the values can be positive or negative.

A negative value corresponds to solute leaving the coating, as illustrated in Fig. 1. A positive value indicates that solute is entering the coating from the substrate. Related measures of the amount of interdiffusion are obtained by adding absolute values of S for each solute and the solvent^[6] or by adding squares of S for each component in the alloy^[7].

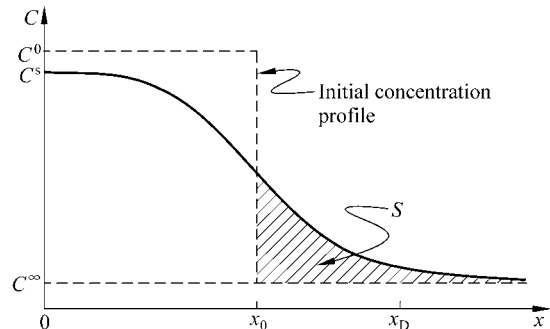


Fig. 1 Concentration profile of a same-phase, coating/substrate system after interdiffusion illustrating three measures of interdiffusion: the diffusion distance, x_D , the amount of interdiffusion, S (cross-hatched area), and the concentration at the coating surface, C^S .

A third measure of interdiffusion is the concentration of components at the surface, C^S . This concentration varies between the initial coating concentration, C^0 , and the final concentration reached, C^F , once the coating has equilibrated with the substrate. There is a value of C^S for each component in the alloy just as there was for S .

3 Same-Phase Approximation

It is possible for a high temperature coating and its substrate to have the same crystal structure, but it is unlikely that the diffusivity will be constant over the entire concentration range of the interdiffusion zone. However, the error introduced by not having a constant D can be minimized by selecting a diffusivity for the calculations that is representative of the concentration at x_0 . Equations for the three measures are given in the following.

3.1 Binary systems

The equations for binary systems can be found in standard textbooks on diffusion, for example Ref. [3].

$$x_D = 2r\sqrt{t_D} \quad (3)$$

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