A Numerical Model of Peritectoid Transformation

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A rigorous numerical model of the diffusion-controlled peritectoid transformation based on the iso-concentration contour migration method is presented here. The model is capable of considering the concentration dependence of diffusivity in the participating phases. The predictions from the model show an encouraging agreement with the experimentally determined peritectoid kinetics in the Zr-Al system and dissolution kinetics in the Ni-Mo diffusion couple. An extensive parametric study through the present formulation indicates that the peritectoid kinetics may be considerably affected by the diffusivities and phase field widths (in the equilibrium diagram) of the concerned solids. In this regard, the field width and diffusivity in the peritectoid phase appear to exert the most significant influence on the reaction rate. The numerically calculated transformation kinetics have been effectively rationalized by means of two dimensionless parameters, ϕ_1 and ϕ_2, which are functions of the concerned phase field widths and diffusivity in the product phase. In addition, these parameters enable prediction of the minimum time required for the completion of peritectoid transformation without going through any rigorous computation.

I. INTRODUCTION

PERITECTOID transformation in a binary system may be described as: $\alpha + \beta \rightarrow \gamma$, where all the participating phases are solids.[1] It is known that the product phase (γ) nucleates heterogeneously only at the α-β interface,[2–4] and grows along the interface to form an intervening layer between the reactants α and β. The transformation proceeds further by solute diffusion through this γ layer following extremely slow growth kinetics[5,6] and, therefore, seldom finds an industrial application. However, several important intermetallic compounds possessing attractive mechanical properties for advanced structural applications, *e.g.*, Zr$_3$Al,[7] may form through peritectoid change. Besides, peritectoid transformation plays a significant role in the evolution of order and decomposition of quasicrystalline phases in several binary/ternary alloys. For instance, order-disorder transformation from Ll$_2$ or Ll$_0$ to Al in near-stoichiometric Fe$_3$Pt is found to evolve from an intermediate phase transition involving the products of an intermediate reverse peritectoid transformation.[8] Similarly, evolution of order in Pd-based rare earth compounds may be attributed to the formation of a Pd$_3$RE phase (RE refers to rare earth elements like Gd, Sm, Ce, Dy, Y, and Eu) through peritectoid transformation.[9–13] These alloys may find applications in optoelectronic devices. Quasicrystalline phases in Al-Mn and Al-Cu-Fe alloys are also found to decompose by peritectoid transformation.[3,4,14]

So far only a limited number of investigations have dealt with the kinetics and mechanism of peritectoid transformation. Experimental studies on the Zr-A,[2,15] U-Si,[15,16] and Fe-Zr[6] systems have revealed that the transformation involves the following consecutive steps: (a) heterogeneous nucleation of γ at the α-β interface, (b) development of γ-rim around the primary particles, and finally (c) γ-rim thickening by concurrent migration of the α-γ and β-γ interfaces in opposite directions through a thermally activated growth process. Empirical analysis of the rim-thickening kinetics has yielded a time exponent of 2.5 in the early stage[16] and 1.5 in the later stage,[2,3,15,16] apparently indicating that the transformation involves both nucleation- and diffusion-controlled growth in the early stage and diffusion controlled growth alone without nucleation in the later stage. Structural refinement is reported to reduce the overall transformation time due to the increased nucleation rate and smaller diffusion distances involved for growth of the peritectoid phase.[17] However, these preliminary observations do not provide a qualitative or quantitative estimate of the kinetics of the transformation and the process parameters influencing the same. Because of the difficulties in generating experimental kinetic data due to the extremely slow growth rate, mathematical modeling may be a complementary investigating tool. In this regard, the only available formulation by Schulson and Graham[2] has employed separate mass balance equations at the respective interfaces of the peritectoid phase. Subsequent integration of the coupled equation has yielded an expression for growth rate of the form $W = B(T)t^{0.5}$, where $B(T)$ is a temperature-dependent parameter, W is the γ-rim thickness, and t is the transformation time. However, such an analysis ignores the time modulation of concentration profiles and impingement of the concerned diffusion fields. This simplification may introduce serious errors in the predicted kinetics at the later stage of the transformation, especially in the presence of closely spaced primary phase particles. The present article reports a more rigorous kinetic model of peritectoid transformation that considers the effects of both time modulation of concentration profiles and overlapping of diffusion fields on the reaction rate. The results have been validated by a suitable comparison with the relevant experimental data for the Zr-Al system reported in the literature.[2] Finally, an attempt has been made to identify the extent of influence of the process parameters on the transformation kinetics and to predict the time for completion of the peritectoid transformation through a suitable rationalization scheme.

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