Alloys oxidation from bi-velocity phase-field method; drift and Kirkendall effect in two-phase zone of ternary system

Bartek Wierzba[a], Patrycja Wierzba, Katarzyna Tkacz-Śmiech

Interdisciplinary Centre for Materials Modelling, FMSci&C, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland.

[a]bwierzba@agh.edu.pl

Abstract. We generalize Morral and Wagner models of alloy oxidation by combining phase field and bi-velocity (Darken) methods. In the proposed approach, local equilibrium (for diffusing components) at all interfaces of each moving phase boundary zone and deviations from the local equilibrium are considered. The method
allows simulating diffusive mass transport in every phase and computing kinetics of the process, concentration profiles, diffusion paths and Kirkendall effect. It can, in particular, predict a formation of two-phase diffusion zone. The solution obtained for a ternary diffusion couple with a two-phase zone provides: 1) diffusion path in the concentration triangle, 2) concentration profiles of the components and 3) drift-velocity distributions. As an example, the interdiffusion in the α|β ternary diffusion couple is modeled and the internal oxidation process discussed. The Kirkendall plane position is predicted and the profiles of the element concentrations are simulated for the considered system.

Keywords: Phase field method, bi-velocity method, mass transport kinetics, Kirkendall plane.