Modelling Cr depletion under a growing Cr2O3 layer on austenitic stainless steel: the influence of grain boundary diffusion

The oxidation behaviour of austenitic stainless steels in the temperature range 723–1173K is strongly influenced by the grain size of the oxidizing alloy. In this work the evolution of the concentration profiles of Cr, Ni and Fe in the substrate below a growing Cr2O3 layer is simulated with a Fisher-type numerical model, which takes both volume and grain boundary diffusion into consideration. The model is based on a two-dimensional control volume-based solution of Fick’s 2nd law for multicomponent diffusion and includes crossterm diffusion coefficients. The oxide layer is assumed to grow according to a parabolic rate law as a consequence of rate limiting diffusion of Cr cations through the oxide layer, the retraction of the oxide/alloy interface associated with the removal of Cr atoms from the substrate is included in the calculations. Numerically, the movement of the oxide/alloy interface is formulated such that the initial mesh can be used throughout the calculation. The calculated concentration profiles of the alloying elements emphasize the importance of grain boundaries in supplying Cr from the alloy to the growing oxide layer. For temperatures of 823 and 923K the simulations predict a significantly lower concentration of Cr atoms in the alloy at the oxide/alloy interface than that predicted by the conventional one-dimensional analytical Wagner solution, where an effective diffusion coefficient at the interface is assumed.

General information
Publication status: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Materials and Surface Engineering
Pages: 035009
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Modelling & Simulation in Materials Science and Engineering
Volume: 17
Issue number: 3
ISSN (Print): 0965-0393
Ratings:
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.16 SNIP 1.163
Web of Science (2009): Indexed yes
Original language: English
DOIs: 10.1088/0965-0393/17/3/035009
Source: orbit
Source ID: 241914
Research output: Contribution to journal › Journal article – Annual report year: 2009 › Research › peer-review