

A Coupled Thermodynamic-Kinetic Model for the Oxidation Kinetics of Ternary Nickel-Rich Alloys

R.T. WU¹, R.C. REED², K. KAWAGISHI³, AND H. HARADA³

¹ICYS, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba City, Ibaraki, JAPAN

²Dept of Metallurgy & Materials, University of Birmingham; Edgbaston, B15 2TT, UK

³High Temperature Materials Center, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba City, Ibaraki, JAPAN

Oxidation of engineering alloys is an important subject of study in the field of high temperature materials. Numerical modelling efforts of these alloys tended to be limited to single binary and dual-phase binary systems due to the difficulty in formulating the composition-dependent oxidation behaviour of ternary systems. Moreover, the competition between formation of oxides of different compositions also present a challenge in deriving numerical procedures.

In this work, a finite difference model has been developed to simulate the assumed one-dimensional diffusion and oxidation processes of a ternary alloy (i.e. Ni-Al-Cr) upon isothermal oxidation exposure with the aim of not only predicting, but also understanding the composition of the oxide scale and the concentration depth profile change in the alloy substrate. Application of the model to the oxidation of a Ni-27Cr-9Al (at %) ternary alloy shows that the formation of a NiAl₂O₄ oxide layer is not likely due to the thermodynamic constraint. The model also shows that the rate of aluminium supply from the bulk alloy towards the oxide reaction interface by inter-diffusion is considerably slower than the rate of aluminium consumption to form oxide during the initial transient oxidation stage. This is in fact, responsible for the aluminium depletion near the interface and its local concentration being essentially very close to zero.