

Modeling Internal Corrosion of High Temperature Alloys

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ABSTRACT

Internal oxidation and nitridation of high-temperature alloys often results in a deep penetration of coarse and sometimes needle-shaped precipitates that act as crack initiation sites, i.e., giving rise to an embrittlement of the surface layer. For well-defined, non-complex conditions, e.g., binary alloys AB, where the concentration of the oxide-/nitride-forming element B is not sufficient to form a superficial scale, internal oxidation and nitridation attack can be predicted by Wagner's theory of internal oxidation, taking the diffusive fluxes of the two reacting species into account. However, formation of precipitates of various thermodynamic stabilities, nucleation and growth effects, short circuit diffusion paths, and stress effects due to differences in the specific volumes, are not included in the original approach.

The present contribution provides an overview about the applicability of numerical approaches to the problem of internal corrosion. Easy to use and versatile solutions are the finite-difference method (FD) and the cellular automata concept (CA). While the FD method substitutes the differential quotients of the diffusion equation by means of differences, the CA concept considers diffusion of the reacting by jump and phase transformation probabilities between discrete cells having certain concentrations of the solvent, the solute and the nitride/oxide compound, respectively. It was shown that both approaches allow the prediction of (i) the internal precipitation depth of nitrides and oxides of different thermodynamic stabilities (FD), (ii) the transition to superficial scale formation (CA) and (iii) transport along various diffusion paths (FD and CA). Reaction kinetics are considered by the simultaneous thermodynamic equilibrium calculation ChemApp implemented in the numerical diffusion treatment