## Coupling diffusion and local equilibrium in modelling oxidation, nitridation and carburisation

S. Gorr, U. Krupp, H.-J. Christ Siegen University

## **Abstract**

High-temperature corrosion is generally known as a material degradation process that occurs at the surface of engineering components. In the case of internal corrosion the corrosive species penetrates into the material by solid-state diffusion leading to the formation of internal precipitates, e.g., oxides (internal oxidation), nitrides (internal nitridation) and carbides (carburization). It is known from numerous publications and technical failure cases that internal corrosion results in a strong deterioration of the materials properties, i.e., near-surface embrittlement or the dissolution of strengthening phases.

To predict such kinds of high-temperature corrosion phenomena a computer model termed INCORR has been developed that combines a numerical finite-difference approach to solve the diffusion differential equations with the thermochemistry software ChemApp. Hence, simulations to be carried out with INCORR account for the local chemical composition and phase composition, the material's microstructure, as well as the solubility and diffusivity of the corrosive species. By several examples it will be shown that the model has been applied successfully to simulate internal nitridation, carburization, and oxidation of high-temperature alloys.