Internal Oxidation and Nitridation of Hot Rolled Steels – A Theoretical Study and its Experimental Verification

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ABSTRACT

The properties and composition of polycrystalline specimens change tremendously during oxidation. While exposing metallic alloys to the ambient at high temperatures (e.g. in steel manufacture), the formation of oxides and nitrides along the grain boundaries and inside the grains is observed.

Our aim is to elucidate the sequence of formed reaction products and to theoretically predict the phase formation in binary and ternary iron alloys [1]. Thermodynamic assumptions are used to determine stability and spatial distribution of oxide [2] and/or nitride [3] phases in order to shine light on the processes which take place at high temperatures.

Simulations were composed as a subsequent 2-step based algorithm, consisting of element migration and chemical reactions, assuming local equilibrium under manufacturing conditions.

This has been realized by coupling the thermochemical subroutine *ChemApp* (GTT-Technologies, Germany) to the numerical program COMSOL (COMSOL Inc., USA). The results are presented as a two dimensional map, indicating the amount and spatial distribution of each considered phase in a given sample microstructure.

These findings will be compared with experimental measurements in low oxygen activity gases (i.e. no wustite formation on the sample) and characterized by surface sensitive techniques such as Scanning Electron Microscopy (SEM) or Energy Dispersive X-Ray Analysis (EDX).

Literature

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