



INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Düsseldorf, Germany

Monday, July 9, 4:30 p.m. **NEW ICAMS building Universitätstr. 90a, Room 0.08**
What do we know about Internal Oxidation in Hot Rolled Steels?
- A Theoretical Study and its Experimental Verification

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 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. Thermodynamic assumptions are used to determine stability and spatial distribution of oxide 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.

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 characterised by surface sensitive techniques such as Scanning Electron Microscopy or Auger Electron Spectroscopy (AES).

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