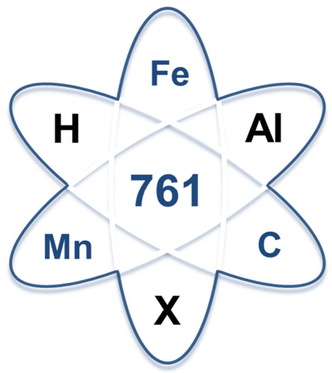
T4 Wasserstoff-Karbid-Wechselwirkung

Einfluss der Mikrostruktur auf die Wasserstoffversprödung in Cr-haltigen hoch-Mn Stählen



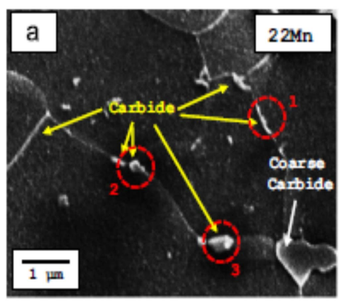
Poulumi Dey, Tilmann Hickel, Jörg Neugebauer
Max-Planck-Institut für Eisenforschung
Zacharias Georgeou, Frank Klose
Salzgitter Mannesmann Forschung GmbH

Transferprojekt

Motivation

- Delayed fracture in high Mn steels caused by HE → unresolved issue
- Fracture surfaces often decorated by inclusions
- Relevance of intergranular cementite:
  - starting point for crack initiation
  - disappear with increased Al content
  - sensitivity to HE decreases strongly

Goals:
- Confirmation of trend for cementite
- Extension to Cr carbides



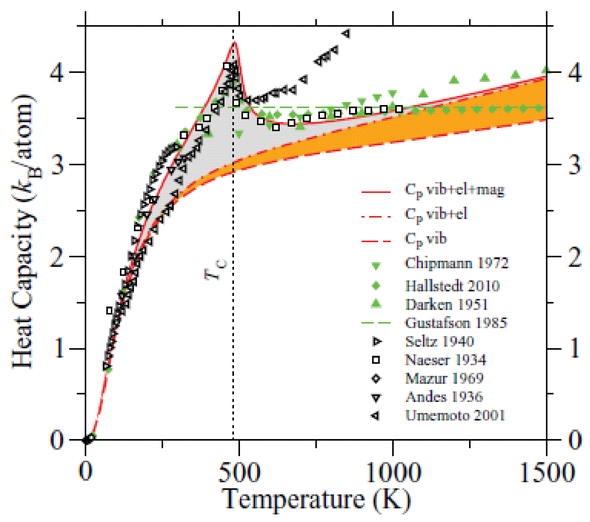
► S. Hong et al., MSE-A 587 (2013).

Methodology

- DFT as implemented in VASP (Vienna b-initio package simulation)
- Coherent interface energy between carbide and matrix obtained using DFT energies in $\gamma = (E_{int} - E_{bulk})/2A$
- Magnetic contribution to free energy of cementite evaluated using spin quantum Monte Carlo scheme
- Spin-space averaging formalism employed to deal with magnetic disorder
- H solution enthalpy obtained using DFT energies in $\Delta H_H = E[XCH] - E[XC] - \mu_H$
- Diffusion of H in high Mn steels studied using kinetic Monte Carlo simulations

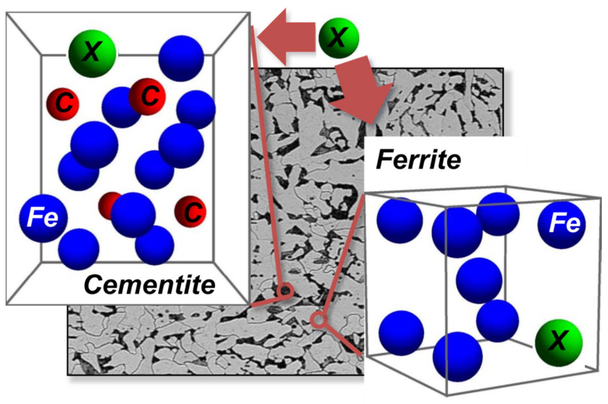
Phase stability

Previous work:
- Thermodyn. properties and formation free energy of Fe_3C
- Partitioning of Al and Si between Fe_3C and bcc matrix



Ab initio calculated heat capacity of cementite vs T

► A. Dick et al., PRB 84 (2011) pp. 125101

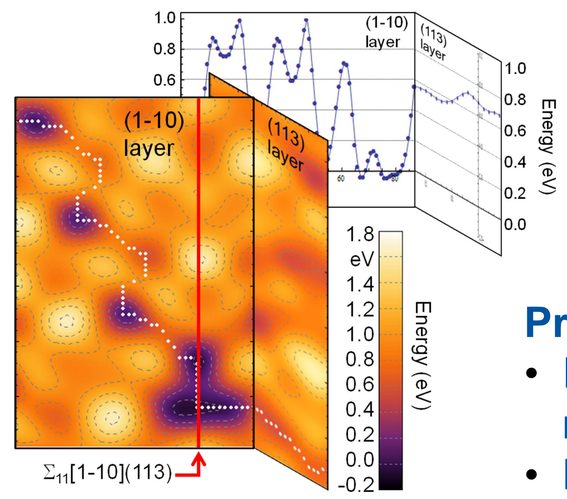


Schematic view of partitioning of Al and Si to cementite and matrix

► K. Hausmann et al., Diploma thesis (2011)

Plans for present project:
- Extension of concepts to partitioning between Fe_3C and austenitic matrix with focus on the mechanisms for Al
- Discussion of role of coherency strain
- Development of methods to calculate semi- and incoherent interface energies

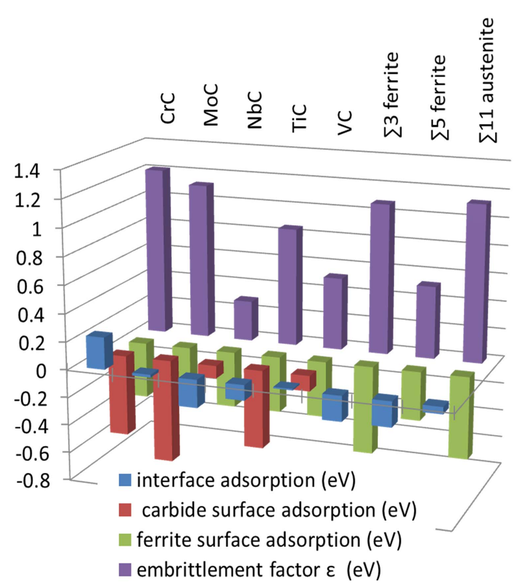
Impact of H



Effective diffusion channel of H in Σ11 grain boundary

► Y.A. Du et al., PRB 84 (2011) pp. 144121.

Previous work:
- Interaction of H with various microstructure features
- Effective diffusion channels for H in grain boundaries
- Analysis of HEDE mechanism for different carbide/matrix interfaces



H solution enthalpies at interface and on respective free surfaces

Plans for present project:
- Extension to the relevant carbides and phase boundaries
- H in bulk carbide
- Consideration of point-defect hydrogen interaction (in bulk and at the interface)

Links to SFB

- Exchange with A1 dealing concerning H interaction with κ-carbide
- Methods developed to investigate thermodynamic properties in A2 are transferred to study thermodynamic stability of carbides
- Intensive exchange with A9 over mechanisms of HE and relevance of microstructure
- APT measurements performed within C8 are employed to detect chemical composition of carbides and matrix

Work packages

- **WP1**: Calculation of TD stability of carbides: *dependence on matrix composition, chemical structure, temperature*
- **WP2**: Structure of carbide/matrix interface: *coherent interfaces, extension to incoherent concepts*
- **WP4**: Determination of interaction between carbides and H: *perfect carbide, point defects, interface*
- **WP5**: Hydrogen enhanced decohesion (HEDE): *coherent (Fe_3C, Cr-carbide) and incoherent (Cr-carbide) interfaces*

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Ein Unternehmen der Salzgitter Gruppe

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