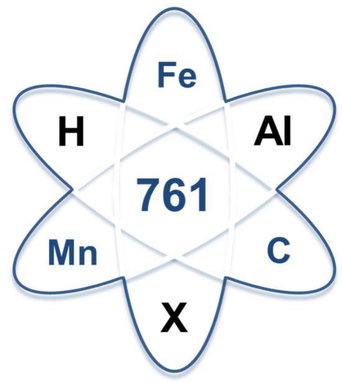
A9 *Ab initio* hydrogen embrittlement

Ab initio based mesoscale simulation of hydrogen embrittlement



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Results 2nd phase

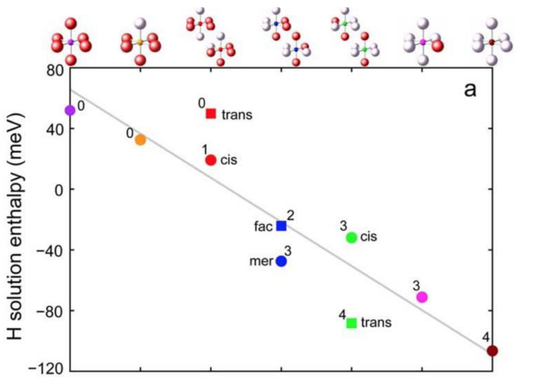
Motivation

Hydrogen embrittlement is a problem for many high strength steels. Next to experimental investigations theoretical approaches and simulations are required to capture the intertwined aspects on all scales. Here we will consequently link aspects on the atomic scale, which will be quantified with *ab initio* methods, to the continuum level, in order to understand the influence of hydrogen also on mesoscopic and macroscopic scales.

Methods

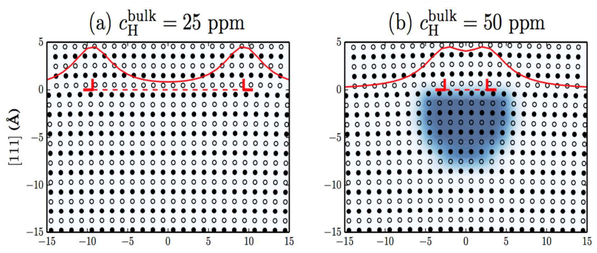
- Ab initio simulations
- Molecular dynamics and Monte Carlo simulations with embedded atom potentials
- Phase field and Cahn-Hilliard models
- Greens function methods
- Finite element methods
- Theory of elasticity
- Analytical methods

H in High Manganese Steels

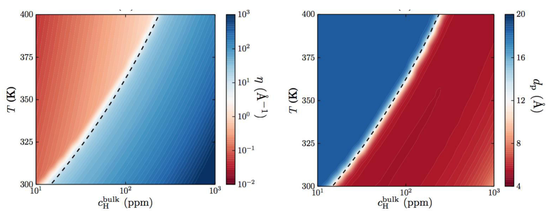


Hydrogen preferentially segregates in mangenese rich environments. This ab initio predicted effect is primarily due to elastic-volumetric zurückzuführen.

Nano hydride formation

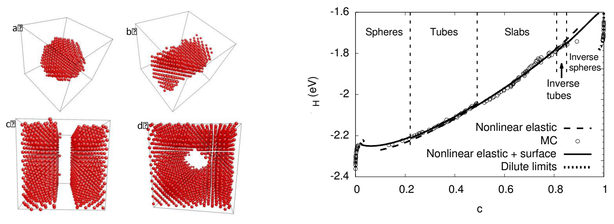


Nano hydride formation at edge dislocations at 300K.



Temperature-hydrogen concentration-phase diagram of nano hydrides for (a) the hydrogen excess and (b) partial dislocation distance.

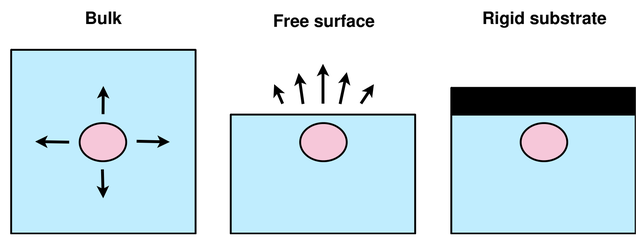
Multiscale modeling

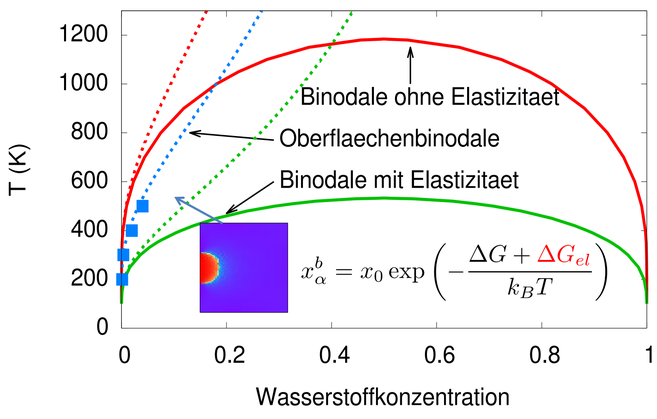


Monte Carlo simulation and quantitative continuum description of hydride formation in Ni.

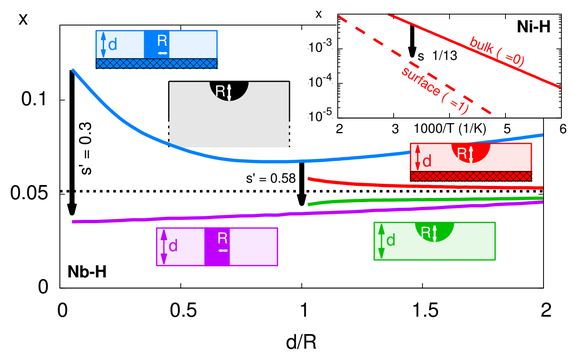
Scale bridging modeling of hydride formation

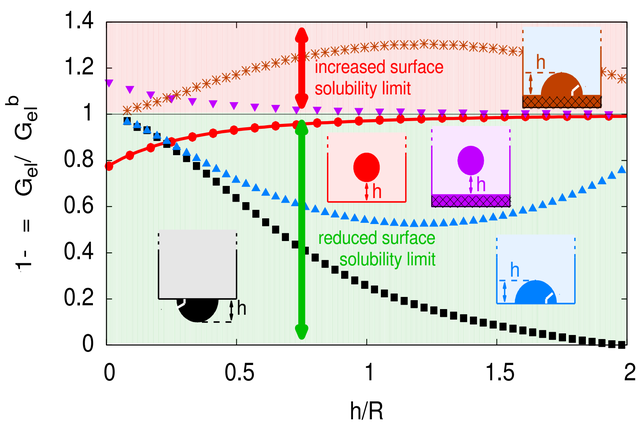
- Phase separation in hydride forming systems will be strongly influenced by elastic effects.
- Near free surfaces elastic stresses can partially relax. This leads to dramatic local modifications of the phase diagrams.





- Coupling of ab initio simulations with mesoscale methods for the prediction of solvus lines in the bulk and near surfaces
- Agreement with thin film experiments





- Solubility limit of hydrogen in fcc iron near free surfaces decreased by two orders of magnitude

Impact

- Scale and project bridging description of hydrogen → **A1, A2, A7, C6**
- (Nano-) hydride formation and hydrogen enrichment at dislocations and surfaces can trigger and enhance hydrogen embrittlement in a HELP and HEDE sense.
- Generic prediction of surface phase diagrams.

► J. v. Appen, R. Dronskowski, A. Chakrabarty, T. Hickel, R. Spatschek, J. Neugebauer: J. Comp. Chem. 35 (2014) 2239.
► T. Hickel, R. Nazarov, E.J. McEnery, G. Leyson, B. Grabowski, J. Neugebauer: JOM 66 (2014) 1399.

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