Interfacial Properties of the FeTi Hydride Formation from First Principles

Ebert Alvares [a], Kai Sellschopp [a], Bo Wang [b], Richmond Odufisan [b] , Shinyoung Kang [b], Tae Wook Heo [b], Paul Jerabek [a], Thomas Klassen [a,c], and Claudio Pistidda [a]

[a] Institute of Hydrogen Technology, Helmholtz-Zentrum hereon GmbH, Max-Planck-Straße 1, D-21502 Geesthacht, Germany
[b] Materials Science Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA
[c] Helmut Schmidt University, Holstenhofweg 85, 22043 Hamburg, Germany

Summary

To understand metal-hydride phase transformations and their impact on hydrogenation kinetics, the interfacial properties between the ß-FeTiH hydride and its parent B2-FeTi matrix were analyzed by :

- Studying the interfaces between the hydride/metallic matrix
- Quantifying separately their chemical and elastic energy contributions
- Analyzing the strain and elastic tensor relationship
- Determining the habit plane of hydride formation
- Implementing the interfacial analysis into KKS phase-field model

Findings:

- Insights into the interplay between chemical and elastic interfacial energies
- Calculation of the habit plane of the ß-phase in the B2-FeTi matrix.
- Support micro-mechanics implementation into phase-field simulations of FeTi alloy hydrogenation.

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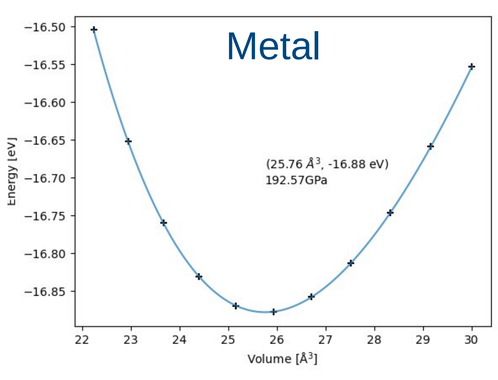
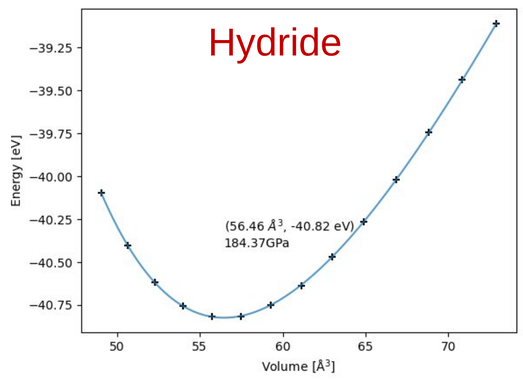
Bulk crystal properties

- At first, the bulk crystal structures were relaxed to their equilibrium volume and had their properties calculated for benchmarking the DFT settings:





- The DFT calculations reproduce reaction enthalpy, cell shape, bulk modulus and elastic properties in good agreement with experimentally measured data.

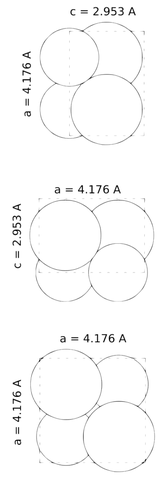
Elastic properties of crystals

- By applying incremental tensile, compressive and shear strain in all directions, the elastic properties of metal and hydride were calculated [GPa].

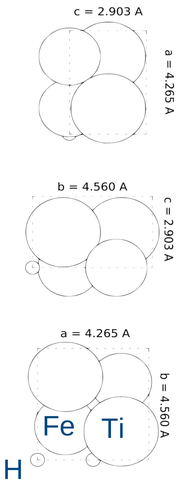
$$^{\alpha}C_{ij} = \begin{bmatrix} 371.45 & 106.08 & 106.08 \\ 121..30 & 371.45 & 142.89 \\ 88.60 & 88.60 & 388.34 \end{bmatrix}$$

$$^{\beta}C_{ij} = \begin{bmatrix} 360.0 & 86.11 & 63.18 \\ 99.45 & 301.98 & 74.54 \\ 82.76 & 173.21 & 313.04 \end{bmatrix}$$

Metal

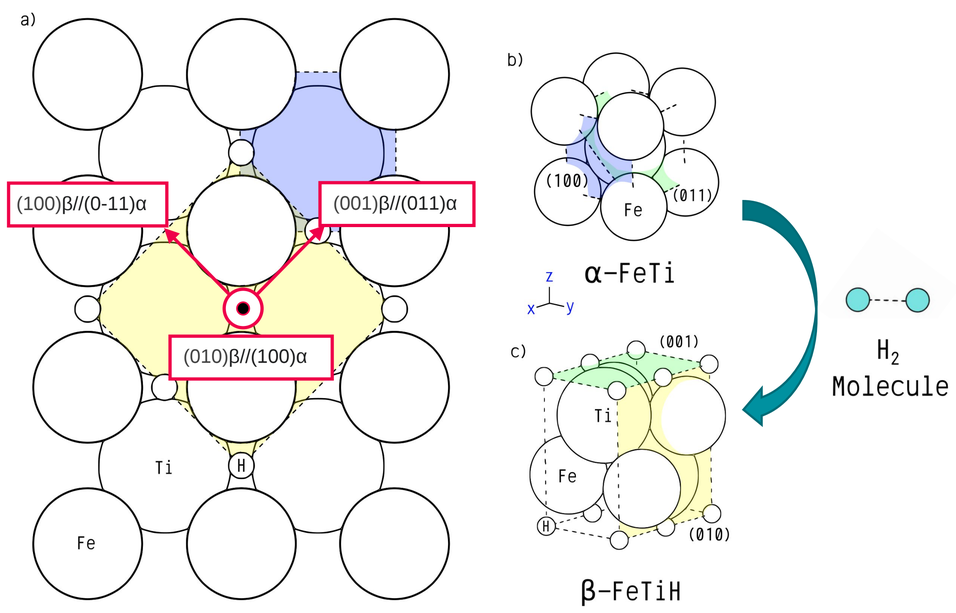


Hydride

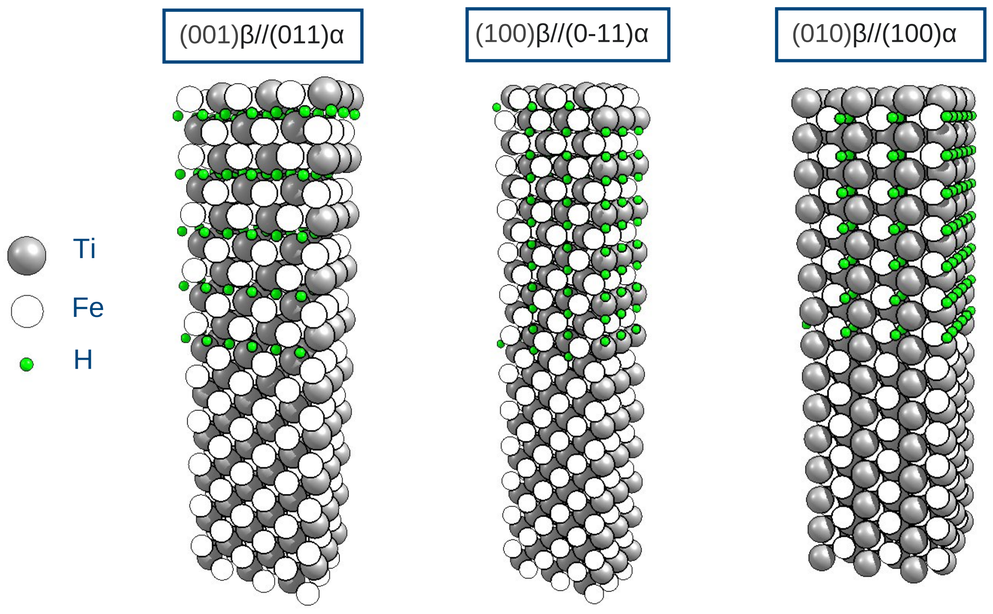


Metal-hydride orientation

- From Westlake[1] work, a purely geometrical model that reduces mismatches was derived and used as initial guess for the metal-hydride orientation relationship



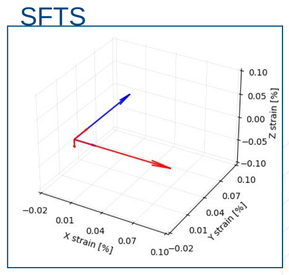
- Based on this, correspondent strained interfacial slab models are used to extract the chemical contribution to the interfacial energy for the three orientations.

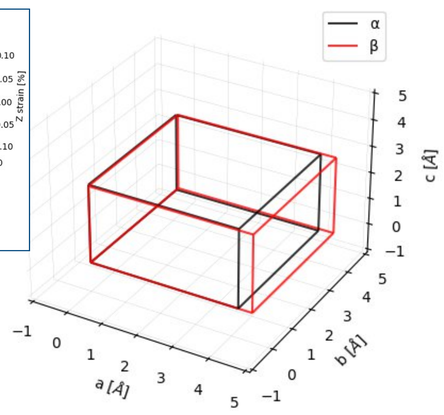


Cell-shape correlation

- Using the hydride phase as frame of reference, a tetragonal to orthorhombic transformation is identified

SFTS





SFTS

$$^{1}E_{ij} = \begin{bmatrix} 0.092 & 0.000 & 0.000 \\ 0.000 & 0.021 & 0.000 \\ 0.000 & 0.000 & -0.017 \end{bmatrix}$$

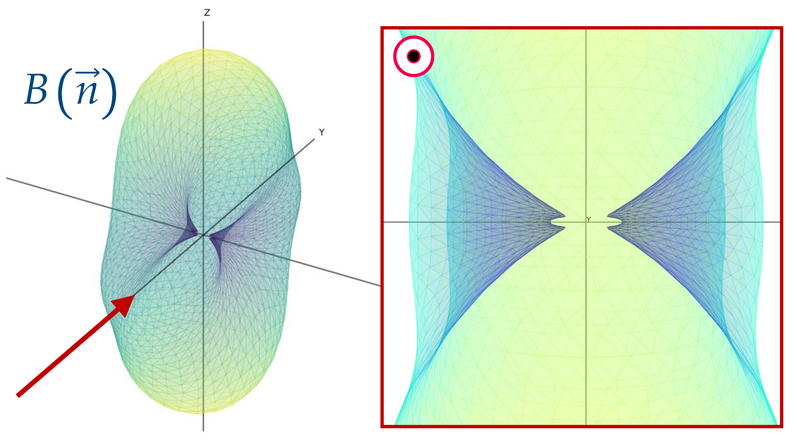
$$^{2}E_{ij} = \begin{bmatrix} 0.021 & 0.000 & 0.000 \\ 0.000 & 0.092 & 0.000 \\ 0.000 & 0.000 & -0.017 \end{bmatrix}$$

- The Stress-Free Transformation Strain (SFTS) is derived based on the lattice mismatch between the metal and the hydride.

B($\vec{n}$) Calculation

$$B(\vec{n}) = C_{ijkl}E_{ij}E_{kl} - n_i\sigma_{ij}\Omega_{jk}\sigma_{kl}n_l$$
$$\sigma_{ij} = C_{ijkl}E_{kl}$$
$$\Omega_{jk}^{-1} = C_{ijkl}n_in_l$$

- Stress-Free Transformation Strain & Elastic properties convolution
- Favorable direction of formation
- Anisotropy in phase-field simulations



References:

[1] D. G. Westlake, Application of a geometric model to the hydrides of FeTi, Journal of Materials Science 19 (1) (1984) 316–326. doi:10.1007/BF02403141.

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He Honoka Hauwai German-NZ Green Hydrogen Centre

Helmholtz-Zentrum Hereon • Institute of Hydrogen Technology • Materials Design • Max-Planck-Straße 1 • 21502 Geesthacht I Germany

Contact: ebert.alvares@hereon.de • /ebertalvares

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