Hydrogen effect on the strength of the Fe_3Al alloy

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Introduction

Quantum-mechanical molecular-dynamics (MD) study of Fe_3Al with and without hydrogen atoms under conditions of uniaxial deformation up to the point of fracture.

T = 300 K (room temperature).

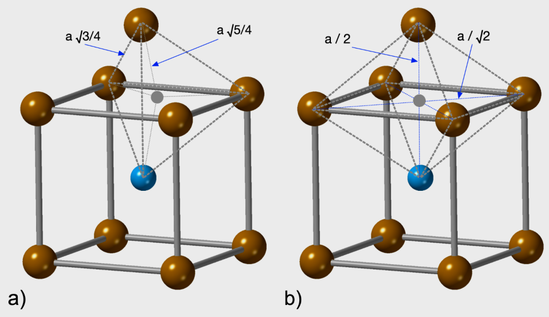
H concentrations range from 0.23 to 4 at. % of H and show a clear preference of H atoms for tetrahedral-like interstitial positions within the $D0_3$ lattice of Fe3Al.

Basic principle of the presented quantum-mechanical molecular-dynamics.

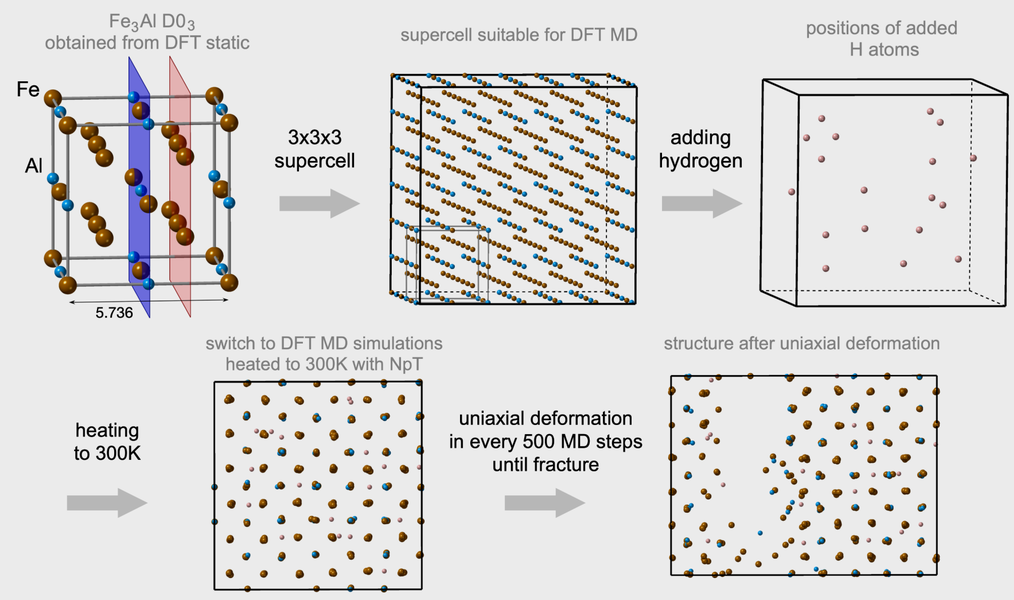
Ab initio MD simulations of uniaxial deformation along the ⟨001⟩ crystallographic direction up to the point of fracture.

Also, static and dynamic H-position in the $D0_3$ structure investigated

Preferable variant **a)** OR **b)**?

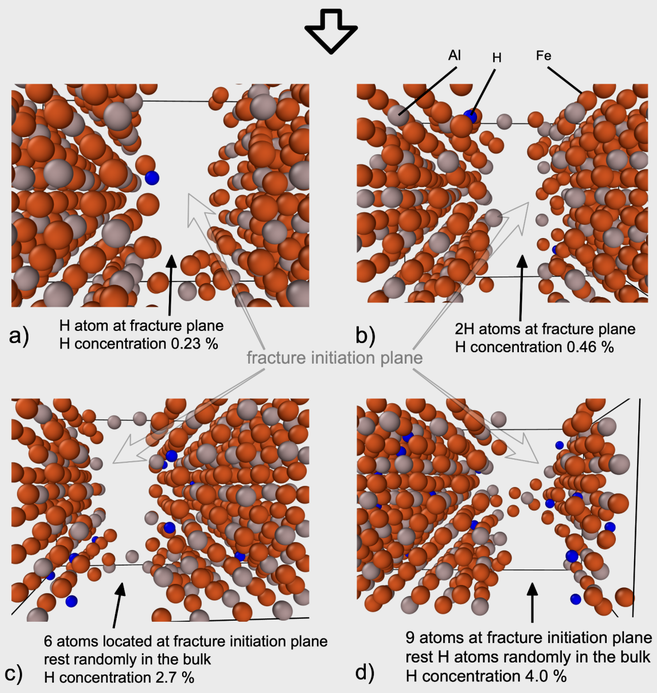


Simulations - Basic principle



Stress-strain behavior

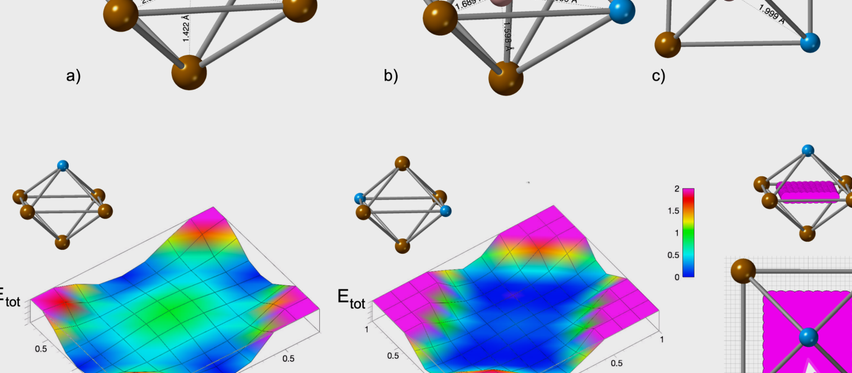
fracture always initiated at a crystallographic plane with H-atom(s)



fracture analysis

stress analysis

presence of hydrogen always decreases the maximum achievable strain

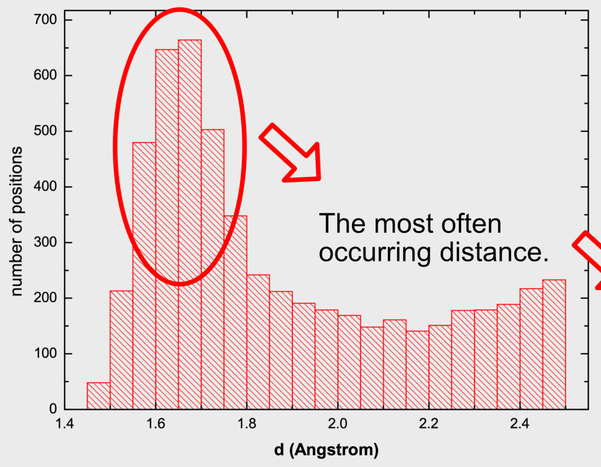


Increasing H-content → decreasing the strain.

Preferable H-position in $D0_3$

molecular dynamics using DFT simulations

A statistical analysis of the distances between H-atom and its neighbors (Al or Fe atoms).



DYNAMICS (T=300K) **vs** STATICS (T=0K)

Preferable position between the tetrahedral and octahedral.

Preferable position between the tetrahedral and octahedral.

Static and dynamic predictions are consistent!

static optimization using the DFT simulations

Summary

- ***Fracture is always initiated at crystallographic planes containing H-atom.***
- ***Increasing the hydrogen concentration decreases the maximum achievable strain.***
- ***Hydrogen atoms occupy the tetrahedral-like positions, i.e. the positions between the tetrahedral and octahedral sites and prefer a higher Al concentration in their close vicinity.***

Entire work can be found in:

Šesták, P.; Friák, M.; Šob, M. *Materials* 2021, 14, 4155

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