Kinetics and ordering of hydrogen at dislocations in bcc iron

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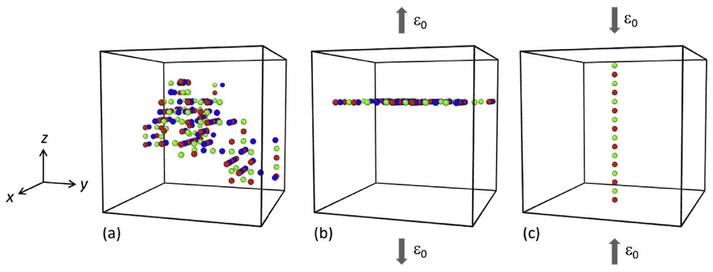
Motivation

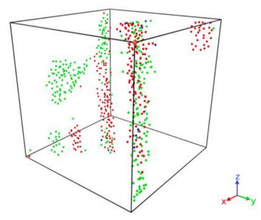
Development of reliable infrastructure for hydrogen-based energy requires improved understanding of mechanisms of hydrogen induced embrittlement. The project is focused on understanding the effect of hydrogen on carbon behaviour in iron based steels. Thermodynamic and kinetic properties of hydrogen atoms in body-centered iron are investigated by using Monte Carlo (MC) simulations [1,2]. Pairwise interactions between carbon atoms are obtained by combining the linear elasticity theory and the state-of-the-art results from density functional theory (DFT). Interaction of interstitials atoms with dislocations is modelled by introduction of corresponding stress fields. The results are compared with the behaviour of carbon [1,2] and possible synergistic effects between both impurities are discussed.

References:
[1] Maugis, P., Chentouf, S., & Connétable, D. (2018). Stress-controlled carbon diffusion channeling in bct-iron: A mean-field theory. Journal of Alloys and Compounds, 769, 1121–1131.
[2] Huang, L., & Maugis, P. (2023). Atomistic simulation of the collective carbon motion in body-centered tetragonal iron: A new insight into the martensite ageing. Acta Materialia, 249, 118846.

Diffusion [1]

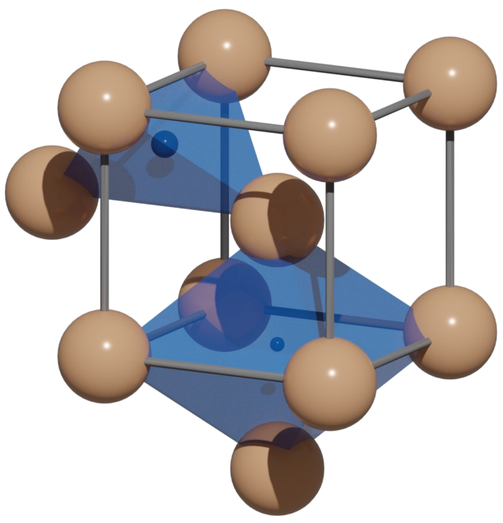


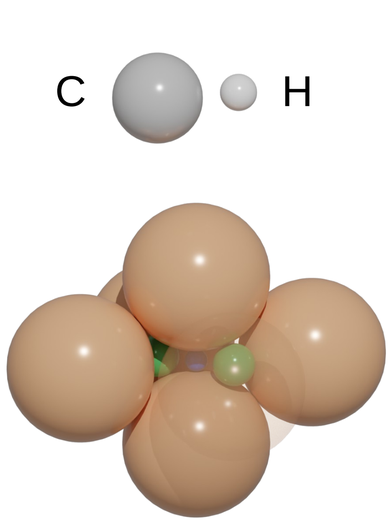
Segregation

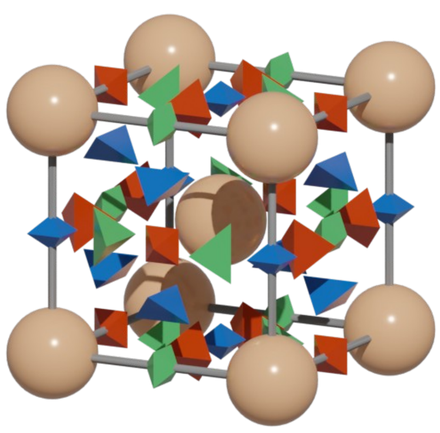


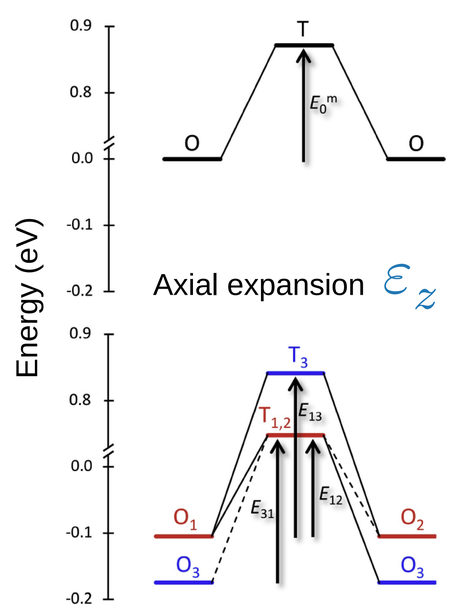
Clustering [2]

Interstitials in bcc iron



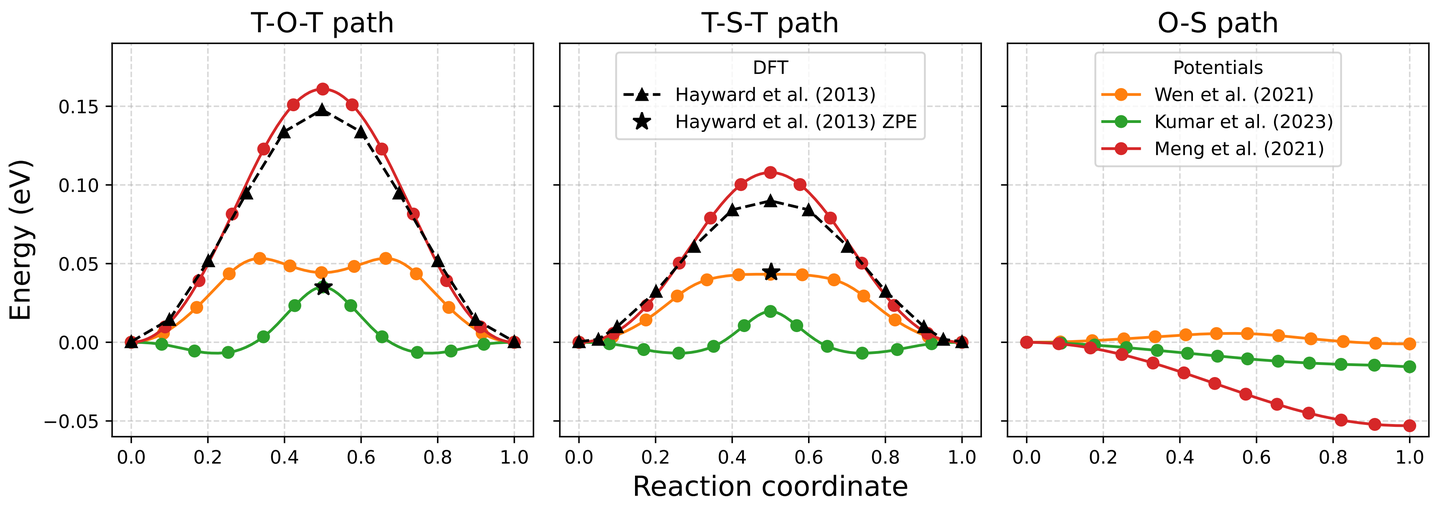




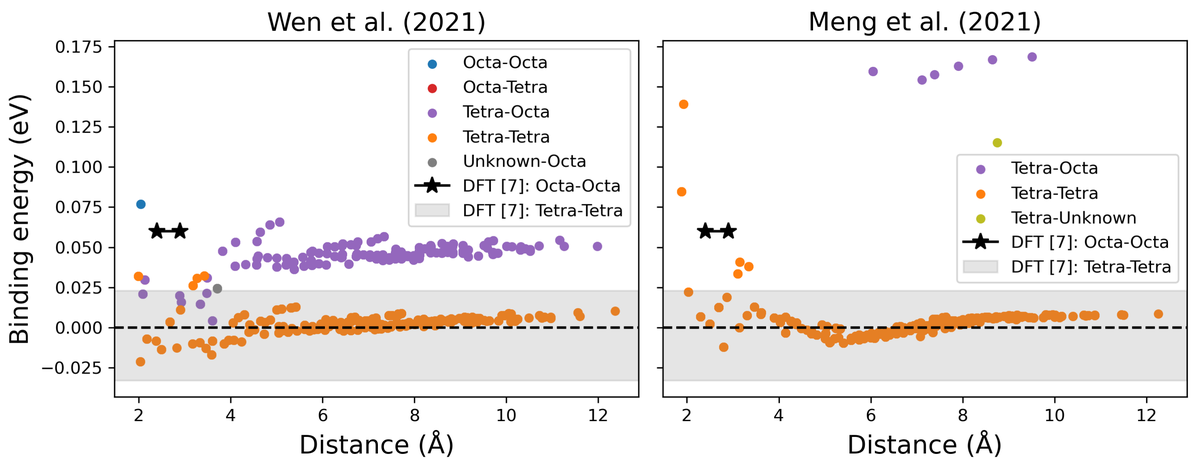


H in bcc iron

Diffusion



Pair interaction



- 5x5x5 unit cells
- 1500 tetrahedral
- 750 octahedral
- $F_{max} = 10^{-3}$ eV/Å
- Final octa/tetra detection by coordination number

Outlook

- Estimation of importance of ZPE for diffusion and pair interaction parametrisation
- Influence of stress on octa/tetra stabilisation and consequences for ordering and kinetics with mean field theory and Monte-Carlo simulations
- Introduction of dislocation stress field
- Parametrisation of diffusion and pair interaction for H-C system to study influence of H on kinetics of carbide precipitation
- Other point and extended defects: vacancies and grain boundaries
- Coupling to experiments with mechanical testing and advanced microstructural characterisation is planned within HyStyle ANR project

[3] Hayward, E., & Fu, C. C. (2013). Interplay between hydrogen and vacancies in α-Fe. Physical Review B - Condensed Matter and Materials Physics, 87(17), 174103.
[4] Wen, M. (2021). A new interatomic potential describing Fe-H and H-H interactions in bcc iron. Computational Materials Science, 197, 110640.
[5] Kumar, P., Ludhwani, M. M., Das, S., Gavini, V., Kanjarla, A., & Adlakha, I. (2023). Effect of hydrogen on plasticity of α-Fe: A multi-scale assessment. International Journal of Plasticity, 165, 103613.
[6] Meng, F. S., Du, J. P., Shinzato, S., Mori, H., Yu, P., Matsubara, K., Ishikawa, N., & Ogata, S. (2021). General-purpose neural network interatomic potential for the α -iron and hydrogen binary system: Toward atomic-scale understanding of hydrogen embrittlement. Physical Review Materials, 5(11), 113606.
[7] Cui, Y., Hu, C., Yu, P., Xie, D., Kong, L., Rong, Y., Wen, M., & Zou, J. (2020). Enhanced H-H binding and consequent H-aggregation around dislocation in α-Fe lattice. Materials Research Express, 7(6), 66518.

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