Atomistic modelling of fracture in iron

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Irradiation and extreme temperatures in nuclear reactor pressure vessels lead to embrittlement of their structural steels. Multiscale models of this complex phenomenon [1] require, at the lowest rung, inputs on fracture properties at the atomic scale. In this talk, I will present simulations of atomistic crack propagation in α-iron using a machine learned interatomic potential (MLIP) [2] that we have iteratively retrained to model fracture. The critical stress intensities and corresponding energy barriers to crack propagation along different crystal planes are mapped via the numerical-continuation technique proposed by Buze et. al. [3], within the plane strain approximation. I will then present an extension of this approach to initialize crack propagation pathways in fully three-dimensional cells. This new approach is employed along with the nudged elastic band method to compute energy barriers to crack propagation via the double kink mechanism. These fracture energy barriers are used to parametrize a temperature dependent model of crack velocity, an essential input to larger scale models of fracture in ferritic steel [1].

References

[1] Mathieu, Jean-Philippe, et al. Journal of Nuclear Materials 406.1 (2010): 97-112.

[2] Zhang, Lei, et al. npj Computational Materials 9.1 (2023): 217.

[3] Buze, Maciej, and James R. Kermode. Physical Review E 103.3 (2021): 033002.