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Ab initio study of cementite – α -Fe interfaces under irradiation

One of the materials that will be investigated in the IFMIF-DONES facility is EUROFER97, the European reference steel for the First Wall and the Breeding Blanket of DEMO, which is a reduced activation ferritic/martensitic (RAFM) steel. This steel is a Fe alloy containing mainly Cr, C, W, Ta, Mn, and V.

It is well-known that C impurities strongly affect point-defect properties in Fe-based alloys. However, many aspects of the mechanisms through which the C atoms arrange in bcc-Fe lattices are not yet clear. We aim at exploring the configuration adopted by C in the presence of cementite, a common carbide that precipitates in steels. For this, we employ Density Functional Theory (DFT) calculations.

Our current focus lies on the bcc-Fe – Cementite (α/θ) interface. It is crucial to understand the behavior and properties of cementite, since carbides can emit C atoms, interact with radiation defects, or even influence the thermal conductivity of steels, whose stability can be affected by irradiation.

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