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

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One of the materials that will be investigated in the IFMIF-DONES facility is EUROFER97, a reduced activation ferritic/martensitic (RAFM) steel and the European reference steel for the First Wall and the Breeding Blanket of DEMO.

It is now well-established that defects generated under neutron irradiation strongly affect mechanical properties, and thus, the material's performance [1]. In particular, while C impurities [2] significantly influence point-defect evolution in Fe-based alloys, many aspects of the mechanisms governing the arrangement of C atoms in a bcc-Fe lattice remain unclear. Our objective is to explore the configuration adopted by C in the presence of cementite, a common carbide that precipitates in steels. To achieve this, we use Density Functional Theory (DFT) calculations and Molecular Dynamics simulations (MD).

Our primary focus lies on the bcc-Fe – Cementite (α/θ) interface. On one hand, understanding the behavior and properties of cementite is crucial, as carbides can emit C atoms, which can alter the evolution of defects generated during irradiation. On the other hand, it is also essential to determine how radiation defects interact with the cementite into the Fe matrix, in particular, whether the α/θ interface can act as a sink as how this would affect their evolution.

In this study, we construct the α/θ interface based on the Bagaryatskii OR. We investigate the effects of strain, the various possible terminating planes, and the relative in-plane positions to determine the most stable structures using MD simulations. Subsequently, these energetically favorable structures are downscaled for DFT, and the interfacial energy is recalculated.

References

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