Modelling of complex Fe-C systems for radiation applications with MLIAPs

Pedro Delgado[1], Pablo Canca[2], María José Caturla[4], Blanca Biel[2,3]

[1]IFMIF-DONES España, Granada, Granada, España

[2] Department of Atomic, Molecular and Nuclear Physics, Faculty of Science, University of Granada, Granada,Spain

[3] Instituto Carlos I de Física Teórica y Computacional, University of Granada, Granada, Spain

[4] Department of Applied Physics, University of Alicante, Alicante,Spain

pedro.delgado@ifmif-dones.es

In recent years there have been notorious advances in fusion technology, such as the proliferation of private startups and international projects such as ITER [1]. In the roadmap of the ITER project and looking forward to the future DEMO [2] reactor, one of the main problems is the design of materials able to withstand the neutron radiation produced inside DEMO being the structural material for the vessel the less studied in comparison with other components. In this context, IFMIF-DONES is born as the infrastructure to test and develop better and new materials for this purpose. [3]

The chosen material will be EUROFER97 steel, which has been heavily tested at low radiation doses. If we want to predict and try to improve the behavior at higher radiation doses, we need to know the effect of radiation on the atomic structure of the steel.

One of the key components in the fragility of steels is the formation of the so-called cementite carbide. Not much is known about the presence of cementite under irradiated steel, such as its effects on the recombination rates of atoms and in the migration of dislocations in the material.

At the moment, due to the variety and complexity of possible combinations of cementite and iron, it is not possible to study these problems with accurate quantum methods such as Density Functional Theory (DFT), as the system size ranges from 500 to more than 40.000 atoms. In addition, in radiation damage studies, the number of defects heavily increases with the radiation energy, and so does the number of atoms needed to describe the system, in order to avoid border effects.

Therefore, these systems must be studied by means of Molecular Dynamics (MD) techniques. One mayor issue is the lack of accurate and general potentials for the multiple combinations of C and Fe structures. In order to solve this problem, we have developed a Machine Learning Interatomic Potential based on the Neuroevolutional Potential (NEP) [4] formalism combined with a Ziegler-Biersack-Littmark (ZBL)interaction potential [5] for the short-range interactions needed in radiation simulations.

After the validation with known structures, we aim to perform calculations of the most studied Bagarytsky interfaces of Fe-Cementite with multiple defects and the study of radiation effects in the nearby region, trying to capture the effects of the presence of the cementite.

References

[1] ITER, https://www.iter.org/
[2] DEMO,https://eurofusion.org/programme/demo/
[3] IFMIF-DONES, https://ifmif-dones.es/es/
[4] Zheyong Fan, *et al,* Phys. Rev. B. 104, 2021 104309
[5] J.F. Ziegler, J. P. Biersack and U. Littmark, Pergamon, Volume 1, 1985.
[6] Liyanage *et al*, Phys. Rev. B, 9, 2014, 094102

Figures

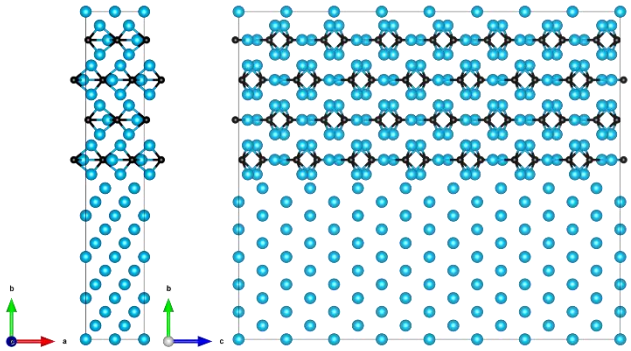

Figure 1. Minimum strain Bagarytsky interface to study within DFT. 416 atoms are needed in order to minimize the strain in the structure so it is suitable to study within DFT. The human computational time is about 10 days using 416 cores.

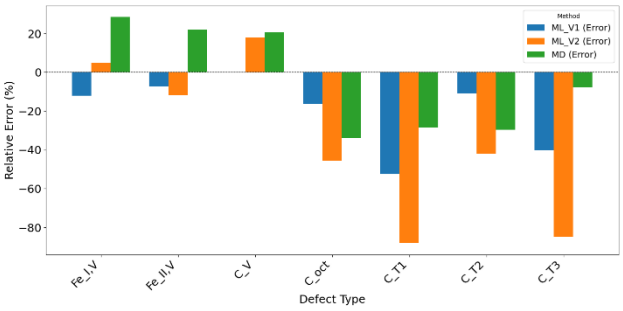

Figure 2. Error comparison of point defect formation energy (vacancies and interstitials) with DFT, for the most used MEAM potential for cementite [4] and two different versions of the potential for common defects in cementite.