Machine Learning Interatomic Potentials for Fusion Oriented Materials

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Machine Learning Interatomic Potentials (MLIAPs) mix the accuracy of *ab initio* methods such as Density Functional Theory (DFT), with the scalability of classical interatomic potentials. Fusion structural materials, employed in the construction of future fusion reactors, experiment high neutron radiation doses. This radiation disturbs the crystal structure, generating defects in the lattice. To better understand the formation and dynamics of these defects in the crystal, we present a MLIAP based on the equivariant neural network MACE [1]. Using this potential, we are able to characterize the formation and binding energies of the most common defects in an iron crystal using a reduced database with only some simple defects. We also include a top layer with a Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion potential in order to perform Primary Knock-on Atom simulations (PKA), giving the potential the capability of study neutron collision cascades.

References

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[2] Barouh, Caroline, et al. "Interaction between vacancies and interstitial solutes (C, N, and O) in α− Fe: From electronic structure to thermodynamics." *Physical Review B* 90.5 (2014)

[3] Fu, Chu-Chun, François Willaime, and Pablo Ordejón. "Stability and mobility of mono-and di-interstitials in α-Fe." *Physical review letters* 92.17 (2004)

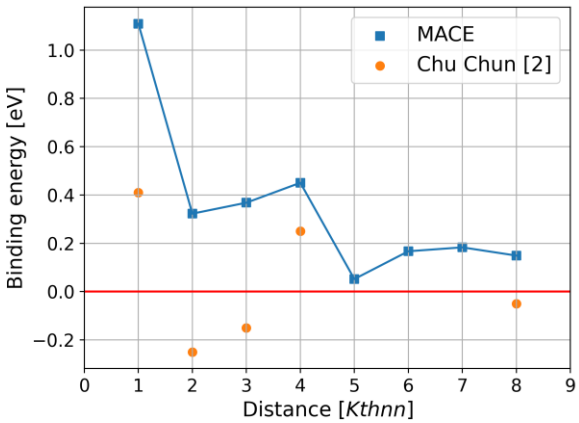

Figure 1. C-V Binding energy for 8 nearest neighbors, and previous DFT study [2]

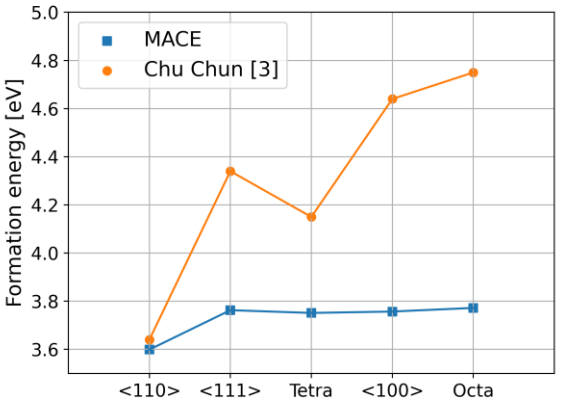

Figure 2. Common interstitial defects formation energies. The lower energy for the <110> is crucial in iron modelling [3]

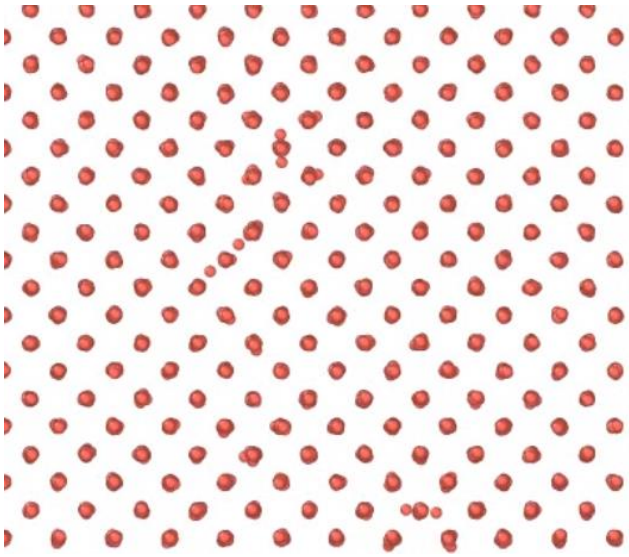

Figure 3. Crystal structure after a PKA of 5 KeV

Figures