Efficient Machine-Learned Graph Neural Network Interatomic Potential for modeling radiation and helium damage in Fe-Cr alloys

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Machine learned interatomic potentials (MLIPs) provide great balance between speed and scale of MD methods with accuracy of DFT. This work focuses on Allegro MLIP. Allegro is a fully local Graph Neural Network (GNN) MLIP based on NequIP MLIP. It provides good training data efficiency, balanced speed and great parallelization across multiple GPUs and compute nodes in contrast to other GNN MLIPs where non or semi locality makes distributed computation less efficient. MLIP was trained on dataset containing relevant defects and atomic structures, including helium derived defects, with chemical composition of host alloy ranging from 0 % to 50 % of Chromium. Limited chemical range was required in order to prevent model errors associated with magnetism of host system.

Current version of MLIP provides excellent data efficiency, correctly predicting [110] grain boundary behaviour despite having only Σ 3 grain boundary in its training dataset. Model correctly predicts formation energies of defects near DFT accuracy[1].

Model was trained with ZBL enabling collision-cascade simulations for modeling of irradiation damage from high energy particles. On single GH200 GPU model achieves 4.2 $\frac{Matoms}{s}$ for large, 120k+ atom supercells in lammps with enabled cuEquivariance acceleration package. Torch-sim provides similar efficiency for large number of small supercells.

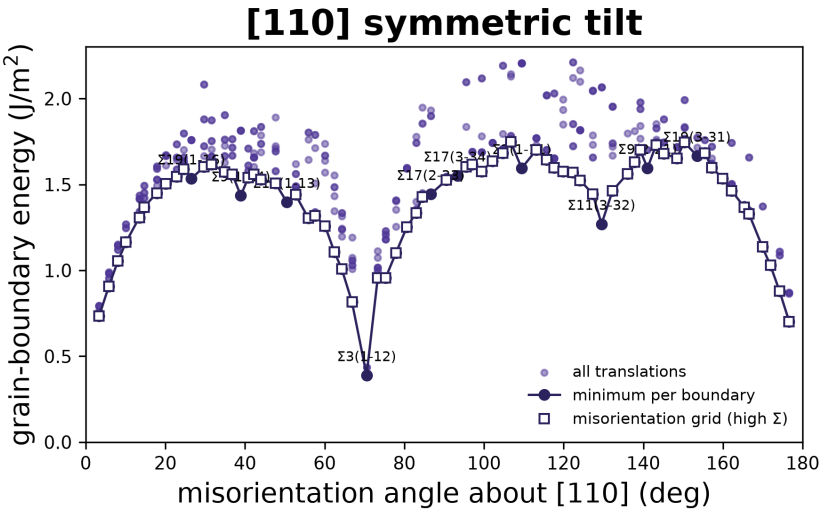

Figure 1: Energy of [110] grain boundaries of pure BCC Fe predicted by MLIP

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References

[1] Marcin R. Zemła, Jan Wróbel and Tomasz Wejrzanowski *Computational Materials Science* (2025).