Evaluating Machine Learning Foundation Models for High Throughput Calculations of Metal-Metal Adhesion Energies

Derek A. Stewart[1, †], **Priyanka B. Shukla**[1], **M. Clelia Righi**[2], **Tiffany S. Santos**[1]

[1]Western Digital Research Center, Western Digital, San Jose CA, United States
[2]Department of Physics and Astronomy, University of Bologna, Bologna, Italy
†corresponding author's email: derek.stewart@wdc.com

Modern electronic devices rely on the construction of complex multilayer stacks of nanoscale material layers. Good adhesion between these layers is essential for device integrity during annealing steps, in-field operation, and long-term device endurance. Protective coatings also require excellent adhesion to prevent film delamination under harsh conditions. Although adhesion is a key design parameter in device development, experimental data on interfacial adhesion energy is limited and it can be costly to perform an extensive experimental search to find the optimal material candidates. First principle approaches, like density functional theory (DFT), can be used to predict the adhesion energy for a given atomic interface. However, identifying the optimal low-strain lattice-matched interface often requires large atomic supercells for structural relaxations, making ab-initio calculations computationally expensive. This makes first principles approaches infeasible for high-throughput screening of interfaces.

The development of machine-learning interatomic potentials (MLIPS) based on DFT training sets has greatly improved the accuracy of large scale atomistic material simulations. Early MLIPS were developed using targeted DFT training for a particular material problem with a small subset of elements. While these MLIPs were effective at their specific tasks, they often were not transferable to other scenarios involving other phases or elements. To address this issue, concerted academic and industry efforts have leveraged vast online DFT crystal structure training sets (MPTrj, Omat24, Alexandria) to create universal machine learning foundation models that cover interactions over 89 elements. These "periodic table" foundation models have demonstrated near DFT-accuracy for crystal structure predictions. However, it is unclear how these models will do at predicting interfacial adhesion.

Here, we evaluate the performance of fourteen different Multi-Atomic Cluster Expansion (MACE) foundation models [1] that have been trained on DFT calculations for an expansive set of materials. To test these models, we compare against DFT (PBE-GGA) reference adhesion energies for 120 metal-metal interfaces calculated by Restuccia et al. [2]. This data set includes a range of fcc, bcc, and hcp crystal structures for sp and transition metals. Predicted adhesion energies range from 0.8 J/m^2 for weak interfaces (Au/Zn) to 5.5 J/m^2 for strong interfaces (Mo/W). Early MACE models, like MACE-MP-0b, have severe difficulties predicting adhesion energies and can have mean absolute errors (MAE) up to 0.92 J/m^2. Recent foundation models (MACE-MATPES-PBE, MACE-MPA-0, MACE-OMAT-0) that build on a broader set of equilibrium and non-equilibrium configurations show superior performance in predicting interface adhesion energy with MAE as low as 0.17 J/m^2. These encouraging results indicate that specific MACE foundation models can be used "off the shelf" for high-throughput investigations of metal-metal interfaces. By comparing MACE model performance for interfaces between different crystal structures (fcc, bcc, hcp) and between different metal families (sp, early transition, late transition), we can also gain insight into potential error sources and use this to further improve these models with targeted fine-tuning. The evaluation procedure developed here can also serve as an important metric for adhesion energy predictions for future machine learning foundation models.

References

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