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Learning a force field for the martensitic phase transformation in Zr HONGXIANG ZONG, Xi'an Jiatong University and Los Alamos National Laboratory, GHANSHYAM PILANIA, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut, TURAB LOOKMAN, Los Alamos National Laboratory — Atomic simulations provide an effective means to understand the underlying physics of martensitic transformations under extreme conditions. However, this is still a challenge for certain phase transforming metals due to the lack of an accurate classical force field. Quantum molecular dynamics (QMD) simulations are accurate but expensive. During the course of QMD simulations, similar configurations are constantly visited and revisited. Machine Learning can effectively learn from past visits and, therefore, eliminate such redundancies. In this talk, we will discuss the development of a hybrid ML-QMD method in which on-demand, on-the-fly quantum mechanical (QM) calculations are performed to accelerate calculations of interatomic forces at much lower computational costs. Using Zirconium as a model system for which accurate atomisctic potentials are currently unvailable we will demonstrate the feasibility and effectiveness of our approach. Specifically, the computed structural phase transformation behavior within the ML-QMD approach will be compared with available experimental results. Furthermore, results on phonons, stacking fault energies, and activation barriers for the homogeneous martensitic transformation in Zr will be presented.

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