Molecular Dynamics Simulations of Multiple Phases and Rare Events with On-The-Fly Machine Learning

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Abstract

Ab initio molecular dynamics is a powerful tool for accurately probing the dynamics of molecules and solids, but it is limited to system sizes on the order of 1000 atoms and time scales on the order of 10 ps. We present a scheme for rapidly training a machine learning model of the interatomic force field that approaches the accuracy of *ab initio* force calculations but can be applied to larger systems over longer time scales. Gaussian Process models are trained on-the-fly, with density-functional theory calculations of the atomic forces performed whenever the model encounters chemical configurations outside of the training set. We demonstrate the flexibility of our approach by testing it on vacancy diffusion in bulk metals.

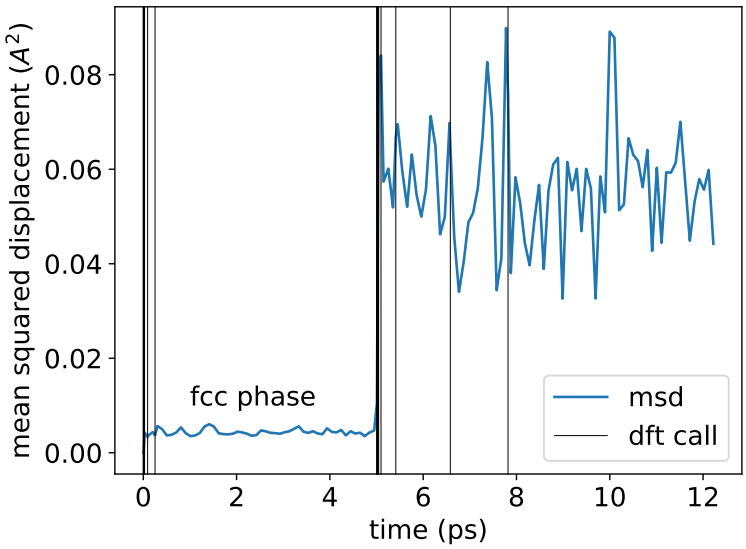

FIG. 1. Mean square displacement of aluminum quench.

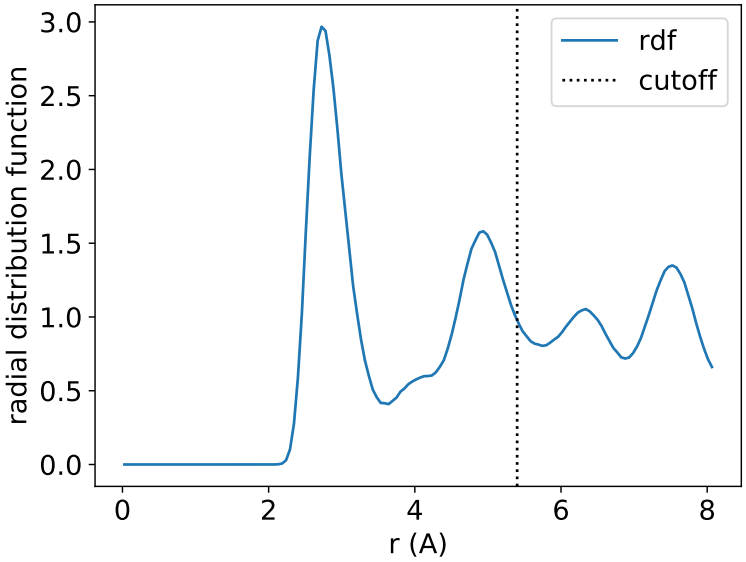

FIG. 2. RDF of Al quench.

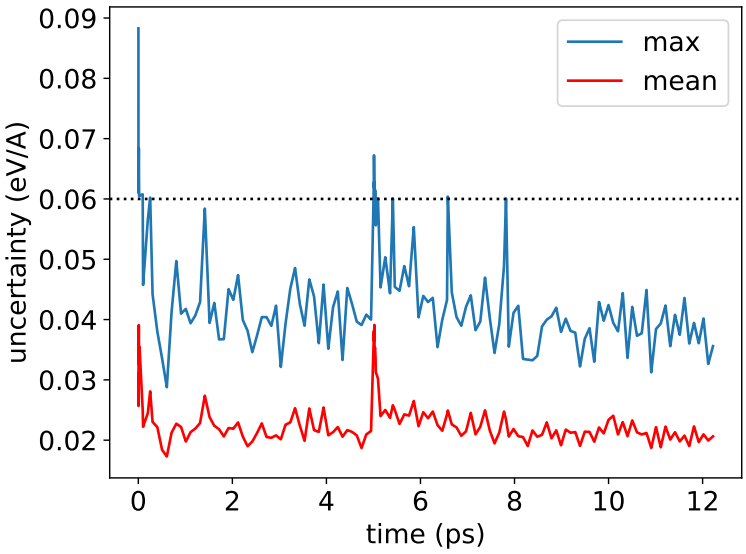

FIG. 3. Mean and max uncertainty.