Detailed instability of BCC Fe via a machine learning potential

Adrian De la Rocha[1], Valeria Arteaga[1], Sofia Gomez[1], Yu-Hang Tang[2], Wibe A. de Jong[2], Jorge A. Munoz[1]

1. The University of Texas at El Paso; 2. Lawrence Berkeley National Laboratory

Abstract

Gaussian process regression on a molecular graph kernel was performed to construct a relation between the total potential and atom displacements of a non-spin-polarized body-centered cubic (BCC) iron (Fe) ab initio simulation. When training on 400 randomly selected molecular dynamics steps, the standard deviation of errors in the testing predictions of the model was of 8meV, while the mean of this errors was 5meV. The resulting machine learning potential of a model trained on 1000 times steps was used to approximate the forces acting upon each atom in the axes of displacement of each first and second nearest-neighbor. The forces were obtained through numerical differentiation according to the central difference approximation and through derivation of a polynomial fit to the potential functional given by the model. The resulting forces are consistent within approximation techniques and show stability in the first nearest-neighbors' axes, but not for the second nearest neighbors. While it is known that the BCC is unstable without magnetism, these observations suggest that the effect of magnetism in the stability of the system of interest is not noticeably affected in the first nearest-neighbor interactions.