Fe Neural Network Interatomic Potential

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Purpose Understanding the mechanism of deformation of BCC iron at the atomic scale.

Outline Neural network interatomic potential (NNIP) construction and demonstration by atomistic simulation

Result Beyond the properties of perfect α-iron crystal, this new NNIP can describe the interactions between various defects in α–iron, including vacancies, surfaces, grain boundaries, and dislocations. Demonstrations show that this NNIP can be applied to, but not limited to, the study of dynamic behavior of the various defects and these interaction in systems in first-principles accuracy.

Computing system: Octopus
        node-hour   1800 node-hour
        memory used   50 GB
        vector per   85 %
        parallelize   2-4 nodes