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Interatomic Potentials for Large-Scale Simulations of High-Pressure, High-Temperature Phenomena[1]

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The use of large-scale atomistic simulations in the study of high-compression, high strain-rate phenomena has dramatically increased in the last decade. Most of this type of simulations utilize classical empirical or semi-empirical potentials to describe the inter-atomic interactions. The regime of validity of most of these potentials is however often limited to a narrow region of the pressure-temperature phase diagram. In the development of accurate inter-atomic potentials for material simulations at high-pressures or temperatures, a high degree of transferability is desirable without resorting to fitting everywhere in phase space. We will review two popular cluster functional models: the embedded-atom-method (EAM) and the modified embedded-atom-method (MEAM). The embedded atom method provides a very good description of metallic properties at a low computational cost and has become the workhorse of large-scale atomistic simulations of metallic systems. The modified embedded-atom-method is an improvement of EAM which includes the effect of angular bonding. We outline inherent limitations of these models and present a systematic approach to improving their transferability and predictive accuracy at high pressures and/or temperatures.

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