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Interatomic Potentials for Large-Scale Simulations of High-Pressure, High-Temperature Phenomena¹

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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 five years. Most of this type of simulations utilize classical empirical or semi-empirical potentials to describe the inter-atomic interactions. The regime of validity of these potentials is however often limited to a narrow region of the pressure-temperature phase diagram. In constructing interatomic potentials for high-pressure high-temperature applications, it is desirable to obtain a high degree of transferability 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 EAM provides a very simple description of the many-body cohesion in metals and MEAM 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.

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