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The Angular-Dependent Embedded Atom Method: Applications to multi-component interactions in nanocomposites

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Abstract: Atomic-scale modeling of many practically important multi-component systems requires interatomic potentials capable of providing an adequate description of interactions with mixed types of atomic bonding. We present a new computationally efficient Angular-dependent EAM (A-EAM) interatomic potential developed by combining the Embedded Atom Method (EAM) potential for metals with the Stillinger a?" Weber (SW) potential for Si/Ge and also with the Tersoff Potential (TF) for Si/Ge/C in a compatible functional form. The cross metal-covalent interactions are fitted to reproduce the energies and structural characteristics of several representative bulk structures and small clusters as obtained from Density Functional Theory (DFT) calculations. The first applications of the A-EAM potential to investigate effects of intermixing and segregation in the Au-Si-Ge ternary system as well as the mechanical properties of metal-covalent (Al/Si) interfaces at the atomic scale using molecular dynamics and Monte Carlo simulation techniques will be presented. The combined potential proves to be computationally efficient and suitable for large-scale MD simulations of metala?"Si/Ge systems, while retaining the properties of the pure components as predicted by the original SW and EAM potentials. The framework of the A-EAM potential also allows for an extension to the Tersoff potential opening possibilities for modeling of metal-carbon systems.