Interatomic potentials for metals

Analysis of dimensionless materials properties reveals intrinsic constraints of EAM-type potentials

The class of interatomic potentials chosen for an atomistic simulation generally limits the adequacy to model a given element. For example, any simple metal modeled with a two-body potential automatically obeys the Cauchy relation: all its elastic tensor elements are identical for a given set of indices, irrespective of their order. However, real metals normally do not obey Cauchy (figure 1). Thus two questions arise: What correlations does the embedded-atom method (EAM) impose – EAM is the most popular type of many-body potential for simple metals – and to what extent do simple metals obey them?

To address these questions, we chose to systematically analyze the Gupta potential and to compare its predictions on the interdependence of different materials properties with experimental data. Gupta is a simple (four-parameter) variant of EAM, allowing one to calculate many properties analytically in the (reasonable) short-range or nearest-neighbor approximation. At the same time, Gupta usually outperforms other, in particular, parameter-laden EAM variants when applied to a broad range of elemental structures encompassing small through high coordination numbers. This is why we consider Gupta as a justifiable representative for the whole class of EAM-type potentials.

In *J. Phys.: Condens. Matter 28 395701 (2016)*, we find that Gupta predicts many properties to correlate in a way conveying the trends revealed by real metals. For example, the ratio of the elastic constants C_{1212} and C_{1122} is less than one and moreover roughly linear if C_{1212} expressed in the units of the bulk modulus B (figure 1). Similarly, Gupta predicts a strong correlation between the vacancy formation energy E_V expressed in units of the fcc cohesive energy E_C. This time, agreement with experimental data is only semi-quantitative for many metals, albeit always considerably better than with any short-range, two-body potential (figure 2).

If a metal strongly deviates from the identified correlations, Gupta, and more generally, EAM cannot provide an accurate description. Even if one could fix some or all of the ratios for one or two crystal structures, this would happen at the expense of deteriorating the description of other structures. The results of our study open up the possibility to estimate based on experimental data alone to what level of accuracy a potentially transferrable EAM-type potential can be constructed, or if modifications are needed.

About the author

The work was carried out by the materials simulation group (http://www.lms.uni-saarland.de) in the Department of Materials Science and Technology at Saarland University during a visit at FZ Jülich. S. Sukhomlinov is a postdoctoral fellow in the materials simulation group, which is headed by M. H. Müser, who is a full professor at Saarland University.

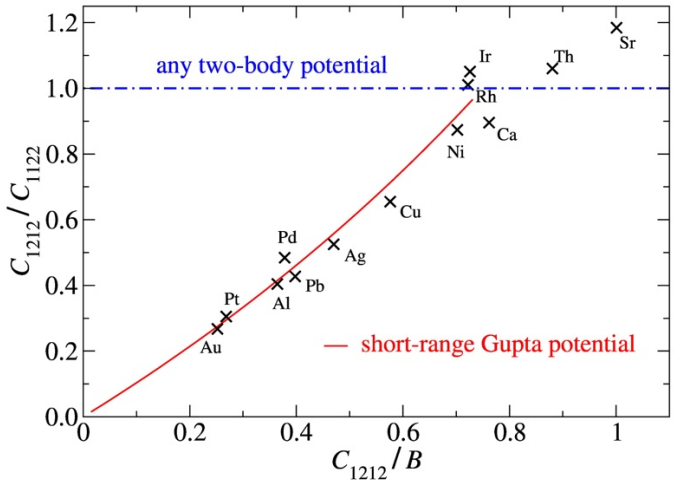

Figure 1:

Short caption: Interdependence of elastic tensor elements

Long caption: Ratio $C_{1212}/\ C_{1122}$ (in Voigt notation $C_{44}/\ C_{12}$) versus C_{1212}/B.

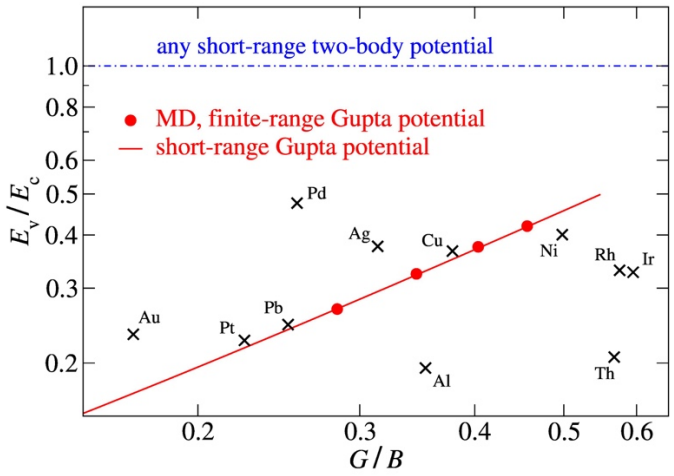

Figure 2:

Short caption: Interdependence of defect energies and elastic properties.

Long caption: Dimensionless vacancy energy E_V/E_C versus dimensionless shear module C_{1212}/B.