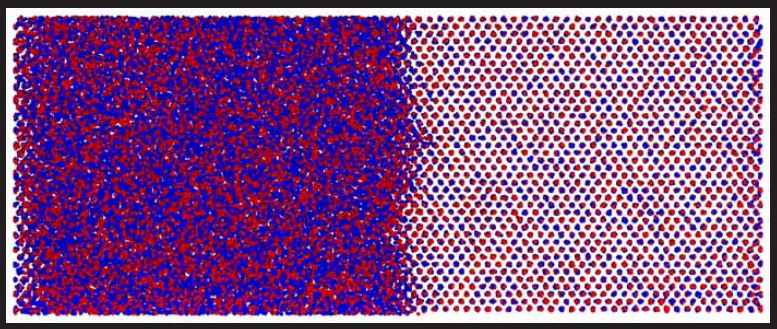
Atomistic Potentials and the Future of Nanomaterials Metrology

Objective



We will provide researchers and designers with a database of evaluated interatomic potentials for metals and alloys; thermodynamic, kinetic, and mechanical materials properties generated for each potential; and experimental or first-principles reference data for comparison. The use of atomistic simulations will thus be facilitated as a tool to predict properties of materials in systems, such as nanomaterials, where direct measurement is time-consuming or extremely difficult.

Impact and Customers

- Computational methods are being used industrially to reduce costs in product development and evaluation. Atomistic simulations can be used to examine properties that are difficult or impossible to measure experimentally, yet these simulations depend critically on the quality and applicability of the underlying atomic interaction potentials employed. Developing and evaluating these interaction potentials is time consuming, with the strong possibility that the model will be inadequate for the problem under consideration.

- We are working with industrial, academic, and government researchers to develop a database of atomic interaction potentials, standard evaluation methods, and reference data to assist researchers in evaluating interatomic interaction models.

CTCMS

NIST Center for Theoretical and Computational Materials Science

- The public NIST Interatomic Potentials Repository (http://www.ctcms.nist.gov/potentials) provides developers and users with a central location to distribute and obtain interaction models for metals and alloys.

- The 2008 NIST/MSEL Workshop on Atomistic Simulations for Industrial Needs provided a forum for developers and users to address barriers to the wider adoption of these atomistic simulation methods in R&D.

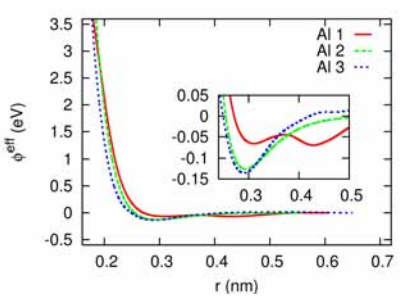
Approach

We are meeting with researchers in industry, government, and academia to determine their highest priorities. These meetings are conducted through conference presentations and workshops, but also through informal discussions with colleagues. In response to these interactions, we created the NIST Interatomic Potentials Repository as the central location for distribution of interatomic interaction models of materials, including metals and alloys. We have also responded to user requests for conversion tools between software formats, and we are defining a standard set of tests and the computational infrastructure necessary to evaluate new and existing potentials as required to verify or complement other measurements. Additionally, we are compiling a database of available experimental measurements, first-principles calculations, and reported properties from atomistic potentials. Our public database of properties will ultimately allow users to compare interatomic potentials and experimental results.

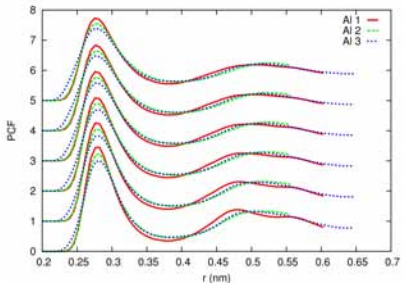
Accomplishments

The success of atomistic simulations depends critically on the fidelity of a specific model of interatomic interactions to the area of application. Interatomic potentials in metallic systems are typically derived and optimized against a small number of validating experiments, and they necessarily work best for specific materials and phases. Thus, they may accurately model one system and range of parameter space but be inappropriate for another. It is therefore essential that engineers and researchers know which interatomic potentials are available and how well they reproduce material properties of interest.

To build and disseminate a database of interatomic potentials, evaluations, and reference data, we have begun by soliciting feedback from researchers in industry, government, and academia to ascertain which properties are most relevant for industrial design processes. Such properties include, but are not limited to, molar volumes, phase stability, microstructural information, thermodynamics of interfaces and surfaces, diffusion, and melting temperatures. Additionally, it is important to know how these quantities change with decreasing size, especially as nanoscale materials become increasingly important.



Effective pair potentials show Al interactions.



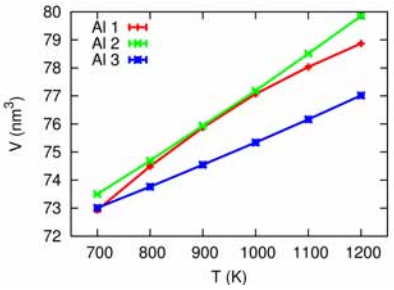
Local atomic structure in the melt from pair correlation functions.

To this end, in April 2008 we hosted the inaugural NIST/MSEL Workshop on Atomistic Simulations for Industrial Needs to facilitate interactions between researchers in industry, academia, and government on issues related to the development and use of interatomic interaction potentials, including accuracy, standardization, and evaluation methods. Participants in this workshop included representatives from Ford Motor Company, GE, General Motors, United Technologies Research Center, Materials Design, NIST, various national laboratories (Sandia, Air Force Research Lab, Ames, Los Alamos), and universities. The workshop planned for 2009 will further address these topics, but it will also include a greater focus on the standardization of interatomic potential formats and discussions about the role of experimental measurements in fitting and validating interatomic potentials.

Among the most requested items during these interactions was the development of a neutral location for the dissemination of interaction models. The NIST Interatomic Potentials Repository (www.ctcms.nist.gov/potentials/) answers this need by posting files of known origin with full citation information and notes about the formatting and use of the files in molecular simulation software. Various element and alloy interatomic potentials are available from multiple developers, and the number continues to grow. Users and developers have also requested conversions of interatomic interaction models between different file formats, and we are working on both the conversions and tools to be released publicly.

We have also performed structural, thermodynamic, and kinetic analyses on several popular models of Aluminum optimized to have good liquid properties but which display qualitatively different crystallization behavior, in order to document these differences in a systematic way. In this way we have examined the pair correlation functions, thermal expansions, and liquid diffusion coefficients, respectively, as functions of temperature. This has helped identify issues related to technical implementation of property evaluations in order to maintain consistency in approach (simulation times, data analysis methods, etc.). We are also examining formats and methods for publishing or disseminating the collected information in a user-friendly way.

This work is the first step in a larger program to provide researchers with the tools to evaluate how well interatomic potentials for multicomponent alloys, as well as interactions of metals with ceramics and polymers, model the properties of real materials. This will help improve the quality of atomistic simulations for design and nano-metrology.



Volume comparisons for liquid Aluminum.

Learn More

Chandler A. Becker
(Metallurgy Division)
(301) 975-5344
chandler.becker@nist.gov
www.nist.gov/metallurgy

Publications

NIST Interatomic Potentials Repository: http://www.ctcms.nist.gov/potentials/

Mendelev MI, Kramer MJ, Becker CA and Asta M *Analysis of Semi-Empirical Interatomic Potentials Appropriate for Simulation of Crystalline and Liquid Al and Cu* Phil. Mag., 88 1723-1750 (2008)

Becker CA, Hoyt JJ, Buta D and Asta M *Crystal-melt Interface Stresses: Atomistic Simulation Calculations for a Lennard-Jones Binary Alloy, Stillinger-Weber Si and Embedded Atom Method Ni* Phys. Rev. E, 75 061610 (2007)

Becker CA, Olmsted D, Atas M, Hoyt JJ and Foiles SM *Atomistic Underpinnings for Orientation Selection in Alloy Dendritic Growth* Phys. Rev. Lett., 98 125701 (2007)