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FINAL REPORT

A Workshop on Developing Potentials for Atomistic Simulations

Air Force Office of Scientific Research AFOSR-91-0142

Prepared by

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12/20/91

UM—AFOSR Workshop:

DEVELOPING POTENTIALS FOR ATOMISTIC SIMULATIONS

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6.	*John Ferrante*	*NASA, Cleveland*
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8.	*William Goddard*	*California Institute of Technology, Pasadena*
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Developing Potentials for Atomistic Simulations

Abstract

A small group of researchers met recently to review the new and rapidly growing field of many-atom potentials for solids. The workshop was held on September 25-27, 1991, in Ann Arbor, MI, and was commissioned by the Air Force Office of Scientific Research. Some classes of materials are being well treated by many-atom potentials, while others are just now being considered. Combinations of materials including more than one type of bond seem clearly beyond our present capabilities. The systematics of many-atom potential development are in their infancy, and progress appears to be rapid.

Introduction

"We could model that for you if we only had an accurate interatomic potential for that material[1]". Scientists and engineers in the materials community who are theoretically or numerically inclined are finding themselves making statements like that more often these days. Solid state physicists, quantum chemists, and materials scientists or engineers are excited by their early successes in collaborations to develop tools to predict the properties of real material defects at the atomic level. Some are now envisioning that if their capabilities continue to develop they may be able, say, to design metal-matrix composites via atomistic numerical simulation. While this excitement is due primarily to advances in simple many-atom potential or energy methods, the need to expand the capabilities of these methods is currently the rate-limiting step in this field. Here we report a summary of a workshop on that subject held at the University of Michigan on September 25-27, 1991. The workshop was commissioned by the Air Force Office of Scientific Research.

In the last 20 years or so it has become possible to compute total energies and electronic structures of extended defects, such as crystalline surfaces, from first principles. The number of non - equivalent atoms that can be treated that way is limited to between 10 and 50. This is indicated schematically[2] in Fig. 1, where first-principles methods are indicated as local density functional. Tight-binding methods, in which Hamiltonian matrix elements are obtained via fitting to first-principles or experimental results, are simpler to apply than first principles methods, and allow the treatment of defects containing up to several hundred atoms. Recently, several groups have proposed simpler methods or expressions for obtaining total energies or forces as a function of atomic arrangements or geometries. These empirical methods often require computational effort comparable to that needed for pair-potential applications, but they nevertheless include the many-atom effects which are now known to be essential. These are denoted as many-atom potentials in Fig. 1, where it is suggested that they could allow the treatment of up to 100,000 inequivalent atoms. While this capability is certainly exciting, there are currently known limitations of many-atom potentials. For example, the treatment of partially ionic - partially covalent bonds is at best approximate. Mixing elements of covalent, ionic, and metallic bonds are even more difficult. A classic example of a system which currently can not be treated reliably via many-atom potentials is a metal/ceramic interface such as one might find in a composite.

Representatives from most of the groups developing many-atom potentials gathered together in Ann Arbor to assess limitations and strengths of these new methods and to attempt to decide how best to proceed to improve their generality and accuracy. In addition, there were in attendance those who specialize in numerical simulations, and they indicated needs or requirements of these new potentials which would be important for their applicability. A list of workshop participants and their addresses is attached. While the group is small, it includes solid state physicists, quantum chemists, and materials engineers, consistent with the interdisciplinary nature of this relatively new field. There were also practitioners present from all three of the types of methods shown in Fig. 1.

Talk Summaries

In this sections we will give a brief summary of talks given by those at the workshop. In the final section we will attempt to summarize the sense of the members of the workshop as to the status of the field and suggestions for how to proceed.

Needs for Potentials in Simulations

Dave Srolovitz led off our discussions by citing needs for interatomic potentials in new atomistic simulation methods. Among other things, he suggested that it was important that potentials be continuous up to at least third derivatives with respect to atomic coordinates so that dynamical matrices can be easily treated. He also cited structural stability of predictions as being critical. For example, one would not want to predict that the known ground-state crystal structure of a material was unstable, as could happen if the potential were not correctly formulated. Finally, he discussed the local harmonic model[3], which is a method for including entropy and hence temperature effects given a many-atom potential, with computational requirements comparable to those needed for the many-atom potential itself. This illustrates a common limitation of many-atom potential methods, namely that strictly speaking they apply only at $T = 0K$, and hence require additional computation to consider the effects of temperature.

Angularly Dependent Many-Atom Potentials

The majority of the talks were devoted to describing methods of including bond-angle effects in a many-atom potential approach. In this section, we briefly summarized eight talks on the subject.

Stephen Foiles argued that the embedded atom method[4], which has been applied with considerable success to fcc metals, is not adequate for bcc metals because of the expectation that angular interactions would be important for the latter. He then proposed a tight-binding approach for bcc metals, which relies on a moments method up to the fourth moment for the electronic density of states and an additive repulsive pair interaction[5]. This is a scalar version of the model proposed by Carlsson discussed below. Six adjustable parameters are fit to 9 experimental quantities. Results for defect properties of Mo show agreement with experiment.

The universal energy relation[6], which is important to several[7-11,20] of the many-atom potentials, was reviewed by John Smith. It has been discovered that the total energy as a function of distance between atoms has the same form for adhesion, cohesion, and chemisorption on metals and covalent semiconductors. This provides an anchoring point for several of the many-atom potentials, as discussed earlier. Smith then discussed the equivalent crystal theory[7], which is derived from a perturbation theory in which the environment of an atom in a defect is taken in lowest order to be a single crystal. The ***equivalent crystal*** is that single crystal whose lattice constant is such that its energy per atom is equal to the energy of the atom in the defect. The energy of the atom in the defect is then simply obtained from the universal energy relation. The perturbation involves an average distance term, as well as 2 atom terms and a small number of 3 and 4 atom terms including nearest neighbors only, but the ease of applicability of the method is comparable to a pair potential calculation. The method is semiempirical, with an input of 6 experimental constants. Results for surface energies, adhesion, and surface atomic relaxations on fcc and bcc metals were found to be in good agreement with experiment and/or first principles computation. A prediction of a new phenomenon in adhesion called avalanche[11] was made. Application of the method to metallic alloys was described by Bozzolo[12], as will be discussed below.

The application of the equivalent crystal theory to semiconductors was next discussed by Tom Perry[7]. He gave results for surface energies and (1x1) atomic relaxations for the (100) surfaces of Si, Ge, and diamond. Predictions are in good agreement with first principles results. Perry then discussed the computation of the (2x1) reconstruction of Si(100). Again results for reconstruction energies and atomic locations agreed well with first principles results. Angular terms, which were found to be relatively unimportant in (1x1) relations on the semiconductors and metals treated, were seen to be significant in the (2x1) reconstruction. Results for internal strain in Si and Ge were in good agreement with first principles calculations and in reasonable agreement with experiment.

John Moriarty presented a set of interatomic potentials including angular 3 and 4-atom potentials. They are based on the first- principles, density functional version of the generalized pseudopotential theory[13]. The pseudopotential theory is extended to surfaces[14] by transforming the total-energy functional to a local-environment representation in which both the volume term and the multi-atom potentials are modulated by local averages of the electron density or the density of states. The coefficient of each d-state contribution is adjusted to fit experimental or theoretical data on cohesive and vacancy formation energies, bulk structural energies, elastic constants, and phonon frequencies. Like the equivalent crystal theory[7], this method goes beyond embedded atom theory[8] by including 3 and 4-atom angular terms. The predicted surface energies[14] seem relatively insensitive to the choice of electron-density or density of states modulation, with the result for Mo in better agreement than for Cu with first principles results. Surface relaxations were found to be sensitive, however, with the density of states modulation providing good agreement with first principles results.

The next author to discuss angularly dependent many-atom potentials was David Pettifor, who formulated his potential within tight-binding Huckel theory[5,15-16]. Pettifor writes his many-atom potential as the sum of a pairwise repulsive term and a bond energy term. The latter term is written as a sum of products of bond integrals and bond orders. The bond energy term is attractive, and contains the angular effects. The bond order is defined as the difference between the number of electrons in bonding and antibonding states, and is calculated explicitly by using the recursion method [17]. The bond integrals were obtained by diagonalizing the two-center Huckel secular equation with nearest-neighbor interactions only. Pettifor found that 3 and 4 - atom contributions are essential for the correct prediction of structural trends.

Like Foiles, Pettifor, and - as we shall see below - Kress, Voter, Baskes, and Ho, Anders Carlsson[18] writes the total energy as the sum of a pairwise repulsive term and an attractive bonding term. Carlsson's method is based on a tight-binding Hamiltonian in which, e.g., fourth moments of the electronic density of states are written in terms of products of interatomic coupling strengths summed over a matrix of hopping paths. As mentioned earlier, Foiles' method is a scalarized version of this, with the bonding energy written as a scalar function of the second and fourth moments. There are only 4 parameters in Carlsson's method, and these are fitted to the cohesive energy, equilibrium lattice constant, and the three independent elastic constants. Predicted vacancy formation energies and bcc - fcc structural energies agree well with experiment for Cr, Mo, and W. A good description of surface structural energetics is demonstrated for W(100), although the reconstruction amplitude appears somewhat sensitive to the choice of fit.

Joel Kress and Arthur Voter[19] also write the total energy as the sum of a bond energy and a pairwise repulsive term. Again the directional bonding effects are incorporated in the bond energy through energy moments evaluated over atomic orbitals. Here only the first two moments are included. The second moment matrix is diagonalized to achieve rotational invariance of the coordinate system, hence the name rotated-second-moment approximation (RSMA). Fcc - hcp energy differences were obtained, even though higher moments were not included. For Ir, potential parameters were fitted to 9 input data values. Tests against Ir data suggested a generalization[20] of the RSMA, in which the bonding energy was required to agree with the form of the universal energy relation[6]. This allowed good agreement with experiment to be obtained for Ir.

The final paper in this section was presented by Mike Baskes. He discussed a modified embedded atom method (MEAM)[21]. As with the other speakers in this section, his goal was to include angular effects, and like many of the speakers he chose to write his total energy as a sum of a pairwise repulsive term and a bonding or embedding term. However, his bonding term is not written as a function of *the electronic* density of states or moments thereof, but rather the argument was taken to be an electron density. So far, this prescription is the same as that followed in the EAM. Baskes then suggested two modifications of EAM. First, the embedding term was taken to be a logarithmic function of the electron density. Secondly, he included in the electron density angle-dependent terms which result in bond-bending forces. He then fitted 8 parameters to experimental data and tested predictions of the method against other experimental data for fcc and bcc metals, as well as C, Si, and Ge. He also discussed applications to alloy systems and including screening effects.

Alloys

Guillermo Bozzolo presented a new semiempirical method[22] for alloys which is based on the equivalent crystal theory[7]. He wrote the total energy of an atom in an alloy as the sum of a strain energy and a chemical energy. The strain energy the atom is computed using equivalent crystal theory, treating all of the atom's neighbors as if they were of the same element as the atom. The chemical energy is then the change in energy due to some neighbors not being of the same element. The experimental input data is the same as for the equivalent crystal method, plus two data points for a binary alloy. The initial choice for the two alloy data points was heats of solution in the two dilute limits. As with equivalent crystal theory, the ease of application is comparable to that of a pair potential calculation. The Connolly-Williams[23] procedure was used to relate the energies of ordered compounds to the disordered ones. Predicted heats of formation and lattice parameters as a function of concentration for 12 binary transition metal alloys were found to agree well with experiment.

Developing and Testing Interatomic Potentials

Jerry Tersoff provided a welcome discussion of methods and strategies for developing and testing many-atom potentials. This kind of information is needed, and is generally omitted from researcher's talks and publications. There were a number of tips made, and a few will be noted here. The functional form of the potential should be at least physically motivated, the data base for parameter fitting should include at least the elastic constants, and the potential should be tested for incorrect ground states by melting and quenching. This last test would be unnecessary for perturbation methods[7] which guarantee the correct ground state, but is essential for most approaches. He suggested setting up a battery of subroutines for routine testing new potential forms against an array of data.

Tight-Binding Methods

Kai Ming Ho described a new[24–25] empirical tight-binding force method for molecular-dynamics simulations of Si and C. He writes his total energy in the familiar (as in the methods described here of Foiles, Pettifor, Kress, Voter, and Carlsson), form of the sum of a band-structure or bonding energy term and a short-ranged two-body potential representing the sum of the ion-ion repulsion and the correction to the double counting of the electron-electron interaction in the band-structure energy term. The band-structure term is computed in a two-center tight-binding approximation following Chadi[26] which takes as input 6 matrix elements determined by fitting to the calculated bulk band structure. A difference between Ho's approach and those described above is that he doesn't make continued fraction or moment's method approximations in computing the electronic density of states. Another difference is that the two-body potential is obtained without fitting to experimental data, rather by subtracting the band-structure term from the universal energy relation[6] for the limiting case of volume changes with a fixed ground-state crystal structure. Molecular dynamical calculations can be done for about 500 atoms with this method. A large array of anharmonic, defect and cluster results were presented for Si and diamond, including the structure and dynamics of the C_{60} buckyball.

A tight-binding LMTO approach to electronic and atomic structure of extended defects in metals was presented by Mirek Sob in collaboration with V. Vitek and Y. Oh. Sob correctly argued that there are cases where ab initio calculations provide information where no experimental data exist, such as segregation of Bi to grain boundaries in Cu. His method begins with the tight-binding LMTO approach of Andersen[27] et al. A difficulty is encountered in an electrostatic term in the total energy, which is dealt with through a warping correction containing two parameters which are adjusted to reproduce the bulk modulus and one of the second-order shear elastic constants. Calculations of twist grain boundaries in Cu are in progress.

Effective Medium Theory

Recent developments in the effective medium theory were discussed by Karsten Jacobsen[28]. This is a method which is based on a local density functional calculation of the energy to embed an atom in a uniform electron gas. It has been shown[6] that the embedding energy in a uniform electron gas as a function of the gas density has a universal form. For an actual solid, the effective uniform electron density is determined by summing electron densities from neighboring atoms. In addition to the embedding energy, the atomic binding energy in a solid includes an overlap energy and a one-electron energy. Several applications were discussed, including computations of surface self-diffusion energies and layer-by-layer contributions to stacking fault energies.

Partially - Ionic Materials

The important but presently very difficult subject of modelling metal - ceramic interfaces was presented by Tony Harker, work in collaboration with A. M. Stoneham, D. M. Duffy, J. H. Harding, and P. W. Tasker. Earlier reviews can be found in Refs. 29 - 30. Harker discussed treating the oxide - metal interfacial interaction by classical electrostatics, including struggling with the known[31] deviation from the image potential at separations of the order of 2 Å or less. Various schemes for calculating oxide potentials were reviewed[30] and results presented for the MgO/Ag interface.

John Ferrante, in collaboration with H. Schlosser, J. R. Smith, W. Leaf, P. Vinet, and J. H. Rose (see Refs. 32 - 35), has investigated limitations and generalizations of the universal binding energy relation[6] as a function of the amount of charge transferred in a partially - ionic bond. The universal binding energy relation has been very useful in simplifying a number of methods discussed above when applied to metals and covalent semiconductors. It would therefore be desireable to understand how it should be used in the case of charge transfer. Studies were first carried out for 150 diatomic molecules, where good spectroscopic data was known to exist. It was found that for all molecules examined which did not contain a halogen atom the usual universal binding energy relation reproduced the experimental data adequately. A simple generalization ensued[33−34], in which a Coulombic term was added to the universal binding energy relation, and this produced good results even for the halogen-containing molecules. This applies also to solids[32,35], with the inclusion of the Madelung constant. This suggests that there is a simple potential form even when there is charge transfer.

What is still needed is a method for simply calculating the charge transfer in selfconsistent manner. This was proposed by William Goddard[36], in collaboration with A. K. Rappe. An atomic chemical potential is constructed from atomic ionization potentials, electron affinities, atomic radii, and shielded electrostatic interactions between all charges. Equilibrium charges that depend on geometry are computed by requiring equal chemical potentials. Results for simple examples of organic, inorganic, biological, and polymer systems seem reasonable.

Gas - Solid Interface

Donald Brenner ended the workshop with what might be called a bang, with a talk on molecular chemistry at the gas - solid interface, including shock and detonation chemistry and reactive hydrocarbon dynamics. Of particular interest was his[37] modification of the Abell[38] - Tersoff[9] formalism to treat radicals as well as single, double, and triple carbon bonding. This would seem to be an attempt to include both global and local information in a quasi-local formulation. Results including detonations, buckyball compressions, and adhesive indentations were presented.

Summary

There are a small but growing number of researchers that are attempting to develop reliable many-atom potentials for materials simulations. Now is an early time in the life of this field, and most found it quite valuable to exhange ideas at this point. It is an interdisciplinary effort by nature and necessity, and exciting progress is being made. This is particularly true of applications to fcc metals and covalent semiconductors like Si. Initial results for bcc metals and binary metal alloys look promising as well. Ceramics and other materials with partially - ionic bonding are just now being considered in a many-atom context and most of the progress there is for the future. Combinations of materials including metallic, covalent, and partially-ionic bonds are clearly beyond our capabilities at present. Systematics for developing new many-atom potentials are also in the exploratory stage. Given the need for such potentials and the quality and variety of backgrounds and tools availabled to the scientists and engineers that are currently pursuing them, it would seem that one should expect rapid progress in this field in this decade.

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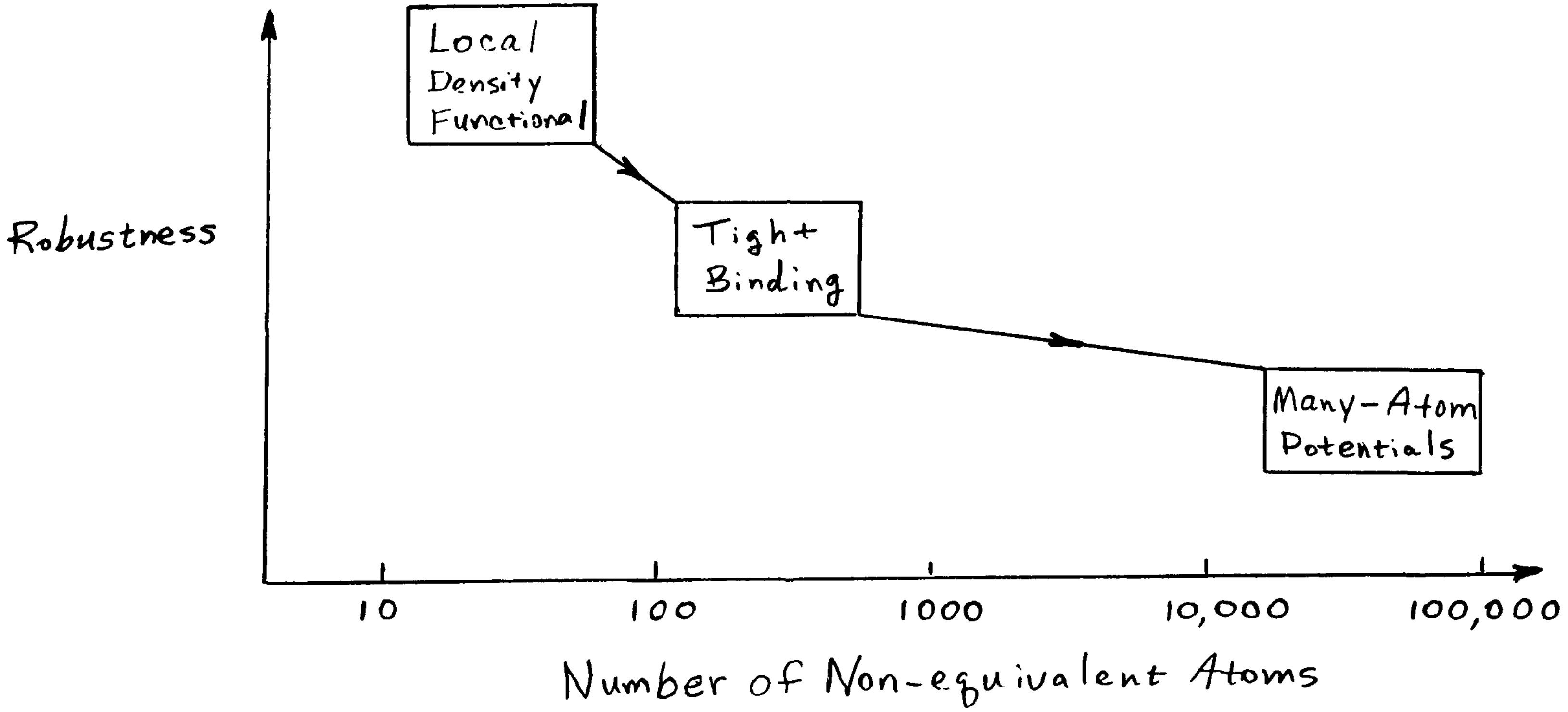
Figure Captions

1. A schematic for three types of methods indicating their robustness versus the number of non-equivalent atoms that is practical to treat with the method. By robustness we mean the variety of material combinations and defect configurations that the method can be relied upon for accurate predictions.


Robustness
Local Density Functional
Tight Binding
Many-Atom Potentials
10
100
1000
10,000
100,000
Number of Non-equivalent Atoms