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Development of lattice inversion modified embedded atom method and its applications

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ABSTRACT

The modified embedded atom method (MEAM) has been widely used in describing the physical properties of elemental crystals, alloys and compounds with multiple lattice structures. We report here the development of a reliable procedure to reduce the complexity of the MEAM formalism by removing the many-body screening function. In the proposed formulation, the interatomic pair potential is obtained by applying Chen-Möbius lattice inversion up to fifth nearest neighbors, so that the cohesive energy curve can be reproduced faithfully. The newly developed model (Lattice Inversion MEAM, LI-MEAM), which can be viewed as a direct extension of the embedded atom method (EAM), no longer requires the computation of many-body screen functions and has fewer adjustable parameters than MEAM. As an illustration, we optimized the potential parameters of body centered cubic iron (bcc-Fe). The values of the calculated physical properties agree well with experimental results. We further investigated the size-dependent melting behavior of bcc-Fe nanoparticles (NPs) with particle size ranging from 725-atom (~25 Å) to 22899-atom (~80 Å) using replica exchange molecular dynamics (REMD) simulations. Our simulations show advantages of LI-MEAM in modeling of the melting process and quantitatively reveals that the liquid skin melting (LSM) process of bcc-Fe NPs.

1. Introduction

Atomistic simulations are powerful techniques to explore the physical properties of materials on micro scales. While simulations with billions of atoms or millisecond time span can be achieved on super computers nowadays [1,2], the reliability and accuracy of the simulation results depend critically on the quality of the interatomic potentials [3]. Many efforts have been devoted to the development of more accurate and reliable potentials for describing the interactions between specific atoms [4–8]. Among the various models, the embedded atom method (EAM) proposed by Daw et al. [4,5] is an elegant and powerful model for describing atomic interactions in bulk metals. To make EAM applicable to more complex systems, several modifications and extensions to EAM were proposed. Johnson and Oh [9,10] developed the analytical embedded atom method by choosing appropriate analytical forms for all the EAM functions (AEAM). Later on, Zhang, Hu and Ouyang [11,12] added an analytical modification term to the AEAM expression of cohesive energy and proposed a modified form of the EAM potential. Lee and Cho [13] extended EAM by introducing a local structural dependent prefactor with three additional parameters to account for the bond characteristics arising from asymmetrical surface atoms. Shan et al. [14] reported an extension of EAM potentials applied to alloy nanoparticles by refining the original EAM embedding and cross-pair functionals. Some works have also been done to improve the EAM accuracy by incorporating the Chen-Möbius lattice inversion [15–19] method into the potential fitting process [20–23]. In summary, most of these extended models could show relatively good performance in describing the properties of specific systems. However, due to the lack of angular electron density dependence, EAM derived models in general lack the transferability to apply to other none-close packed structures,

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complex oxides, or systems with partial covalent bonding characteristics [3].

Aimed at improving the description of directional bonding in solids, Baskes et al. [24–27] modified the EAM by considering three directional partial electron densities in addition to the original spherical component, which conceptually represent p, d, f orbitals with different angular momentum, and put forward the modified embedded atom method (MEAM). Due to the consideration of the interactions from only the first nearest neighbors, it is also named as the first nearest-neighbor MEAM (1NN MEAM). The 1NN MEAM stands out for its universality and accuracy, and could describe the properties of a variety of metals and alloys accurately [26,27]. However, it faces difficulties in modeling some bcc transition metals, such as incorrect ordering among low-index surface energies and structural instability [28]. In order to mitigate these shortcomings, Lee et al. [28] modified 1NN MEAM by extending the interactions to the second nearest neighbors, and proposed the second nearest-neighbor MEAM (2NN MEAM). Compared to 1NN MEAM and previous EAM models, 2NN MEAM is a more accurate model for describing metals, alloys and covalent systems. Much efforts have also been made by Lee et al. [28–31] and other researchers [32,33] on building up a database of potential parameters based on 2NN MEAM.

In the practical application of MEAM (If not specified below, MEAM refers to both 1NN MEAM and 2NN MEAM.), an additional many-body screening function must be introduced to cutoff the interactions from neighbors beyond first or second nearest neighbors on the electron densities and pair energies, which increases the complexity of this model [26–28]. Furthermore, there seems to be a lack of systematic way for the determination of the parameters associated with the many-body screening function. For pure element, there are two parameters, $C_{\max}$ and $C_{\min}$, which are related to screening function. But the parameter set quickly grow into a large set as a total of eight parameters of $C_{\max}$ and $C_{\min}$ (A-A-B, B-B-A, A-B-A, A-B-B) are needed for binary AB alloys, and the parameter size increase exponentially for multicomponent systems [3,31,33]. In MEAM formalism where the interaction is limited to first or second neighbors, the many-body screening function is needed as a practical approach to obtain the desired accuracy. In the present work, we report the reformulation of the MEAM model by using Chen-Möbius lattice inversion method (Lattice Inversion MEAM, LI-MEAM). By incorporating the lattice inversion technique, we have successfully removed the many-body screening function, which makes MEAM formalism simpler. From another point of view, it provides transparent physics, which can be viewed as a direct extension of EAM by considering the directional partial electron densities. Also, the number of adjustable parameters has been reduced. In order to validate the developed LI-MEAM model, the potential was parameterized for body centered cubic iron (bcc-Fe), which is a classical benchmark for many body potentials. Some key physical properties of Fe were calculated and compared with the results of experiments and other potential models. Furthermore, the size-dependent melting behavior of bcc-Fe nanoparticles (NPs) was investigated using replica exchange molecular dynamics (REMD) simulations [34,35].

2. Methodology

2.1. Chen-Möbius lattice inversion

Chen-Möbius inversion formula was first derived by Chen based on the number theory [15] and then applied to a variety of inverse problems in physics [36–38]. Later on, Chen et al. [17–19] developed a series of lattice inversion methods by inverting cohesion for interatomic potential in bulk materials and adhesion for interatomic potential across interfaces. The following is a brief introduction to the fundamentals of Chen-Möbius lattice inversion.

Theoretically speaking, any cohesive energy for a multidimensional crystal lattice can be expressed as a sum of many-body interactions, which include two-body, three-body, …, n-body interactions. If only two-body interactions are considered, the expression for cohesive energy per atom, E, can be simplified as the following:

$$E = \frac{1}{2}\sum_{j(\neq i)} \Phi(r_{ij}), \tag{1}$$

where r_{ij} represents the lattice vector from site i to site j, $\Phi(r_{ij})$ is the corresponding pair potential. Considering a standard reference structure, such as bcc or fcc, $\Phi(r_{ij})$ can be expanded along the orders of nearest neighbors, then Eq. (1) can be written as:

$$E(r) = \frac{1}{2}\sum_{m=1}^{\infty} Z_0^{(m)} \Phi\left(a_0^{(m)} r\right), \tag{2}$$

where m is the order of the nearest neighbors and ranges from 1 to infinity, $Z_0^{(m)}$ is the actual number of m-th nearest neighbors, $a_0^{(m)}$ is the ratio of the distance of m-th nearest neighbors to r, which is the distance for the first nearest neighbors.

In order to apply Chen-Möbius lattice inversion to obtain pair potential function from Eq. (2), a mathematic technique is used to extend the original series $\{a_0^{(m)}\}$ to a multiplicative semi-group $\{a^{(m)}\}$ such that, for any two integers i and j, an integer k always exists which satisfying:

$$a^{(i)}a^{(j)} = a^{(k)}. \tag{3}$$

Then Eq. (2) can be rewritten as:

$$E(r) = \frac{1}{2}\sum_{m=1}^{\infty} Z^{(m)} \Phi\left(a^{(m)} r\right), \tag{4}$$

where

$$Z^{(m)} = \begin{cases} Z_0\left(a_0^{-1}\left[a^{(m)}\right]\right) & a^{(m)} \in \left\{a_0^{(m)}\right\} \\ 0 & a^{(m)} \notin \left\{a_0^{(m)}\right\} \end{cases}. \tag{5}$$

Note that $\{Z_0^{(m)}\}$ is the actual numbers of the m-th nearest neighbors, and $\{Z^{(m)}\}$ is the extended group which contains $\{Z_0^{(m)}\}$ with all the additive elements equal to zeros. Eq. (4) is a standard form available for applying Chen-Möbius lattice inversion directly to invert the relationship between the two involved functions, saying $E(r)$ and $\Phi(r)$. The inverted equation is shown as:

$$\Phi(r) = 2\sum_{m=1}^{\infty} I^{(m)} E\left(a^{(m)} r\right), \tag{6}$$

where the inversion coefficient $I^{(m)}$ is given by:

$$\sum_{a^{(m)}|a^{(k)}} I^{(m)} Z\left[a^{-1}\left(\frac{a^{(k)}}{a^{(m)}}\right)\right] = \delta_{k1}, \tag{7}$$

and δ_{k1} is Kronecker delta function.

Fig. 1 shows the scheme about how to obtain the pair potential from the cohesive energy by applying Chen-Möbius lattice inversion. The arrows in the figure represent the determinant relationships between the involved parameters or physical quantities. In details, the cohesive energy $E(x)$ can be obtained from experiments