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Comparative investigation of a newly optimized modified embedded atom method potential with other potentials for silicon

Bin Liu [a,b], Hao Zhang [b], Junyong Tao [a,*], Xun Chen [a], Yun'an Zhang [a]

[a] Science and Technology on Integrated Logistics Support Laboratory, College of Mechanics and Automation, National University of Defense Technology, Changsha 410073, China
[b] Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB T6G 2V4, Canada

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ABSTRACT

Genetic algorithm (GA) is used to optimize the parameter set of the second nearest-neighbor modified embedded atom method (2NN MEAM) interatomic potential for silicon (Si). The optimization is carried out by tuning the parameters to match a set of physical properties including elastic constants, point defect formation energy, phase transformation, surface formation/relaxation and stacking faults. Besides the physical properties for optimization, other molecular dynamics (MD) predictions such as surface reconstruction, point defect diffusion, dislocations and thermal properties are also calculated to test the robustness of the new potential. Another purpose of this work is to compare various physical properties of available MEAM potentials for Si (and Tersoff and SW where necessary). It is shown that the new potential gives a better description in surface, stacking fault and dislocation. Finally, extensive discussion is given to specify the applicability of this potential and the validity of the potentials on fracture simulation.

1. Introduction

In technological areas such as integrated circuit (IC), micro-electro-mechanical systems (MEMS), Si is a very important material. Besides, as a representative covalent element, it has great significance in theoretical research. With the great progresses in semiconductor processing technologies, Si micro/nano structures are fabricated at ever-decreasing length scales, making it necessary to understand material behaviors at nano or even atomic scale.

Several techniques enable investigation of atomic interactions, among which quantum mechanics-based density functional theory (DFT) and empirical method molecular dynamics (MD) are most widely used. DFT can accurately describe covalent nature, which, however, cannot deal with a system with thousands of atoms despite of rapid development of computers technologies. Somehow, many physical phenomena, such as dislocation emission and expansion, can be only observed in large systems. Therefore, (semi-)empirical potentials play a critical role in simulation experiments.

Over 30 (semi-)empirical potentials for Si can be found in published Ref. [1], mainly in SW [2], Tersoff [3], EDIP [4], EAM [5], MEAM [6] formalisms. MEAM is a semi-empirical one and able to maintain the brittle nature of Si [7–9]. Though a modified SW can describe the brittleness of Si [10], it reproduces much worse elastic constants and melting point than the original one. In addition, MEAM can predict many physical attributes as good as other empirical approaches, like elastic constants, surface relaxation/reconstruction, phase transformation [11]. Hence MEAM is a better choice for simulating mechanical properties of Si.

By adding angular terms in the EAM model [5], Baskes et al. initially proposed MEAM formalism [6] that has been constructed for 26 elements [12], including gas elements nitrogen, oxygen and hydrogen. The original MEAM just took the first nearest neighbor atoms into consideration, thus showed some drawbacks when applied for BCC crystals [13]. To fix this, Lee and Baskes developed the 2NN MEAM [13], a more generalized version. MEAM model for Si has been modified for different purposes. For example, Lee [11] improved the description of surface relaxation, thermal expansion and amorphous structure; Swadener et al. [14] modified the potential parameters to get a better description of vacancy clusters; Ryu's version [15] gives a better agreement with melting point and latent heat.

Effects of surface and dislocation on the mechanical performances become increasingly prominent as the scale decreases. Stacking fault is closely related to dislocation which is inseparably linked with mechanical behaviors such as fracture, residual stress and fatigue failure. As a brittle material, Si is extensively deemed

* Corresponding author.
E-mail address: taojunyong@gmail.com (J. Tao).

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to be inaccessible to fatigue fracture. Nevertheless, it has been experimentally confirmed that Si would fatigue and generate dislocations under ambient condition [16,17]. To our knowledge, there is still no MEAM potential that is optimized considering stacking fault of Si. Lenosky et al. [18] developed a new MEAM formalism known as HOEP that gave better stacking fault formation energies than the other MEAM potentials for Si though it was not specially optimized for stacking fault. Anyhow, we think the agreement is not good enough and needs improvement. As for surface, the most concerned are formation, relaxation and reconstruction properties, which are closely related to grain boundary, twin and surface effects. In engineering fields, silicon usually exists in polycrystal. Therefore, for a better description of polycrystal Si structures, MEAM should basically predict surface properties well enough. As mentioned above, though Lee [11] has optimized the parameter set to better predict surface properties, we intend to go further in this research.

This paper mainly reports two aspects. First, the parameters of 2NN MEAM potential for Si are optimized using GA, and various MD predictions are compared with experimental values, first principle calculations, and other MEAM counterparts. Moreover, we calculated some other properties, like melting point and enthalpy change, to test the reliability of this new potential. Second, as MEAM model cannot describe every physical property very well with a specified set of parameters, the respective advantages of MEAM potentials from Baskes et al. [6], Lee [11], Jelinek et al. [19], Ryu et al. [15], Lenosky et al. [18], Cui et al. [20], Swadener et al. [14] are figured out, so that researchers can choose the appropriate parameter set according to investigation targets.

2. Methodology

2.1. 2NN MEAM interatomic potential

The complete 2NN MEAM theory can be found in Ref. [21]. Here we introduce its primary frame and illustrate the differences from other related literatures. In the 2NN MEAM model, the total energy of a system is calculated as

$$E = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j\neq i}\phi(R_{ij}) \right] \tag{1}$$

where $F_i(\bar{\rho}_i)$ is the embedding function, $\bar{\rho}_i$ is the background electron density at site i, and $\phi(R_{ij})$ is the pair interaction between atoms i and j at a distance R_{ij}. Lenosky's MEAM formalism is slightly different from (1). Details can be found in Ref. [18].

The embedded function is given by

$$F(\bar{\rho}) = AE_c(\bar{\rho}/\bar{\rho}^0)\ln(\bar{\rho}/\bar{\rho}^0) \tag{2}$$

where A, E_c and $\bar{\rho}^0$ are respectively adjustable parameter, sublimation energy and background electron density for the reference structure.

The background electron density $\bar{\rho}$ consists of spherically symmetric partial electron density $\rho_i^{(0)}$ and angular contributions $\rho_i^{(1)}$, $\rho_i^{(2)}$ and $\rho_i^{(3)}$ with the following expression

$$\left(\rho_i^{(0)}\right)^2 = \left[\sum_{j\neq i}\rho_j^{a(0)}(R_{ij})\right]^2 \tag{3}$$

$$\left(\rho_i^{(1)}\right)^2 = \sum_{\alpha}\left[\sum_{j\neq i}(R_{ij}^{\alpha}/R_{ij})\rho_j^{a(1)}(R_{ij})\right]^2 \tag{4}$$

$$\left(\rho_i^{(2)}\right)^2 = \sum_{\alpha,\beta}\left[\sum_{j\neq i}(R_{ij}^{\alpha}R_{ij}^{\beta}/R_{ij}^2)\rho_j^{a(2)}(R_{ij})\right]^2 - \frac{1}{3}\left[\sum_{j\neq i}\rho_j^{a(2)}(R_{ij})\right]^2 \tag{5}$$

$$\left(\rho_i^{(3)}\right)^2 = \sum_{\alpha,\beta,\gamma}\left[\sum_{j\neq i}(R_{ij}^{\alpha}R_{ij}^{\beta}R_{ij}^{\gamma}/R_{ij}^3)\rho_j^{a(3)}(R_{ij})\right]^2 - \frac{3}{5}\sum_{\alpha}\left[\sum_{j\neq i}(R_{ij}^{\alpha}/R_{ij})\rho_j^{a(3)}(R_{ij})\right]^2 \tag{6}$$

where $\rho_j^{a(h)}$ is the atomic electron densities of j at a distance R_{ij} relative to the site i, and R_{ij}^{α}, R_{ij}^{β}, R_{ij}^{γ} are components of the distance vector between atoms i and j.

The total background electron density is calculated by combining the contributions in a specified form. In this work, we use the most widely used form:

$$\bar{\rho}_i = \rho_i^{(0)}G(\Gamma) \tag{7}$$

where Gamma function $G(\Gamma)$ can be expressed in different ways

$$G(\Gamma) = \frac{2}{1+\exp(-\Gamma)} \tag{8.1}$$

$$G(\Gamma) = \begin{cases} \sqrt{1+\Gamma}, & \Gamma \geqslant -1 \\ -\sqrt{|1+\Gamma|}, & \Gamma < -1 \end{cases} \tag{8.2}$$

where Γ is calculated as

$$\Gamma = \sum_{h=1}^{3} t^{(h)}\left[\rho_i^{(h)}\Big/\rho_i^{(0)}\right]^2 \tag{9}$$

It is worth noting that (8.1) is used in this work. Some other literatures [12,14,19] used (8.2). $t^{(h)}$ are adjustable parameters. The atomic electron density is given by

$$\rho^{a(h)}(R) = \rho_0 \exp\left[-\beta^{(h)}(R/r_e - 1)\right] \tag{10}$$

where $\beta^{(h)}$ are adjustable parameters, r_e is the nearest neighbor distance in the equilibrium reference structure. The scaling factor ρ_0 has no effect on pure element system, thus usually set 1.

In reference structure, the energy per atom is a function of nearest-neighbor distance R, which can be written as [22]

$$E^u(R) = -E_c(1 + a^* + d\cdot(a^*)^3)\mathrm{e}^{-a^*} \tag{11}$$

$$a^* = \alpha(R/r_e - 1) \tag{12}$$

$$\alpha = (9B\Omega/E_c)^{1/2} \tag{13}$$

$$d = \begin{cases} d_{\text{repuls}}, & a^* < 0 \\ d_{\text{attrac}}, & a^* > 0 \end{cases} \tag{14}$$

In (11), the universal function $E^u(R)$ is used to describe a uniform expansion or contraction in the reference structure, B is the bulk modulus, Ω is the equilibrium volume per atom, d_{repuls} and d_{attrac} are adjustable parameters, which in most published literatures were set $d = d_{\text{repuls}} = d_{\text{attrac}}$. However, we have found that d_{repuls} has great impact on surface, self-interstitial and stacking fault, and d_{attrac} on stacking fault and phase transformation. We can get much better stacking fault predictions when d_{repuls} and d_{attrac} are dealt with independently.

In 2NN MEAM frame, $E^u(R)$ can also be expressed as

$$E^u(R) = F[\bar{\rho}^0(R)] + (Z_1/2)\varphi(R) + (Z_2S/2)\varphi(aR) \tag{15}$$

where Z_1 and Z_2 are respectively the number of first- and second-nearest neighbor atoms, a is the ratio between the first- and second-nearest-neighbor distances, and S is many-body screening factor decided by two adjustable parameters $C_{\max}$ and $C_{\min}$, see Ref. [23].