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Development of a second-nearest-neighbor modified embedded atom method potential for silicon–phosphorus binary system

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ABSTRACT

Phosphorus (P) is one of the most common impurities in silicon (Si). To investigate the effects of P on the mechanical properties of Si at nano or atomic scale, the second-nearest-neighbor Modified Embedded Atom Method model (2NN MEAM) potentials for pure P and Si–P binary system are developed using genetic algorithm (GA). The reference physical properties for the parameterization for pure P include cohesive energies, lattice constants, bulk moduli and first order pressure derivatives of experimentally-existing phases. The van der Waals interactions in P are not considered since it's beyond the description of MEAM and it's less important in covalently bonded Si–P compounds. For Si–P binary system, cohesive or formation energies, lattice constants and elastic constants of typical Si–P structures, properties of point defects and P–vacancy pairs are considered. The robustness of the newly developed potentials is examined by testing the thermal stability and transformation from non-equilibrium to ordered phase. The effects of P on the tensile behaviors of bulk Si are demonstrated. Results show that phosphorus lowers the fracture threshold and stiffness of bulk Si.

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1. Introduction

Si is a technologically important material in integrated circuit (IC), micro-/nano- electro-mechanical systems (MEMS/NEMS), solar cell, etc. As a representative covalent element, it has great significance in theoretical research and has drawn much attention during the past decades. In engineering, P is one of the most common dopants in Si and plays a critical role in its electrical properties. In addition, P significantly influences the mechanical [1] and thermal [2] properties of Si, about which many experimental reports [1,3–5] can be referred to. In order to reveal the underlying mechanisms behind the experimental phenomena, it's essential to raise an atomistic-scale technique.

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 provides the most reliable information about materials at atomistic-scale, which, however, cannot deal with a system with thousands of atoms despite of rapid development of computer technologies. Somehow, many physical phenomena, such as dislocation emission and expansion, can be only observed in large systems. Therefore, empirical potentials are applied extensively in simulation experiments.

Only a few empirical potentials for Si–P binary system can be referenced in the literatures [2,6]. Lee and Hwang [2] developed a SW potential for Si–P binaries to better describe the effects of P impurities on the thermal conductivity of Si. Wilson et al. [6] investigated the diffusion of P on the surface of Si crystal using Environment-Dependent Interatomic Potential (EDIP) model. In addition, some other P-based multi-element potentials can be referred to. For example, Ackland et al. [7] developed a Fe–P potential based on DFT calculations. This model, as the authors pointed out, is unable to describe covalent materials, thus is only suitable for low P concentration systems. Above-mentioned empirical models are applicable for only a few elements and have unsatisfactory extendibility for the other elements. Moreover, they are incapable of maintaining the brittle nature of Si. Although Hauch et al. [8] observed brittleness using the modified SW potential, some other important properties such as elastic constants and melting point become unacceptable. Mattila et al. [9,10] and Sheng et al. [11] developed a potential for Ni–P binary system using Embedded Atom Method (EAM) model which has been applied successfully for many elements and multi-element systems. However, it cannot perform well in describing amorphous Si. Mattila's and Sheng's work have enlightened us that EAM model can be used for

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P-based system, then the MEAM model developed from EAM can accordingly be applied in our work. A 2NN MEAM potential for pure P has been developed by Ko et al. [12]. Considering the critical role of reference structure in the thermal stability of Si crystal with high P concentration, we have to develop a new parameter set for P according to the specific requirements in this work. MEAM potential can maintain the brittleness of Si [13–15], and give good predictions for thermal [16], vacancy [17], phase stability [18], stacking faults [19] and amorphous [18] properties. It is thus clear that MEAM is a solid choice for our work.

MEAM was constructed by Baskes et al. [20] by adding angular terms to EAM formalism [21], and has been extensively applied in a wide range of fields. Currently, 26 elements have been covered by MEAM [22], including metal materials, semiconductors, gas elements like nitrogen (N), oxygen (O), hydrogen (H), which shows the universality of MEAM formalism. Lee and Baskes developed a more generalized version, second-nearest-neighbor modified embedded atom method model (2NN MEAM) [23], which has been widely used for binary and ternary systems [24]. Up to now, Si-based multi-element MEAM potential include Si–Ni [25], Si–Li [26], Si–Al/Fe/Cu/Mg [27].

To lay the foundation of investigating the effects of P impurities on the mechanical properties of Si in our future work, this article reports the development of 2NN MEAM potentials for pure P and Si–P binary system using genetic algorithm (GA). The reference physical properties for parameterization are all from experiments or higher level calculations. The van der Waals interactions (existing in white (α) P, black P (A17) and a transformed phase (A7)) are omitted by only taking single molecule white (α) P (written P4), single layer A17 and A7 into account. Then the potential is extended to the Si–P binary system to describe various structural arrangements including typical diamond-like compounds, phases reported in phase diagram, and dopant P related defects. The robustness of the newly developed potentials is examined by testing the thermal stability and transformation of Si crystal with high P concentration from non-equilibrium to ordered arrangement. Last, the effects of P on the tensile behaviors of Si are tested to give explanations to experimental phenomena.

2. Methodology

2.1. 2NN MEAM interatomic potential

The complete 2NN MEAM theory can be found in Ref. [24]. Here we introduce its primary framework and illustrate the differences from other related literatures. In the 2NN MEAM model, the total energy of a system is given as:

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

where $F_i(\bar{\rho}_i)$ is the embedding function, $\bar{\rho}_i$ is the background electron density at site i. S_{ij} and $\phi(R_{ij})$ are respectively the screening function and the pair interaction between atom i and j separated by a distance R_{ij}. The background electron density $\bar{\rho}$ consists of four terms (one spherically symmetric partial term $\rho_i^{(0)}$ and three angular contributions $\rho_i^{(1)}$, $\rho_i^{(2)}$ and $\rho_i^{(3)}$) associated by the adjustable parameters $t^{(h)}$ (h = 1–3).

Background electron density $\bar{\rho}$ is calculated as follows:

$$\bar{\rho}_i = \rho_i^{(0)} G(\Gamma) \tag{2}$$

Gamma function $G(\Gamma)$ can be expressed as:

$$G(\Gamma) = \frac{2}{1+\exp(-\Gamma)} \tag{3.1}$$

$$G(\Gamma) = \begin{cases} \sqrt{1+\Gamma}, & \Gamma \geqslant -1 \\ -\sqrt{|1+\Gamma|}, & \Gamma < -1 \end{cases} \tag{3.2}$$

where Γ combines $\rho_i^{(0)}$, $\rho_i^{(1-3)}$ and $t^{(1-3)}$, see Ref. [24]. (3.1) is used in this work, while some other literatures applied (3.2) [17,22,27].

The atomic electron density is given by:

$$\rho^{a(h)}(R) = \rho_0 \exp[-\beta^{(h)}(R/r_e - 1)] \tag{4}$$

where $\beta^{(h)}$ (h = 0–3) are adjustable parameters, r_e is the first neighbor distance of the reference structure. The scaling factor ρ_0 has no effect on pure element systems while greatly affect multi-element systems.

In MEAM formalism, pair interaction $\phi(R)$ doesn't have any formula. Instead, it is evaluated from the values of the total energy per atom in the reference structure, where individual atoms are on the exact lattice point, and the embedding energy, as a function of the nearest-neighbor distance. The total energy per atom is estimated from the zero-temperature universal equation of state of Rose et al. [28]. Reference structure is crucial for a MEAM potential since it directly influence its reliability [29]. The reference structure applied in this work is diamond-structured, i.e. interlaced FCC for alloy, with the Space Group F$\bar{4}$3m, see Fig. 1(a), which has been reported to experimentally exist [30]. We have tested B1-NaCl structure, the most commonly used reference structure [24,27,29], which can well reproduce the reference physical properties. However, the thermal stability of Si7P (Fig. 1(b)) is not acceptable. B2, l12 and C11 are also considered and passed for the same reason. F$\bar{4}$3m gives overall better predictions on various properties, especially lattice constant of F$\bar{4}$3m, elastic constants of Si7P, thermal stability and transformation from non-equilibrium to ordered arrangement of Si7P. For F$\bar{4}$3m -SiP structure, the total energy per atom (1/2Si + 1/2P) is given as:

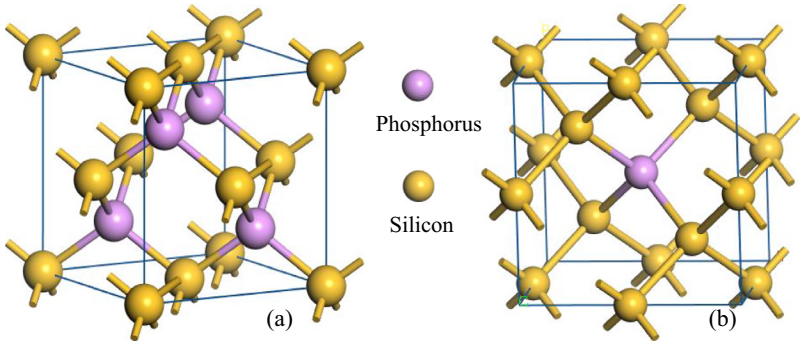

Fig. 1. Schematic view of (a) F$\bar{4}$3M and (b) Si7P.

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