Double lattice potential for silicon for molecular dynamics simulation

Hui Zhang,a) Chongyang Wei, Zhongwu Liu, Xichun Zhong, Dongling Jiao, Wanqi Qiu, and Hongya Yu
School of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, People’s Republic of China

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Double lattice (DL) potential, which is constructed from two interatomic potentials for face centered cubic (fcc) lattice, is proposed for molecular dynamics (MD) simulations of silicon. The potential for fcc lattice is simply the well-known Lenard-Jones (LJ) potential. The DL potential, as well as Tersoff potential, Stillinger and Weber (SW) potential, environment-dependent interatomic (EDI) potential, charge optimized many-body (COMB) potential, and modified embedded-atom (MEAM) potential has been applied for the validity test in MD simulations. By calculating the distribution functions of the distances between atoms and the angles between the lines linking an atom with its nearest neighbors and comparing the results with that of perfect silicon crystal, the crystal lattice of simulated system can be identified. The crystal lattice, the crystallization temperature, binding energy, and elastic constants for the above potentials have been calculated from MD simulations. The results have shown that the systems with Tersoff, SW, EDI, COMB, and MEAM potentials could not show the diamond structure as the one with DL potential shows. The physical parameters obtained from the simulations with DL potential are in agreement with the experiments. The paper is helpful for rethinking the nature of chemical bond and the formation of crystal.

I. INTRODUCTION

Silicon is a technologically important semiconductor element and one of the most heavily studied materials. During the past decades, atomistic computation methods have played an important role in the research of semiconductor Si and its compounds along with the experimental methods. With the decrease in silicon chip size, the experimental investigation on both physical and chemical behaviors of these nano silicon clusters becomes more and more difficult and the atomistic computation methods become especially more important. However, silicon is a covalent crystal and the description for the covalent bond in atomistic computation methods is a hard issue. Theoretically, the density functional theory (DFT) may give the most accurate result, but the time and the computation power required for the system consisting of a few hundred of atoms are very huge and expensive. Therefore, DFT may not be a good choice. A feasible approach instead is to construct an empirical potential, and then to calculate both the physical and chemical parameters of the system with the application of this potential in MD simulations.

So far, the interatomic potentials for silicon include Tersoff potential, Stillinger and Weber (SW) potential, environment-dependent interatomic (EDI) potential, charge optimized many-body (COMB) potential, and modified embedded-atom (MEAM) potential. Among these, Tersoff potential, SW potential, EDI potential, and COMB potential are many body potentials. In these potentials, in addition to the pair term for the interatomic coupling between two atoms, there is a three-body term that can describe the interatomic coupling among three atoms or define the so-called bond angles. Furthermore, COMB potential also takes into account the effect of charge. It is expected that these many-body potentials could present an appropriate description for silicon. For this purpose, the authors have calculated the relevant parameters required for the potentials, and tested the validity which includes the elastic constants, binding energy, radial distribution function, and so on. These physical parameters tested are important for one substance, but what’s most important is whether the diamond structure could be reproduced with the interatomic potential applied in MD simulations.

In fact, the diamond structure could not be formed in MD simulations even if the physical parameters given with one interatomic potential are in good agreement with the experimental data. For instance, for the embedded-atom (EAM) potential which is successfully applied in the metallic elements and alloys, the crystal lattices in agreement with the experiments could be reproduced with the corresponding EAM potentials in MD simulations. However, for silicon showing the diamond structure, with the above-mentioned interatomic potentials applied in MD simulations, no simulated systems can show the diamond structure and these potentials could not pass the validity test of crystal structure. Therefore, our goal is to construct a new interatomic potential for silicon. With this potential the diamond structure could be reproduced in MD simulations and the physical parameters are accordingly obtained.

The diamond structure could be regarded as the penetrating of two fcc lattices and there are eight atoms in its crystal cell. It is reasonable to reproduce the diamond structure from two fcc interatomic potentials and one interatomic potential between two lattices. So far there mainly exist EAM potentials for fcc lattice. However, too many parameters introduced in EAM potentials make it difficult to define the interatomic coupling

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a)Electronic mail:zhope@scut.edu.cn
between two fcc lattices. Here, we only take into account the simple Lenard-Jones (LJ) potential. Recent investigation has shown that the ground state of LJ potential corresponds to the hexagonal close packed lattice \((c/a \approx 1.633, a \) and \(c \) being lattice constants of hcp lattice) by MD simulations, and the systems could also show the meta-stable fcc lattice under some simulation circumstances\(^{12}\). The Bravais lattices have been identified by comparing the results from simulated systems with those of perfect hcp and fcc lattices. Further investigations have indicated that with the combination of several LJ potentials and without setting any initial Bravais lattices, the diamond and graphite structures\(^{13}\) and more complex perovskite \(\text{ABO}_3\) structure\(^{14}\) have been reproduced in MD simulations. These results are helpful for understanding and rethinking the significance of LJ potential and the formation of crystal structure.

In this paper, double lattice (DL) potential has been constructed to reproduce the diamond structure of silicon. DL potential and the above mentioned interatomic potentials have been applied in MD simulations, and the crystal structure, the crystallization temperature, lattice constants, binding energy, and elastic constants have been obtained and compared with the experiments.

II. MODELLING AND SIMULATIONS

A. The modelling

For the description of the crystal structure of silicon, simple LJ potentials are used and can be expressed as:

\[
U(r) = 4\epsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right) \tag{1}
\]

where \(\epsilon\) is the depth of the potential well, \(\sigma\) is the finite distance at which the inter-particle potential is zero, and \(r\) is the distance between particles.

In the model, two types of atoms denoted as A and B are introduced in and they are physically identical to each other. They may be corresponding to two spin configurations for a silicon atom. For example, there are four spins up for A atom and four spins down for B atom. A and B atoms should show their own lattices, and their lattices and lattice constants are the same. Here, unlike other models in which all Si atoms are the same, A and B atoms in our model are treated as two distinguishable Si atoms. There are interactions between A and B lattices, which can be simply treated with the same description as that for A atoms (B atoms). Here, LJ potential is used for A lattice, B lattice, and the interaction between A and B lattices, and the equilibrium distance between atoms and the crystallization temperature are determined by LJ potential.

B. Simulation detail

In the simulation, without setting any initial Bravais lattices, A and B atoms are equally and randomly created in the simulation box and the boundary conditions are applied. For LJ potential, the cutoff is denoted as \(r_c\). The maximum temperature for the system is not high above the temperature \(T_0\) (3000 K), and then an energy minimization procedure follows. NPT operation is implemented at \(T_0\) for 1 picosecond with a timestep of \(10^{-16}\) picosecond. The temperature of the system \(T\) decreases from \(T_0\) with a temperature step \(n\), and then one NPT operation is implemented for 0.1-1 picosecond at each temperature \(T\). The parameters for LJ potentials in MD simulation are listed in Table I.

To obtain the stress versus strain relations for Si crystal from MD simulations, a perfect Si crystal is created. The initial fcc lattices for A and B atoms with the same lattice constants of 5.414 Å are created and the relative displacements of A lattice with respect to B lattice are 0.25, 0.25, and 0.25 in the \(x\), \(y\), and \(z\) directions, respectively. One NPT operation is implemented for 1 picosecond at 300 K, and then small deformations of the system follow. The values for the stress caused by the deformations are calculated and the stress versus strain relation is obtained. Consequently, the elastic constants \(c_{11}, c_{12},\) and \(c_{44}\) are calculated and the in-script can be referred to Ref. [15]. Some physical parameters from DL potential are also compared with those from other potentials such as Tersoff, SW, EDI, COMB, and MEAM potentials.

The numbers of atoms for the simulations are 512, 1000, and 8000, respectively. MD simulations are carried out with the aid of lammmps software\(^{18}\) and the in-script can be referred to Ref. [12-14]. The visualization is done with VESTA software\(^{17}\).

C. Identification of the crystal structure of the system

To test the validity of DL potential, the first thing to do is to check whether the system shows the diamond structure. Here the distribution functions of distances between atoms and the angles between the lines linking an atom with its nearest neighbors \(\rho(d)\) and \(\rho(\theta)\) are calculated for the simulated system and a reference system consisting of perfect silicon crystal, and then the difference between simulation and the reference systems is checked for the lattice identification. For perfect Si crys-

| Atom | \(\epsilon\) (eV) | \(\sigma\) (Å) | \(r_c\) (Å) |
|------|----------------|-------------|-----------|
| A    | 0.22           | 3.58        | 3\(\sigma\) |
| B    | 0.22           | 3.58        | 3\(\sigma\) |
| AB   | 0.22           | 1.94        | 3\(\sigma\) |

TABLE I. The parameters for LJ potentials in MD simulations.
tal, the distribution functions consist of a small number of discrete values. If the distribution functions from the simulations show non-zero values at these corresponding positions, then the system shows the same crystal structure as that for perfect Si crystal. This is similar to the phase identification in x-ray diffraction (XRD). In the simulation, the coordinate of any atom at any temperature at any time \((x, y, z)\) is known so that both the distances between atoms and the angles between the lines linking an atom with its nearest neighbors can be calculated. The distribution function \(\rho(d)\) (or \(\rho(\theta)\)) means the count values or intensity of the distances \(d\) (or the angles \(\theta\)) in the range of \(d-d+\Delta d\) (or \(\theta-\theta+\Delta \theta\)). In the calculation, if the distances between one atom \(R\) and its nearest neighbors are \(d_R\), then the minimum distance of these distances \(d_R\) is found to be \(d_m\) for the number of the nearest neighbors of one atom is always more than one and the values for \(d_R\) are different. As a result, the atom is regarded as one of the nearest neighbors of atom \(R\) if \(d_R/d_m < 1.1\).

The distribution function \(\rho(d)\) is similar to the conventional radial distribution function \(g(r)\), but their algorithms are different. The angle \(\theta\) is the bond angle for some crystal structures like the diamond structure. In the case of silicon, for the calculation of distribution functions, A and B atoms are treated as one type of atoms for the whole system, and also can be treated separately for A (B) subsystem.

**III. RESULTS AND DISCUSSIONS**

**A. The phase transition and identification of the crystal structure**

Several different interatomic potentials have been proposed for the description of silicon during the past several decades, and they include Tersoff, MEAM, EDI, SW, and COMB potentials. There are also some modified versions for some potentials, for example, Tersoff-Mod (TM) potential\(^{18}\) from Tersoff model, and MEAM-Spline (MEAMS) potential\(^{19}\) from MEAM. Figure 1 shows the dependence of energy per atom and volume per atom on the temperature. As shown in Fig. 1, for Tersoff potential case, the system is always in a simple crystalline state. The simulation fails because the volume of the system quickly increases to infinity once the temperature is above 1800 K (see Fig. 1(a)). This means that the system with Tersoff potential will never enter into a liquid state and always shows the diamond structure. In the case of TM potential, the system can enter into a liquid state. As shown in Fig. 1(a), the energy per atom deceases with the decrease in temperature until the temperature approaches about 1300 K, and there is an abrupt change in energy, indicating that there is a phase transition. However, there is a sudden increase in the volume. This happens for the simulations with EDI, MEAM, MEAMS, SW, and COMB potentials. There is also a clear thermal hysteresis, especially for the simulation with DL potential. For DL potential case, both the energy and volume decrease when cooling from high temperature, and there is a liquid-crystalline phase transition. This is in agreement with the experiments. As shown in Fig. 1(a), the energy per atom in the case of DL potential is about 2.18 eV at 100 K, only about half those from other potentials. The value for the volume is in good agreement with experimental data. For the simulations with EDI, MEAM, MEAMS, SW, TM, and COMB potentials, the energy per atom is the binding energy of one Si atom. In the case of DL potential, the energy per atom means the binding energy between A and A atoms (or A and B atoms), and the binding energy for A (or B) atom equals that of A atom plus that of B atom. Here, for \(\epsilon_A=\epsilon_B=\epsilon_{AB}\), the binding energy for one Si atom is two times that of A atom, i.e., \(2\times2.18=4.36\) eV. The value for binding energy is close to the accurate value of 4.63 eV for silicon at 0 K\(^{20}\).

Figures 2 and 3 show the distribution functions of the distances between atoms and the angles between the lines
FIG. 2. The distribution functions of the distances between atoms and the angles between the lines linking one atom with its nearest neighbors ρ(d) (a) and ρ(θ) (b) with different interatomic potentials applied in MD simulations at T=100 K. Note that for COMB potential T=50 K.

The stability of the diamond structure is linked to the potential used. For the Tersoff potential, the system shows a clear change, with a peak at 109.5° at T=100 K, but it is not crystalline from ρ(d) as shown in Fig. 2(a). At T=4000 K, these peaks disappear, and all the systems are in a liquid state (see Fig. 3(a)). Figure 4 shows the atomic configurations with different interatomic potentials applied in MD simulations at T=100 K. As shown in Figs. 4(e) and 4(f), the system with Tersoff potentials is still crystalline, and the one with TM potential is clearly disordered. The abnormal change in energy may mean a transition from one liquid phase to another non-crystalline phase, as shown in Fig. 1. However, the sudden increase in volume does not agree with the experiments. The behaviors of the systems with EDI, MEAM, MEAMS, SW, and COMB potentials are also similar to that for TM potential (see Figs. 2, 3, and 4). Now, it can be seen from Figs. 1, 2, 3, and 4 that with MEAM, MEAMS, SW, EDI, TM, and COMB potentials the diamond structure could not be reproduced in MD simulations, and accordingly there are no lattice constants.

In Fig. 2, with DL potential, ρ(d) and ρ(θ) are in agreement with experimental data, even though the seventh peak of ρ(d) shows a small deviation. As shown in Fig. 3, ρ(d) and ρ(θ) at T=4000 K are similar to those for MEAM, MEAMS, SW, EDI, TM, and COMB potentials. In Fig. 4(h), it can be seen that every green atom has four black nearest atoms, and every black atom has also four green nearest atoms. Therefore, the system with DL potential is checked to show the diamond structure. As indicated in Fig. 1, the crystallization temperature (the temperature for the transition of liquid phase to crystalline phase) is 1780 K, and the lattice constant is 5.509 Å, slightly higher than its experimental values of 1687 K and 5.430 Å.

B. The relation between the diamond structure and fcc sublattice or hcp sublattice

Previous investigation has shown that the ground state for LJ potential corresponds to the hcp lattice. However, because the energy for fcc lattice is slightly higher...
FIG. 4. The atomic configurations with different interatomic potentials applied in MD simulations at $T=100$ K. Note that for COMB potential $T=50$ K.

FIG. 5. Dependence of energy per atom (a) and volume per atom (b) on the temperature with different temperature steps $n$ in MD simulations for DL potential. In Fig. 5, for $n=5$ K the system shows the lowest energy and volume, and the highest crystallization temperature of 1780 K. The volume increases slightly with increasing temperature step.

Figure 6 shows the distribution functions of the distances between atoms and the angles between the lines linking one atom with its nearest neighbors $\rho(d)$ and $\rho(\theta)$ with different temperature steps $n$ applied in MD simulations at low temperatures for DL potential. At $n=5$ K, A and B subsystems both show the hcp lattice. However, there are also a number of atoms in A and B subsystems showing the fcc lattice when the temperature step increases. For instance, at $n=40$ K, during the heating, there is a transition of fcc phase to hcp phase (see Fig. 6(a)). However, not all the atoms in the simulation box are showing the hcp lattice, and instead a mixture of fcc and hcp lattices coexists. Figure 7 shows the atomic configurations for the system at $n=40$ K and $T=50$ K for DL potential. The atomic arrangements for the fcc lattice are ABCABC····, and the hcp lattice shows ABAB··· arrangements, where A, B, and C are the close packed atomic layers, as indexed by dotted and dashed circles in Fig. 7. In Figs. 6(c) and 6(e), for A (or B) subsystem, the lattice constant of the crystal cell is $a_f$, which cor-
FIG. 6. The distribution functions of the distances between atoms and the angles between the lines linking one atom with its nearest neighbors $\rho(d)$ (a) and $\rho(\theta)$ (b) with different temperature steps $n$ applied in MD simulations at low temperatures for DL potential. (a)-(b) are for the whole A+B system, and (c)-(d) and (e)-(f) for A and B subsystem, respectively. In (a), (c), and (e), ad and af stand for the lattice constants for the diamond structure and fcc lattice, respectively, as indicated by the arrows.

responds to the $d_2$ value at which the subsystem shows the second peak in $\rho(d)$. The $d_1$ value is the shortest distance of the distances between atoms. As seen from $\rho(d)$ for the diamond structure, the lattice constant for the diamond cell is $a_d$, and $a_d$ is equal to $a_f$. There are four distances in one diamond cell. $d_2$ and $d_4$ are accordingly $d_1$ and $d_2$ for subsystems, and $d_1$ and $d_3$ are the distances between A and B atoms. $d_1$ and $d_2$ have been defined in LJ potentials, but the distances between A and B atoms from the simulations are slightly different from those defined in LJ potentials. The angles are $60^\circ$, $90^\circ$, and $120^\circ$ for fcc sublattice, and $60^\circ$, $90^\circ$, $109.5^\circ$, and $120^\circ$ for hcp sublattice. With the diamond lattice formed from two hcp lattices or two fcc lattices, the distribution functions are changing significantly.

C. A comparison of DL model with experiments

Table II lists the crystallization temperature, lattice constant, binding energy, and elastic constants obtained with different interatomic potentials applied in MD simulations. For other potentials, the simulations have revealed that the systems could not show the diamond structure. As listed in Table II, the elastic constant $c_{11}$ is about 13% larger than the experimental data, and $c_{12} = c_{44}$. Despite this, in contrast with the results from other potentials, the agreement between the simulated results and the experimental data proves the validity of DL potential. The values for the binding energy from other potentials such as Tersoff potential are in good agreement with experimental data, but there is no diamond structure reproduced in MD simulations. This indicates that the crystal structure should be the first criterion for the validity test for the interatomic potentials.

LJ potential has been used in MD simulations several decades ago, and is thought to be only for rare gas or close packed atom systems by most researchers. With the crystal structure as the first criterion for the validity test, our previous results have shown that with one single LJ potential one can reproduce only the hcp or fcc lattice, and never reproduce other Bravais lattices such as body centered cubic (bcc) lattice\textsuperscript{12,23} or perovskite (ABO$_3$) structure\textsuperscript{14}. This demonstrates that LJ potential must be of significant importance in the construction of interatomic potentials.

For Tersoff and EDI potentials, except the pair term,
TABLE II. The crystallization temperature $T_c$, lattice constant $a$, binding energy $E_b$ at 100 K, and elastic constants ($c_{11}$, $c_{12}$, and $c_{44}$) obtained with different interatomic potentials applied in MD simulations. Experimental data are from Ref. [20].

| Potential | $T_c$(K) | $a$(Å) | $E_b$(eV) | $c_{11}$(GPa) | $c_{12}$(GPa) | $c_{44}$(GPa) |
|-----------|----------|--------|-----------|--------------|--------------|--------------|
| EDI       | 4.44     | 165.83 | 69.86     | 112.09       |              |              |
| MEAM      | 4.34     | 157.08 | 63.44     | 194.65       |              |              |
| MEAMS     | 4.46     | 113.24 | 62.45     | 86.72        |              |              |
| SW        | 4.12     | 149.37 | 75.91     | 108.36       |              |              |
| Tersoff   | 4.60     | 120.62 | 82.33     | 85.24        |              |              |
| TM        | 4.42     | 154.59 | 68.41     | 116.17       |              |              |
| COMB      | 4.40 (50 K) | 138.45 | 73.17     | 113.78       |              |              |
| DL        | 1770     | 5.509  | 4.36      | 187.26       | 106.22       | 106.03       |
| EXP       | 1687     | 5.430  | 4.63 (0 K) | 165.78       | 63.97        | 79.62        |

FIG. 7. The atomic configurations for the system at $n=40$ K and $T=50$ K for DL potential. ABAB··· atomic arrangements are circled by dashed lines, and ABCABC··· arrangements by dotted lines, where A, B, and C are the close packed atomic layers.

three-body term has been introduced in to define the bond angle and actually shown its power in the formation of the bond angle of 109.5° in MD simulations, as shown in Fig. 2(b). Unfortunately, the introduction of a three-body term does not lead to the diamond structure. So does the charge taken into account in COMB potential.

In order to reproduce the diamond structure in MD simulations with DL potential, three factors must be satisfied. First, two types of atoms must be created even though they are physically identical to each other. This actually means that Si atoms in diamond structure must be distinguishable as there are no distinguishable Si atoms in other potentials. Second, these two types of atoms must show their own sublattices. Here, A and B atoms can show the hcp lattice, or the fcc lattice. Third, the distance between A and B atoms determines the resulting crystal structure in MD simulations. If the shortest distance for A (B) atoms is $d_A$, and the shortest distance between A and B atoms is $d_{AB}$. When the ratio of $d_A/d_{AB}$ is in the range of 1.2-1.3, one can obtain CsCl structure. $d_A/d_{AB}$ values lie in the range of 1.3-1.6 for NaCl structure, 1.7-1.9 for the diamond structure, and 1.9-2.1 for graphite structure. For graphite structure, A and B atoms may show the hcp or fcc lattices, accordingly leading to $\alpha$ graphite or $\beta$ graphite. In the graphite structure, every single layer is a graphene.

Very interestingly, even though the ground state for LJ potential corresponds to the hcp lattice, the lattice for the subsystem can be self-adaptive to form an ordered structure when the distance between A and B atoms changes. In the case of CsCl structure, the sublattice is the simple cubic (sc) lattice with $d_A/d_{AB}$=1.2, and for NaCl structure, sublattice is only the fcc lattice with $d_A/d_{AB}$=1.4. This means that in MD simulations with LJ potentials, the systems can self-adapt its sublattice to form an energetically favorable ordered structure. However, because LJ potential shows a spherical symmetry, the resulting self-adaptive sublattice also shows the spherical symmetry.

IV. CONCLUSIONS

The results have indicated that with Tersoff, TM, SW, EDI, COMB, MEAM, and MEAMS potentials the diamond structure cannot be reproduced in MD simulations as the system with DL potential has successfully shown the diamond structure. The crystallization temperature, lattice constant, binding energy, and elastic constants have been obtained from the simulations with DL potential, and are in agreement with experimental data. This paper is helpful for rethinking and understanding the nature of chemical bond and the formation of crystalline matter.

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