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An analytic bond-order potential for the Fe–Cu system

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Abstract

An angular-dependent analytic bond-order potential (ABOP) for copper and Fe–Cu system was developed, based on the ABOP of pure iron introduced by Müller *et al* (2007 *J. Phys.: Condens. Matter* **19** 326220). The potential parameters for the present ABOP model of copper were determined by fitting to the experimental data of the basic properties of fcc Cu and *ab initio* calculated properties of bcc Cu. The model predicts the vacancy formation energy in good agreement with the experimental result, although no vacancy formation information was used in the fitting of the model parameters. The melting point of Cu is also properly reproduced. The Fe–Cu binary system was described by adding two independent cross parameters in the potential model. The cross parameters were fitted using the *ab initio* data of the formation energies and lattice parameters of fictitious Fe–Cu alloys. The potential was applied to investigate the point defects and small defect clusters in dilute Fe–Cu alloys. The results were compared with the *ab initio* data and the values obtained with other potentials.

1. Introduction

Copper precipitation is one of the most significant contributors to the irradiation embrittlement of reactor pressure vessel (RPV) ferritic steels. It is essential to obtain a detailed understanding of the precipitation process and the evolution of the precipitate structure in Fe–Cu alloys. The classic atomic scale simulation methods such as molecular dynamics (MD) and Monte Carlo (MC) enable a detailed investigation of the material process and phenomena at the atomistic level. However, the reliability of the results of such atomistic simulations is dependent on a reliable interatomic interaction model. Constructing a fully reliable empirical potential model for Fe alloys remains a great challenge, although Fe alloys are the most commonly used material for structural applications.

For pure iron, various potential models have been developed. In 1984, Finnis and Sinclair proposed an N -body potential for some bcc metals which is the so-called FS potential [1]. Ackland *et al* [2] developed a widely used potential of the FS form for bcc Fe and Fe–Cu alloys in 1997. Since 2000, some new potentials of iron have been established. Mendelev *et al* [3] published a set of potentials based on the embedded-atom method (EAM) [4], and a large set of experimental and first-principles calculated data was used for fitting and examining the potentials. The work of Mendelev was considered a significant advancement in describing the structure and properties of bcc Fe [5]. Dudarev and Derlet [6] proposed a ‘magnetic’ potential, in which an explicit magnetic contribution to the interaction energy of α -Fe atoms was introduced. Chamati *et al* [7] constructed their EAM potential which can reproduce the lattice properties, surface energies and point defect energies for both bcc and the high temperature fcc phases of Fe with satisfactory accuracy. Apart from these potentials based on a central force description, some angular-dependent interaction models were also developed [8–10]. As compared with the standard EAM potentials, the angular-dependent potentials can give an improved description of some properties of iron. In particular, a new angular-dependent analytic bond-order potential (ABOP) for iron was introduced by Müller *et al* [11]. The ABOP is taken to have the form of the Tersoff potential [12] which is usually used for modeling the energetics of covalent systems. It was found that the ABOP performs well in describing the various properties of Fe both in the bcc and fcc phases. The attractive feature of this model is that it can properly reproduce the α - γ - δ phase sequence of iron with rising temperature. Recently, the ABOP model was extended to describe the iron–carbon system [13].

For the Fe–Cu alloy, the most widely used potential model may be the FS potential of Ackland *et al* [2]. An EAM potential was developed by Luwdis *et al* [14]. Lee *et al* [15] developed a modified embedded-atom method (MEAM) potential. Recently, Pasianot and Malerba [16] proposed a new EAM potential which is based on the pure Fe potential of Mendelev *et al* [3] and the pure Cu potential of Mishin *et al* [17], and the cross potential is produced using the Ising formalism and the cluster variation method. It provides a good description of the thermodynamic properties of the Fe–Cu alloy as well as the interaction between Cu atoms and point defects in Fe, and has become a part of the potential model of the Fe–Cu–Ni ternary system [18].

To the best of our knowledge, at present only the ABOP developed by Müller *et al* [11] has the ability to reproduce the phase transformations of iron from bcc to fcc and then back to bcc before melting. Considering the success of the angular-dependent ABOP in describing the structures and properties of iron in various phases, we extended the angular-dependent ABOP to model the Fe–Cu alloy. The potential parameters of Fe were taken from the paper by Müller *et al* [11]. In this work, an ABOP of Cu is established and parametrized, then the Fe–Cu cross potential parameters are adjusted. The validity of the potential is inspected and discussed.

2. Potential model

The formalism of the present ABOP of Cu metal and Fe–Cu alloy is taken as the Tersoff potential [12, 19] in which the energy is modeled as a sum of pair-like interactions including an attractive term and a repulsive term. The coefficient of the attractive term plays the role of a bond order; it depends on the local environment and has a many-body form. The total energy E of a single component system is written by

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij}, \quad (1)$$

$$V_{ij} = f_C(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})]. \quad (2)$$

Table 1. Parameters for the ABOP of Cu.

A (eV)	B (eV)	λ (Å)	μ (Å)	β	m	n
37188.422	66.846	4.870	1.011	0.007338	3	1
η	c	d	h	R (Å)	S (Å)	
0.991	6.649	0.2315	0.2254	3.65	4.00	

where V_{ij} is the bond energy between atom i and j , and r_{ij} is the distance between the two atoms. The functions f_R and f_A represent a repulsive and an attractive pair potential, respectively. The functions b_{ij} represents a measure of the bond order between atom i and j . The bond order is dependent on the geometry, and thereby converts an apparent two-body interaction into a many-body one. The extra term f_C is a smooth cutoff function.

$$f_R(r) = A \exp(-\lambda r), \quad (3)$$

$$f_A(r) = -B \exp(-\mu r), \quad (4)$$

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-\frac{1}{2n}}, \quad (5)$$

$$f_C(r) = \begin{cases} 1, & r < R, \\ \frac{1}{2} \left[1 + \cos \left(\frac{r - R}{S - R} \pi \right) \right], & R < r < S, \\ 0, & r > S. \end{cases} \quad (6)$$

Here A , B , λ , μ , β , n , R and D are adjustable parameters of the potential. The function ζ_{ij} is taken as

$$\zeta_{ij} = \sum_{k \neq i, j} f_C(r_{ik}) g(\theta_{ijk}) \exp[\eta^m (r_{ij} - r_{ik})^m], \quad (7)$$

$$g(\theta) = \left(1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{[d_i^2 + (\cos \theta_{ijk} - h_i)^2]} \right), \quad (8)$$

where η , m , c_i , d_i and h_i are the potential parameters to be determined, and θ_{ijk} is the bond angle between bond $i-j$ and $i-k$.

The potential parameters for Cu are obtained by fitting to the structure and properties of copper. Both the experimental data for fcc Cu and the *ab initio* calculated data for bcc Cu are used in the fitting process. The fitting is carried out with the software GULP (general utility lattice program) [20]. An objective function is defined by the sum of squares:

$$F = \sum_{i=1}^{N_{\text{obs}}} w_i (f_i^{\text{obs}} - f_i^{\text{calc}})^2, \quad (9)$$

where N_{obs} is the number of observables, f_i^{obs} and f_i^{calc} are the fitted and calculated values of the i th observable, respectively, and w_i is the weighting factor for the given observable. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm is used for minimizing the objective function F . The empirical quantities used in the fitting include the lattice parameter, the cohesive energy, the elastic moduli, etc. The parameters of the potentials obtained by this approach are summarized in table 1. As mentioned by Yu *et al* [21], the ABOP cannot distinguish the fcc and hcp structures of Cu if only the first nearest neighbors interactions are included. To reproduce the relative stability of fcc and hcp Cu, the second nearest neighbors interactions are included in the ABOP model.

For binary systems, a new parameter χ was added by Tersoff [19], and equation (2) was modified as

$$V_{ij} = f_C(r_{ij}) [f_R(r_{ij}) + \chi_{ij} b_{ij} f_A(r_{ij})]. \quad (10)$$

Here $\chi_{ii} = 1$, and $\chi_{ji} = \chi_{ij}$, so there is only one independent parameter between different atom types in the above equation. Any ‘chemistry’ of atom pairs is included in this parameter. In this work, however, an additional parameter κ is used with $\kappa_{ii} = 1$ and $\kappa_{ji} = \kappa_{ij}$. Now equation (2) is written as

$$V_{ij} = f_C(r_{ij}) [\kappa_{ij} f_R(r_{ij}) + \chi_{ij} b_{ij} f_A(r_{ij})]. \quad (11)$$

In equation (11), the heteropolar bonds are strengthened or weakened by two parameters κ and χ , which are used to adjust the repulsive term and the attractive term respectively. Following the method of Ackland *et al* [2], the cohesive energies and lattice parameters of the fictitious alloys Fe₃Cu and Cu₃Fe with L1₂ structure calculated by the *ab initio* method are used to fit κ and χ . The potential parameters of Fe are taken from the paper of Müller *et al* [11]. The obtained values are $\kappa_{ij} = 1.180855$ and $\chi_{ij} = 0.725140$. Further mixed parameters are defined as

$$A_{ij} = \sqrt{A_i A_j}, \quad B_{ij} = \sqrt{B_i B_j}, \quad (12)$$

$$\lambda_{ij} = (\lambda_i + \lambda_j)/2, \quad \mu_{ij} = (\mu_i + \mu_j)/2, \quad (13)$$

$$R_{ij} = \sqrt{R_i R_j}, \quad S_{ij} = \sqrt{S_i S_j}. \quad (14)$$

3. Verification

3.1. Cu

Since the properties of Fe calculated with ABOP have been reported by Müller *et al* [11], in this paper we only discuss the ABOP model of Cu and Fe–Cu alloy. The predicted structural and cohesive properties of bcc Cu and fcc Cu by the present angular-dependent ABOP as well as the experimental and *ab initio* calculated data are listed in table 2. The results obtained from the potential proposed by Ackland *et al* [2] are also listed. The vacancy formation energy E_v^f was computed as the energy difference between the system with and without a single vacancy at constant number of atoms [5]. The E_v^f of fcc Cu predicted by ABOP is consistent with experimental data, even though the information of vacancy formation energy was not used for parameter fitting.

It is well known that the Cu precipitates have a bcc structure in the first stage of precipitation of Cu in bcc Fe. Thus, an investigation of the properties of bcc Cu is necessary. The energy difference between bcc Cu and fcc Cu is about 25 meV predicted by the ABOP, which is consistent with the values obtained by [2] and the *ab initio* calculated data. On the other hand, the optimized lattice parameter a_0 of the bcc Cu phase is 2.864 Å which can be compared with the a_0 value of 2.860 Å of bcc Fe predicted by the ABOP [11]. The lattice parameters of bcc Cu and bcc Fe predicted by [2] are 2.961 Å and 2.866 Å, respectively. As a result, in an atomic simulation the stresses around bcc Cu precipitates in bcc Fe obtained by the ABOP may be considerably lower than the results calculated by [2]. Furthermore, ABOP predicts that the lattice parameter of bcc Cu is larger than that of bcc Fe, which is in agreement with the result of the *ab initio* calculation of Becquart and Domain [31]. As for the tetragonal shear modulus, $C' = (C_{11} - C_{12})/2$, the *ab initio* calculations carried out by Liu *et al* [29] and Wang *et al* [30] showed that the unstable bcc Cu exhibits $C' < 0$. This phenomenon is not predicted by [2]. The value of C' of bcc Cu predicted by ABOP is in agreement with the result of Wang *et al* [28]. The structure of the hcp Cu was also optimized by the ABOP model. We obtained that the hcp/fcc energy difference is 0.008 eV, which is consistent with the value predicted by Mishin’s EAM potential [17].

In addition, the melting point of fcc Cu has been calculated with MD simulation. A straightforward two-phase simulation technique [32, 33] was used. With this method, two

Table 2. Properties of Cu predicted by the ABOP and compared with either experimental or *ab initio* data.

Description	ABOP	Ack97 ^a	Exp./ <i>ab initio</i>
<i>fcc-Cu</i>			
a_0	3.6050	3.615	3.6029 ^b
E_c	-3.49	-3.519	-3.49 ^c
B	150.3		137 ^c
C_{11}	180.5	168	176.2 ^d
C_{12}	135.2	121	124.9 ^d
C_{44}	82.5	75	81.8 ^d
E_v^f	1.20	1.19	1.03 ^e , 1.19 ^f , 1.30 ^g
<i>bcc-Cu</i>			
a_0	2.864	2.961	2.80–2.87 ^h
$\Delta E_{fcc-bcc}$	0.025	0.023	0.007–0.049 ^h
B	167.2	160	160–168 ^h
C_{11}	156.1	286	
C_{12}	172.8	190	
C_{44}	118.1	145	95.9 ⁱ , 112 ^j
C'	-8.4	48	-14.5 ⁱ , -6 ^j
E_v^f	1.15	1.34	

^a [2]; ^b [22]; ^c [23]; ^d [24]; ^e [25]; ^f [26]; ^g [27]; ^h [28]; ⁱ [29]; ^j [30].

Note: The *ab initio* data are in italics. a_0 : lattice parameter (Å); E_c : cohesive energy (eV/atom); B : bulk modulus (GPa); C_{ij} : elastic constants (GPa); C' : tetragonal shear modulus (GPa), $C' = (C_{11} - C_{12})/2$; $\Delta E_{bcc-fcc}$: cohesive energy difference between bcc and fcc structures (eV/atom); E_v^f : monovacancy formation energy (eV).

coexisting liquid and solid phases with an explicit interface is included in the MD cell. In the simulation if the temperature and pressure are close to the coexisting conditions of the system, it naturally evolves to the equilibration. Otherwise, either melting of the solid phase or solidification of the liquid phase can occur when the applied temperature of the system is significantly higher or lower than the melting point. In this work a series of constant-pressure constant-temperature (NPT) MD simulations were performed with the present ABOP model using the MD software LAMMPS [34]. The simulated melting temperature of Cu at zero pressure is 1150 ± 25 K, which is lower than the experimental melting point of 1358 K [23]. Using the same method we obtained that the melting points of bcc and hcp Cu are 1175 ± 25 K and 1150 ± 25 K, respectively. The predicted melting point of bcc Cu is even slightly higher than fcc Cu, which indicates that the present ABOP model is not perfect for reproducing the stability of the fcc copper at high temperatures.

3.2. Fe–Cu

The formation energies and lattice parameters of some fictitious Fe–Cu ordered alloys were calculated using the ABOP model. The results are listed in tables 3 and 4. The first-principles linear muffin-tin orbital (LMTO) data of $L1_2$ Fe₃Cu and FeCu₃ in table 3 were included in the Fe–Cu cross parameter optimization procedure. The values of lattice parameters for the $L1_2$ Fe₃Cu and FeCu₃ compounds calculated by Ackland *et al* [2] using the LMTO method were 3.546 Å and 3.555 Å, respectively. Considering the systematic underestimate of the lattice parameter introduced by the local-density approximation (LDA), the authors corrected the values to be 3.6493 Å and 3.6795 Å based on the computational error for pure Fe and Cu. The corrected data were used in the present fitting procedure. The predicted properties of some

Table 3. Calculated lattice parameters and formation energies of $L1_2$ Fe_3Cu and $FeCu_3$.

	Method	a_0 (Å)	E_f (eV/atom)	Reference
$L1_2$ Fe_3Cu	LMTO	3.6493 [†]	0.125	[2]
	MEAM	3.6345	0.158	[15]
	EAM	3.729	0.183	[14]
	ABOP	3.6656	0.140	This work
$L1_2$ $FeCu_3$	LMTO	3.6795 [†]	0.102	[2]
	MEAM	3.6378	0.133	[15]
	EAM	3.7144	0.178	[14]
	ABOP	3.6624	0.126	This work

Table 4. Calculated properties of bcc-based Fe–Cu ordered alloys.

	Method	V_0	E_f	B	Reference
$D0_3$ Fe_3Cu	PAW	12.0	0.153		[27]
	PAW	11.8	0.162	166	[29]
	FLAPW	12.0			[35]
	ABOP	12.3	0.153	167	This work
$D0_3$ $FeCu_3$	PAW	12.1			[27]
	PAW	12.1	0.180	143	[29]
	FLAPW	12.4			[35]
	ABOP	12.4	0.164	160	This work
B_2 $FeCu$	PAW	12.1	0.275	139	[27]
	PAW	12.0	0.281	134	[29]
	FLAPW	12.2			[35]
	ABOP	12.8	0.276	157	This work

Note: V_0 : atomic volume ($\text{\AA}^3$); E_f : formation energy (eV/atom); B : bulk modulus (GPa). PAW means the first principles projector-augmented wave method, FLAPW stands for the first principles full-potential linearized augmented plane-wave method.

fictitious bcc-based Fe–Cu ordered alloys are shown in table 4 for comparison. These data were not included in the parameter optimization, but the values predicted with the present ABOP model are in good agreement with the results obtained by first-principles calculations.

The substitutional energy of a single Cu atom in bcc Fe was also calculated. Following the calculating method of Domain and Becquart [36], the substitutional energy is defined by $E(nFe + 1Cu)_{\text{bcc}} - n \times E(Fe)_{\text{bcc}} - E(Cu)_{\text{fcc}}$, where $E(nFe + 1Cu)_{\text{bcc}}$, $E(Fe)_{\text{bcc}}$ and $E(Cu)_{\text{fcc}}$ are the energy of a supercell containing n Fe atoms and 1 Cu atom, the cohesive energy of α -Fe, and the cohesive energy of fcc Cu, respectively. In our calculation the lattice was relaxed isotropically during the energy minimization procedure, using the conjugate gradient algorithms implemented in the LAMMPS code [34]. We obtained the substitutional energy of 0.65 eV with a supercell containing 6750 atoms. We also used a large supercell containing 16 000 atoms and the result was 0.69 eV. The experimental value was 0.59 eV [36].

The binding energies between two entities (vacancies or substitutional Cu atoms) in a bcc Fe matrix are rather important characteristic energies, which reflect the relative stability of these entities. The binding energies E_b^{A-B} is defined as the difference between the formation energy of the system when the two involved objects (A and B) are far apart and close to each other [5]. A and B may be the first nearest neighbor, the second neighbor and so on. Some of the binding energies were calculated for a supercell containing N Fe atoms using the formula given by Becquart and Domain [31]:

$$E_b^{A-B} = E_{(N-1+A)} + E_{(N-1+B)} - E_{(N-2+A+B)} - E_{(N)}, \quad (15)$$

Table 5. Binding energies (eV) for the vacancy–vacancy (V–V), vacancy–Cu (V–Cu), and Cu–Cu in the bcc Fe matrix, compared with calculations of *ab initio* [31], EAM potentials of Ludwig [14, 31] and Ackland [2, 15], and MEAM potential [15]. Xnn means the Xth nearest neighbor.

	ABOP	<i>ab initio</i>	EAM (Ludwig)	EAM (Ackland)	MEAM
V–V (1nn)	0.14	0.14	0.16	0.14	−0.13
V–V (2nn)	0.20	0.28	0.21	0.19	0.02
V–V (3nn)	−0.10	−0.02	−0.04		
Cu–V (1nn)	0.07	0.17	0.19	0.087	0.098
Cu–V (2nn)	−0.09	0.28	−0.03	0.04	0.103
Cu–V (3nn)	0.02	0.04	−0.01		
Cu–Cu (1nn)	0.18	0.15	0.19	0.075	0.11
Cu–Cu (2nn)	0.03	0.04	−0.02	0.035	0.039
Cu–Cu (3nn)	−0.002	−0.01	−0.01		

where $E_{(N)}$ is the energy of the supercell of bcc Fe without defects, $E_{(N-1+A)}$ and $E_{(N-1+B)}$ are the energies of the supercell containing only one defect A and B , respectively, $E_{(N-2+A+B)}$ is the energy of the supercell containing both A and B . Obviously, the binding energy represents the change in energy before and after putting A and B together, and a positive binding energy indicates attraction between A and B , for the energy increases by separating them from each other. A supercell containing 6750 atoms was used in our calculation. The atoms were relaxed and the energy of the system was minimized at a constant volume. The results are shown in table 5, compared with the data obtained by *ab initio* calculation and by other potential models. The mean discrepancy between the results of ABOP and *ab initio* is the binding energy of Cu–V when the Cu atom is the second nearest neighbor to the vacancy. The *ab initio* calculation predicts that the Cu–V pair in the second nearest neighbor is more stable, which disagrees with the results of the ABOP and the EAM potentials but is consistent with the result of MEAM potential. However, the MEAM potential seems to underestimate the stability of the V–V pair.

The formation energies for different configurations of small vacancy clusters and Cu clusters as well as the Cu₂–V clusters in bcc Fe are shown in figure 1, compared with the results of the *ab initio* computation performed by Becquart and Domain [31]. In this work the formation energies of Cu clusters $E_f(\text{Cu})$ is calculated by $E_f(\text{Cu}) = E_{\text{cell}} - (N-n)E_{\text{c}(\text{bcc-Fe})} - nE_{\text{c}(\text{fcc-Cu})}$, where E_{cell} is the energy of the bcc Fe supercell containing N lattice sites and n -atom Cu cluster, $E_{\text{c}(\text{bcc-Fe})}$ and $E_{\text{c}(\text{fcc-Cu})}$ are the cohesive energies of bcc Fe and fcc Cu respectively. A 6750 atom bcc Fe supercell was used in our calculation. The energy minimizations of the supercell were performed with and without the relaxation of box. During the full relaxation the shape of the cell was maintained. One can see from figure 1 that our ABOP results are in good agreement with the *ab initio* data reported by Becquart and Domain [31].

4. Summary

In summary, an angular-dependent analytic bond-order potential has been developed for the Fe–Cu system based on the ABOP introduced by Müller *et al* [11]. The potential can give a good description of the properties of Fe–Cu alloys and the point defect system. These results suggest that the potential can be used to simulate the behavior of copper atoms in dilute Fe–Cu alloys. As far as Cu is concerned, many EAM potential for Cu have been established up to now (for example, see [17, 37, 38]). Obviously, describing Cu with an EAM potential is more

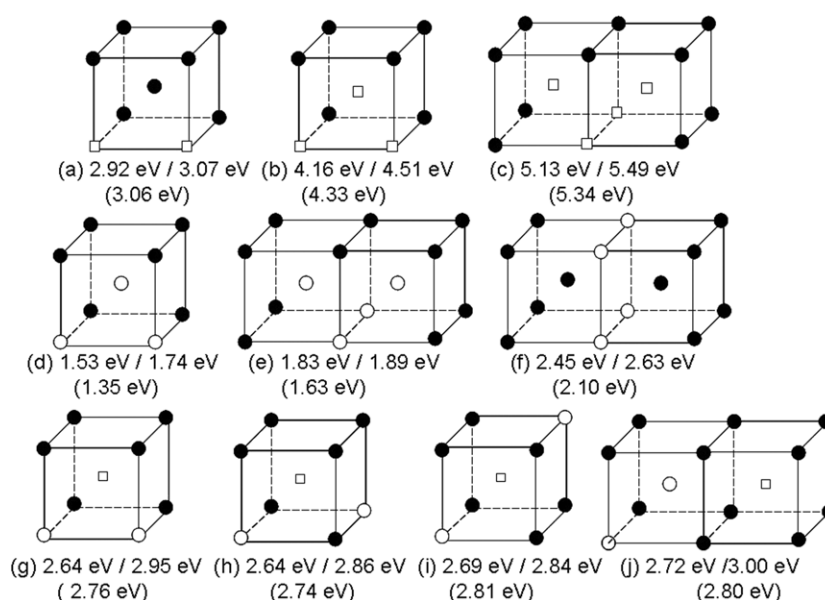


Figure 1. Formation energies of small vacancy clusters and small Cu clusters calculated with constant volume relaxation and box size variable relaxation. The solid circles are Fe atoms, the empty squares are vacancies, the empty circles are Cu atoms. The values in parentheses are the results of *ab initio* calculation for 128 atom supercells performed by Becquart and Domain [31].

feasible than the case of Fe. But it is indicated by this work that the basic properties of Cu can also be described well by the Tersoff formalism of angular-dependent ABOP. Although the EAM potential and the Tersoff potential are usually used for different types of systems, EAM is suitable for describing the metallic systems and the Tersoff ABOP is originally developed for covalent systems, it was pointed out by Brenner [39] that the two potentials are formally identical for a reasonable choice of functional forms and parameters. The Tersoff ABOP has explicitly angular-dependent, in this sense it may have some connections to the MEAM potential [40, 41], which has been applied to a large number of metallic and covalent systems. Recently, ABOP have been used for the systems beyond semiconductors, especially for metal-semimetal systems [13, 42]. In our ongoing work we will attempt to build the model of other iron alloys such Fe–Ni and Fe–Si.

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