New MAEAM Potential Models for BCC, FCC and HCP Metals

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Abstract The calculation results of structure energy differences misfit the experiment data for BCC, FCC and HCP metals in the original modified analytic embedded atom method (MAEAM) theory [1]. To resolve this problem, we not only adopt an end processing function and an enhanced smooth continuous condition, but also adjust parameters of multi-body potential model by fitting cohesion energies, mono-vacancy formation energies, Rose equation curves for total energy as a function of lattice parameter, energy differences between several typical structures, elastic parameters, equilibrium conditions of crystals.
Key words BCC metal, FCC metal; HCP metals, EAM

Introduction

The great leader Comrade **Kim Jong Il** said as follows.

"**Now is the age of science and technology, which is the basis of economic progress**."
（"**KIM JONG IL** SELECTED WORKS" Vol. 10 P. 22）

The modified analytic embedded atom method (MAEAM) was suggested to resolve the negative Cauchy pressure problem of Jonson's model [1]. And the farther neighbor atoms are considered to improve the correctness of the calculation results by this method [2, 3]. But this MAEAM still has some points to improve, including the structure stabilities of noble metals, the properties of the end parts the derivatives of the pair potential function, and the misfitting problem of the calculation results of energy differences between several structures with experimental data.

In this paper, new pair potential forms and a new end processing method are suggested for the three kinds of typical structures of metals (BCC, FCC, HCP metals) in the framework of MAEAM theory. In order to resolve the misfitting problem between calculated results and experimental data for the energy differences between several structures of metals, input data include one of these differences. Two model parameters become unnecessary because of the adoption of the end processing function. Through adjusting one of these two parameters, the many-body potential becomes fit to the experimental data of one structure energy difference. Through adjusting another parameter, we can fit the potential to the experimental data of phonon frequency at a certain value of the vibration number for several metals.

1．New Pair Potential Forms and Model Parameters

The basic equations of MAEAM for the total energy of a system of atoms are as follows [2].

$$E_t = \sum_{i=1}^{n} E_i \tag{1}$$

$$E_i = F(\rho_i) + \frac{1}{2}\sum_j \phi(r_{ij}) + M(P_i) \tag{2}$$

where E_t is total energy of system, E_i is the contribution from the atom at site i, $F(\rho_i)$ the embedded atom energy, $\phi(r_{ij})$ the pair potential between the atoms at sites i and j, and $M(P_i)$ the energy medication term.

Considering farther neighbor atoms, the three basic functions become [2－4].

$$F(\rho) = -F_0\left[1 - \ln\left(\frac{\rho}{\rho_e}\right)^n\right]\left(\frac{\rho}{\rho_e}\right)^n \tag{3}$$

$$M(P) = \alpha\left\{1 - \exp\left[-\left(\ln\left|\frac{P}{P_e}\right|\right)^2\right]\right\} \tag{4}$$

for BCC metals

$$\phi(r) = \sum_{j=-1}^{4} k_j\left(\frac{r}{r_1}\right)^j \tag{5}$$

for FCC metals

$$\phi(r) = k_0 + k_1\left(\frac{r}{r_1}\right) + k_2\left(\frac{r}{r_1}\right)^2 + k_3\left(\frac{r}{r_1}\right)^6 + k_4\left(\frac{r}{r_1}\right)^{-12} + k_5\left(\frac{r}{r_1}\right)^{-1} \tag{6}$$

for HCP metals

$$\phi(r) = \sum_{j=-1}^{6} k_j\left(\frac{r}{r_1}\right)^j \tag{7}$$

where ρ is

$$\rho = \sum_m f(r_m) \tag{8}$$

for BCC and FCC metals P is

$$P = \sum_m f^2(r_m) \tag{9}$$

and for HCP metals, P is

$$P = \sum_m f^2(r_m)\frac{r_{mx}^2 + r_{my}^2 + \beta r_{mz}^2}{r_m^2} \tag{10}$$

where m means all the neighbor atoms in the cutoff distance for the electron density function $f(r)$.

The new pair potential forms and a new end processing method are as follows.

1.1. New potential model of MAEAM for BCC metals

A new pair potential form for BCC metals is

$$\phi(r) = \begin{cases} \displaystyle\sum_{j=-1}^{4} k_j \left(\frac{r}{r_1}\right)^j, & r \le r_2 \\[3mm] \displaystyle\sum_{j=0}^{7} l_j \left(\frac{r}{r_2}-1\right)^j, & r_2 < r \le r_c \\[3mm] 0, & r > r_c \end{cases} \tag{11}$$

and an enhanced smooth continuous condition is

$$\phi(r_c) = 0, \ \phi'(r_c) = 0, \ \phi''(r_c) = 0, \ \phi'''(r_c) = 0,$$
$$\phi_1(r_2) = \phi_2(r_2), \ \phi_1'(r_2) = \phi_2'(r_2), \ \phi_1''(r_2) = \phi_2''(r_2), \ \phi_1'''(r_2) = \phi_2'''(r_2). \tag{12}$$

The relations between $l_j (j = 0\sim3)$ and $k_j (j = -1\sim3)$ are

$$l_0 = \sum_{j=-1}^{3} k_j s^j, \quad l_1 = \sum_{j=-1}^{3} j k_j s^j, \quad l_2 = \frac{1}{2}\sum_{j=-1}^{3} j(j-1)k_j s^j, \quad l_3 = \frac{1}{6}\sum_{j=-1}^{3} j(j-1)(j-2)k_j s^j. \tag{13}$$

The relations between $l_j (j{=}4\sim7)$ and $l_j (j{=}0\sim3)$ are

$$l_4 = -\frac{35l_0}{d^4} - \frac{20l_1}{d^3} - \frac{10l_2}{d^2} - \frac{4l_3}{d}, \quad l_5 = \frac{84l_0}{d^5} + \frac{45l_1}{d^4} + \frac{20l_2}{d^3} + \frac{6l_3}{d^2},$$
$$l_6 = -\frac{70l_0}{d^6} - \frac{36l_1}{d^5} - \frac{15l_2}{d^4} - \frac{4l_3}{d^3}, \quad l_7 = \frac{20l_0}{d^7} + \frac{10l_1}{d^6} + \frac{4l_2}{d^5} + \frac{l_3}{d^4} \tag{14}$$

where

$$s = r_2 / r_1, \ d = r_c / r_2 - 1 \tag{15}$$

where r_c is the cut-off distance for pair potential which is as follows.

$$r_c = r_2 + 0.6(r_3 - r_2) \tag{16}$$

The cut-off distance for electron density function r_{cf} is

$$r_{cf} = r_5 + 0.75(r_6 - r_5). \tag{17}$$

The difference between the above cut-off distances supports the smoothness and continuity of total energy as a volume function $r_i \ (i{=}1\sim6)$ represents the ith neighbor distances respectively.

The unrelaxed vacancy formation energy can be represented with the pair potential approximation for fitting process.

$$E_{1f} \approx -\frac{1}{2}\sum_{m} \phi(r_m) \tag{18}$$

Then the cohesion energy is

$$E_c = F_0 - \frac{1}{2}\sum_{m} \phi(r_m) \approx F_0 - E_{1f} \tag{19}$$

The equilibrium condition can be expressed as a requirement that there is no stress in the crystal and this condition leads to the following equation.

$$\frac{1}{2}\sum_m \frac{(r_{mx})^2}{r_m}\phi'(r_m)=0 \tag{20}$$

The elastic constants, C_{ijkl}, can be calculated with

$$\Omega_0 C_{ijkl}=F''(\rho)\sum_m\frac{r_{mi}r_{mj}}{r_m}f'(r_m)\sum_m\frac{r_{mk}r_{ml}}{r_m}f'(r_m)+\sum_m\frac{r_{mi}r_{mj}r_{mk}r_{ml}}{r_m}\left[\phi''(r_m)-\frac{\phi'(r_m)}{r_m}\right]$$
$$+4M''(P)\sum_m\frac{r_{mi}r_{mj}}{r_m}f(r_m)f'(r_m)\cdot\sum_m\frac{r_{mk}r_{ml}}{r_m}f(r_m)f'(r_m) \tag{21}$$

There are three independent elastic constants C_{11}, C_{12} and C_{44} for BCC metals and thus we get three equations. By combining the three equations for the elastic constants with the equation for the cohesive energy and the equation of the equilibrium condition, the five parameters such as $k_0 \sim k_3$ and α can be determined.

The computational cell is a crystal sphere of radius $2a$ with 65 atoms, in which a is a lattice constant of the considered metal. In order to resolve the misfitting problem between calculated results and experimental data for the energy differences between several structures of transition metals, input physical data include one of these differences. Two model parameters become unnecessary because of the adoption of the end processing function, through adjusting one of these two parameters (k_{-1} in this paper, k_4 is unnecessary and set to zero), the many-body potential becomes fit to the structure energy difference.

In [8] they obtained a universal equation of energy versus volume empirically for a broad range of materials. To ensure reasonable behavior for atom–atom interactions inside the equilibrium spacing, this empirical relationship is fitted by adjusting parameter n, the value of n is accepted as a model parameter which provides the minimum value of ΔS in the follow expression

$$\Delta S=10^3\cdot\sum_{i=1}^{21}\left[E(a_i)-E_R(a_i)\right]^2/e^{20|a_i/a-1|}$$
$$a_i=[0.9+0.01\cdot(i-1)]\cdot a \tag{22}$$

where $E(a_i)$ and $E_R(a_i)$ are the calculation result of our model and the Rose equation respectively. The volume change is smaller, the difference between the two results has a greater effect upon the sum in the above expression by the adoption of exponential function. If there is no minimum of ΔS in $0<n<1$, the mono-vacancy migration energy becomes the object of fitting.

After k_{-1} and n are determined，$k_0 \sim k_3$ and α can be obtained by solving the five linear equations. The input parameters used in this paper are the lattice constant a, cohesive energy E_c, mono-vacancy formation energy E_{1f}, elastic constants C_{11}, C_{12} and C_{44}, and structure energy difference E_{fb} (between FCC and BCC structures) and the calculated model parameters n, α, F_0, and $k_{-1} \sim k_3$ are listed in tables 1 and 2 respectively for seven bcc metals (Cr, Fe, Mo, Nb, Ta, V and W).

Table 1. Input parameter for BCC metals [2, 4, 8]

	a /nm	E_c /eV	E_{1f} /eV	C_{11} /GPa	C_{12} /GPa	C_{44} /GPa	E_{fb} /eV
Cr	0.288 46	4.10	1.80	346.0	66.0	100.0	0.09
Fe	0.286 64	4.28	1.79	230.0	135.0	117.0	0.08
Mo	0.314 68	6.82	3.10	459.0	168.0	111.0	0.28
Nb	0.330 24	7.47	2.75	252.7	133.1	31.9	0.22
Ta	0.330 26	8.10	2.95	262.0	156.0	82.6	0.26
V	0.303 11	5.30	2.10	232.4	119.4	46.0	0.15
W	0.315 60	8.90	3.95	517.0	203.0	157.0	0.33

Table 2. Model parameters for BCC metals

	k_0	k_1	k_2	k_3	k_{-1}	α	n	F_0
Cr	−202.616 4	281.058 2	−178.014 9	43.311 7	56	−0.297 3	0.87	2.30
Fe	−183.137 8	229.417 3	−129.480 3	27.930 6	55	−0.056 2	0.56	2.49
Mo	−494.104 2	685.091 2	−427.906 9	101.470 4	135	−0.203 2	0.90	3.72
Nb	−340.951 3	480.409 5	−302.665 4	71.829 2	91	−0.001 3	0.77	4.82
Ta	−459.003 8	619.317 4	−374.160 1	85.412 8	128	−0.013 8	0.65	5.15
V	−220.072 1	304.520 5	−189.246 0	44.509 2	60	−0.014 2	0.72	3.30
W	−1181.862 5	1631.331 0	−1005.490 3	233.443 3	322	−0.224 4	0.77	4.95

n is dimensionless, F_0, α and k_i are in eV

1.2. New potential model of MAEAM for FCC metals

A new pair potential parameters for FCC metals is as follows.

$$
\phi(r) = \begin{cases} k_0 + k_1\left(\dfrac{r}{r_1}\right) + k_2\left(\dfrac{r}{r_1}\right)^2 + k_3\left(\dfrac{r}{r_1}\right)^6 + k_4\left(\dfrac{r}{r_1}\right)^{-12} + k_5\left(\dfrac{r}{r_1}\right)^{-1}, & r \le r_4 \\[2mm] \sum\limits_{j=0}^{7} l_j\left(\dfrac{r}{r_4} - 1\right)^j, & r_4 < r \le r_c \\[2mm] 0, & r > r \end{cases}
\tag{23}
$$

The relations between $l_j\,(j = 0 \sim 3)$ and $k_j\,(j = -1 \sim 3)$ are

$$
\begin{aligned}
l_0 &= k_0 + k_1 s + k_2 s^2 + k_3 s^6 + k_4 s^{-12} + k_5 s^{-1}, \\
l_1 &= k_1 s + 2k_2 s^2 + 6k_3 s^6 - 12k_4 s^{-12} - k_5 s^{-1}, \\
l_2 &= k_2 s^2 + 15k_3 s^6 + 78k_4 s^{-12} + k_5 s^{-1}, \\
l_3 &= 20k_3 s^6 - 364k_4 s^{-12} - k_5 s^{-1}
\end{aligned}
\tag{24}
$$

where s and d are

$$
s = r_4 / r_1, \quad d = r_c / r_4 - 1.
\tag{25}
$$

where r_c is the cut-off distance for pair potential

$$
r_c = r_5 + 0.6(r_6 - r_5)
\tag{26}
$$

and the cut-off distance for electron density function r_{cf} is

$$
r_{cf} = r_6 + 0.75(r_7 - r_6).
\tag{27}
$$

The relations between $l_j\ (j=4 \sim 7)$ and $l_j\ (j=0 \sim 3)$ agree with the expressions (14).

Table 3. Input parameters for FCC metals [6, 7]

	a /nm	E_c /eV	E_{1f} /eV	C_{11} /GPa	C_{12} /GPa	C_{44} /GPa
Ag	0.408 57	2.95	1.10	123.0	92.0	45.2
Al	0.403 20	3.36	0.68	114.0	61.9	31.6
Au	0.407 80	3.93	0.98	197.0	165.0	45.0
Cu	0.361 47	3.49	1.17	169.0	122.0	75.3
Ir	0.383 90	6.94	3.50	582.0	241.0	262.0
Ni	0.352 36	4.44	1.45	247.0	153.0	122.0
Pd	0.389 07	3.89	1.30	224.0	173.0	71.6
Pt	0.392 39	5.84	1.20	347.0	251.0	76.5
Rh	0.384 01	5.75	2.90	412.6	193.5	184.1

Table 4. Model parameters for FCC metals

	k_c	k_0	k_1	k_2	k_3	k_4	k_5	α	n	F_0
Ag	0.3	−1.527 064	1.865 247	−0.589 960	0.002 479	0.086	0	0.055 1	0.66	1.85
Al	0.4	−2.295 089	2.934 249	−0.945 803	0.003 637	0.080	0	0.002 1	0.56	2.75
Au	0.6	−2.160 974	2.827 772	−0.946 730	0.004 675	0.080	0	0.160 5	0.80	2.91
Cu	0.4	−2.203 440	2.825 760	−0.932 802	0.004 486	0.097	0	0.074 2	0.34	2.32
Ir	0.5	−16.800 98	22.881 900	−7.883 247	0.041 526	0.408	0	−0.203 8	0.64	3.44
Ni	0.3	−4.478 908	5.989 708	−2.040 219	0.010 551	0.143	0	0.000 3	0.42	2.99
Pd	0.1	7.836 509	−5.587 166	1.432 133	−0.006 026	0.156	−4	0.251 3	0.36	2.49
Pt	0.1	13.324 160	−10.520 990	2.895 426	−0.013 288	0.188	−6	0.359 9	0.53	4.41
Rh	0.6	12.256 400	−7.706 841	1.752 638	−0.005 345	0.307	−7	−0.031 0	0.40	2.85

k_c and n are dimensionless, F_0, α and k_i are in eV.

The computational cell is a crystal sphere of radius $2a$ with 141 atoms, the method of determining model parameters is very similar to the one used for BCC metals: k_4 is determined by fitting one of structure energy differences, k_5 is set to zero for Ag, Al, Au, Cu, Ir and Ni. For Pd, Pt and Rh, k_5 is determined by fitting the experimental data of the crystal wave frequency corresponding to the wave number vector $(2\pi/a\ 0\ 0)$, which are 6.7THz, 5.9THz, and 9.5THz respectively [8]. Rose equation is fitted in calculation of n, for Al, Au, Ni and Rh, there no exist the minimum of ΔS in the variation range of n, therefore the experimental data of mono-vacancy migration energy are fitted, which are 0.645, 0.854 1.55 and 2.967eV respectively [8]. After k_4, k_5 and n are determined, $k_0 \sim k_3$ and α can be obtained by solving the equations (19)~(21). The input parameters are the lattice constant a, cohesive energy E_c, mono-vacancy formation energy E_{1f}, elastic constants C_{11}, C_{12} and C_{44}, and structure energy difference E_{bf} (between BCC and FCC structures) and E_{hf} (between HCP and FCC structures) used in this paper and the calculated model parameters n, α, F_0, and k_0 to k_5 for nine FCC metals are listed in tables 3 and 4 respectively.

2. New Potential Model of MAEAM for HCP Metals

A new pair potential form and multibody potential parameters for HCP metals are as follows.

$$\phi(r) = \begin{cases} \displaystyle\sum_{j=-1}^{5} k_j \left(\frac{r}{r_1}\right)^j, & r_1 \le r < r_5 \\[2ex] \displaystyle\sum_{j=0}^{7} l_j \left(\frac{r}{r_5}-1\right)^j, & r_5 \le r < r_c \\[2ex] 0, & r > r_c \end{cases} \tag{28}$$

The relations between l_j ($j=0\sim3$) and k_j ($j=-1\sim3$) are

$$l_0 = \sum_{j=-1}^{5} k_j s^j, \quad l_1 = \sum_{j=-1}^{5} j k_j s^j,$$

$$l_2 = \frac{1}{2}\sum_{j=-1}^{5} j(j-1)k_j s^j, \quad l_3 = \frac{1}{6}\sum_{j=-1}^{5} j(j-1)(j-2)k_j s^j \tag{29}$$

where s and d are

$$s = r_5/r_1, \; d = r_c/r_5 - 1 \tag{30}$$

where r_c is the cut-off distance for pair potential

$$r_c = \frac{1}{4}(6a + \sqrt{a^2+c^2}) \tag{31}$$

and the cut-off distance for electron density function r_{cf} is

$$r_{cf} = 2a + \frac{3}{4}\left(\sqrt{\frac{13}{3}a^2 + \frac{1}{4}c^2} - 2a\right) < 2.2a \approx r_9. \tag{32}$$

The relations between l_j ($j=4\sim7$) and l_j ($j=0\sim3$) agree with the expressions (14).

In view of the HCP crystal symmetries, the equilibrium conditions are expressed by：

$$\frac{1}{2}\sum_{m} \frac{r_{mx}r_{mx}}{r_m}\phi'(r_m) = 0,$$

$$\frac{1}{2}\sum_{m} \frac{r_{mz}r_{mz}}{r_m}\phi'(r_m) = 0 \tag{33}$$

The elastic constants C_{ijkl} can be calculated with：

$$\Omega_0 C_{ijkl} = F''(\rho)\sum_{m}\frac{r_{mi}r_{mj}}{r_m}f'(r_m)\sum_{m}\frac{r_{mk}r_{ml}}{r_m}f'(r_m) + \sum_{m}\frac{r_{mi}r_{mj}r_{mk}r_{ml}}{r_m^2}\left[\phi''(r_m) - \frac{\phi'(r_m)}{r_m}\right] +$$

$$+ 4M''(P)\sum_{m}\frac{r_{mi}}{r_m^2}f^2(r_m)\left(r_{mx}\delta_{xj} + r_{my}\delta_{yj} + \beta r_{mz}\delta_{zj} - 7r_{mj}\frac{r_{mx}^2 + r_{my}^2 + \beta r_{mz}^2}{r_m^2}\right). \tag{34}$$

$$\cdot \sum_{m}\frac{r_{mk}}{r_m^2}f^2(r_m)\left(r_{mx}\delta_{xl} + r_{my}\delta_{yl} + \beta r_{mz}\delta_{zl} - 7r_{ml}\frac{r_{mx}^2 + r_{my}^2 + \beta r_{mz}^2}{r_m^2}\right)$$

Table 5. Input parameters for HCP metals [3, 5, 8]

	a /nm	c /nm	E_c /eV	E_{1f} /eV	C_{11} /GPa	C_{12} /GPa	C_{13} /GPa	C_{33} /GPa	C_{44} /GPa	E_{bh} /eV
Be	0.228 56	0.358 32	3.32	1.11	292.3	26.7	14.0	246.0	162.5	0.068 0
Co	0.249 70	0.406 90	4.39	1.35	295.0	159.0	111.0	335.0	71.0	0.005 0(E_{fh})
Hf	0.319 46	0.505 11	6.44	1.80	181.0	77.0	66.0	197.0	55.7	0.059 0
Mg	0.320 94	0.521 05	1.51	0.58	59.3	25.7	21.4	61.5	16.4	0.031 0
Re	0.276 00	0.445 80	8.03	2.30	616.0	273.0	206.0	683.0	161.0	0.163 6
Ru	0.270 57	0.428 16	6.74	1.85	563.0	188.0	168.0	535.0	181.0	0.075 5
Sc	0.330 80	0.526 70	3.90	1.15	99.3	39.7	29.4	107.0	27.2	0.050 1
Ti	0.295 06	0.467 88	4.85	1.50	160.0	90.0	66.0	181.0	46.5	0.070 0
Y	0.364 74	0.573 06	4.37	1.25	77.9	28.5	21.0	76.9	24.3	0.044 0
Zr	0.323 12	0.514 77	6.25	1.70	144.0	74.0	67.0	166.0	33.4	0.061 0

There are five independent elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44} for hcp metals and thus we get five equations. By combining the four equations for the elastic constants with the one equation for the cohesive energy and the two equations of the equilibrium condition, the seven parameters $k_0 \sim k_5$ and α can be determined. The equation for C_{13} is not considered in the composition of linear equations set, because elastic constants are not linear with respect to one parameter β.

Table 6. Model parameters for HCP metals

	k_{-1}	k_0	k_1	k_2	k_3
Be	301	−1 343.333 8	2 470.327 2	−2 399.268 7	1 298.589 7
Co	306	−1 356.870 1	2 481.983 3	−2 397.465 9	1 289.280 6
Hf	270	−1 181.109 4	2 133.392 7	−2 040.695 7	1 090.750 5
Mg	104	−455.025 9	821.366 6	−783.925 4	417.325 7
Re	572	−2 462.561 1	4 359.932 0	−4 071.896 4	2 118.777 9
Ru	377	−1 635.048 3	2 920.084 6	−2 760.020 5	1 459.796 6
Sc	192	−810.868 1	1 408.208 5	−1 290.011 5	658.241 3
Ti	266	−1 182.098 2	2 169.455 2	−2 105.064 9	1 138.203 3
Y	175	−737.925 5	1 281.434 7	−1 176.232 6	602.772 3
Zr	231	−995.210 2	1 770.005 9	−1 666.001 0	875.436 0

	k_4	k_5	α	β	n	F_0
Be	−371.377 2	43.838 8	−0.482 0	1.00	0.98	2.23
Co	−365.888 5	42.811 6	0.013 8	−1.23	0.58	3.06
Hf	−308.800 1	36.160 0	0.016 6	−0.93	0.32	4.64
Mg	−117.488 9	13.665 3	−0.038 4	3.77	0.75	0.93
Re	−582.975 6	66.310 9	0.090 5	−0.55	0.39	5.73
Ru	−410.099 1	47.813 5	−0.229 1	1.21	0.58	4.89
Sc	−177.520 4	19.778 8	−0.147 1	1.76	0.70	2.75
Ti	−324.938 2	38.251 2	0.030 4	−0.94	0.48	3.35
Y	−163.629 9	18.388 6	−0.127 6	2.36	0.55	3.12
Zr	−243.444 3	27.982 3	0.006 2	−1.02	0.53	4.55

n is dimensionless, F_0, α, β and k_i are in eV.

The computational cell is a crystal sphere of radius $2.5a$ with 87 atoms, the method of determining model parameters is also similar to the one used for BCC metals: k_{-1} is determined by fitting one experimental value or reliable calclulation result of structure energy differences, and through fitting the experimental value of C_{13} and the Rose equation curve, β and n are determined respectively. After k_{-1}, β and n are determined，$k_0 \sim k_5$ and α can be obtained by solving the equations (19), (33), and (34). The input parameters are the lattice constant a, cohesive energy E_c, mono-vacancy formation energy E_{1f}, elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44}, and structure energy difference E_{bh} (between BCC and HCP structures) and E_{fh} (between FCC and HCP structures) used in this paper and the calculated model parameters n, α, β, F_0, and k_{-1} to k_5 for ten HCP metals are listed in tables 5 and 6 respectively.

Conclusion

In the present paper, the traditional MAEAM theory considering farther neighbor atoms is improved for three structures of metals. The pair potential functions are truncated by adopting a new function form and an enhanced smooth continuous condition. The parameters of multi-body potential model are also adjusted to fit the experimental data of cohesive energy, elastic constants, the result from Rose equation, structure energy difference, and equilibrium conditions of crystals for the 26 kinds of metals. Resultantly, the calculation results from these potentials show good agreement with experimental results for the structure energy differences, the bi-vacancy bind energies, the bulk phonon dispersion, the specific heats, and so on.

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