

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/248185630>

Modified embedded-atom method interatomic potentials for the Fe-Ti-C and Fe-Ti-N ternary systems

ARTICLE *in* ACTA MATERIALIA · JUNE 2009

Impact Factor: 4.47 · DOI: 10.1016/j.actamat.2009.03.019

CITATIONS

27

READS

87

3 AUTHORS, INCLUDING:



Byeong-Joo Lee

Pohang University of Science and Technology

177 PUBLICATIONS 3,454 CITATIONS

SEE PROFILE

Modified embedded-atom method interatomic potentials for the Fe–Ti–C and Fe–Ti–N ternary systems

Hyun-Kyu Kim^a, Woo-Sang Jung^b, Byeong-Joo Lee^{a,*}

^a Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

^b Materials Science and Technology Research Division, Korea Institute of Science and Technology, Seoul 136-791, Republic of Korea

Received 29 January 2009; received in revised form 10 March 2009; accepted 10 March 2009

Available online 9 April 2009

Abstract

Modified embedded-atom method (MEAM) interatomic potentials for the Fe–Ti–C and Fe–Ti–N ternary systems have been developed based on the previously developed MEAM potentials for sub-unary and binary systems. An attempt was made to find a way to determine ternary potential parameters using the corresponding binary parameters. The calculated coherent interface properties, interfacial energy, work of separation and misfit strain energy between body-centered cubic Fe and NaCl-type TiC or TiN were reasonable when compared with relevant first-principles calculations under the same condition. The applicability of the present potentials for atomistic simulations to investigate nucleation kinetics of TiC or TiN precipitates and their effects on mechanical properties in steels is also demonstrated.

© 2009 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Modified embedded-atom method; Interatomic potential; Interface property; Fe–Ti–C; Fe–Ti–N

1. Introduction

Titanium carbides and nitrides are two of the most important precipitates for strengthening steels. To obtain the desired mechanical strength in steels, it is important to control the size distribution of the precipitates and to understand the interactions between precipitates and dislocations. The size distribution of the precipitates is determined by the nucleation kinetics, which depends on the metal/precipitate interfacial energy and the misfit strain energy. To estimate the effect of precipitates on microstructural evolution, it is also necessary to quantitatively understand the interaction between precipitates and grain boundaries or other defects.

All of the above-mentioned properties are rather difficult to measure experimentally, but can be estimated efficiently by atomic scale simulation/calculation techniques. First-principles calculations provide the most reliable

information on the atomic or sub-atomic scale properties of materials. Recently, many first-principles calculations have been devoted to metal/carbide or nitride systems [1–9]. However, these studies were mainly for computation of coherent interface energies between Fe matrix and carbides or nitrides. This is because of the size (or number of atoms) limit that first-principles calculations have. In order to be able to investigate large systems (interactions between precipitates and grain boundaries or dislocations, for example), other approaches, based on (semi-)empirical interatomic potentials, which can deal with more than a million atoms, need to be used. In this case, it is important that the interatomic potentials reproduce various fundamental physical properties of relevant materials systems correctly.

Even though many atomistic simulation studies have been performed to investigate atomic scale materials phenomena of metallic materials, none has been done for carbide or nitride systems such as Fe–Ti–C or Fe–Ti–N systems. This is because of the difficulty in developing (semi-)empirical interatomic potentials that can deal with

* Corresponding author. Tel.: +82 54 2792157; fax: +82 54 2792399.

E-mail address: calphad@postech.ac.kr (B.-J. Lee).

all the different elements, Fe, Ti, C and N, and alloy systems composed of those elements using a common mathematical formalism. To the best knowledge of the present authors, the (semi-)empirical interatomic potential formalism that can deal with all the above-mentioned elements simultaneously is the second nearest-neighbor modified embedded-atom method (2NN MEAM) formalism proposed by Lee and Baskes [10,11] by generalizing the MEAM [12]. In addition to the pure elements Fe [11], Ti [13], C [14] and N [15], the 2NN MEAM has been applied to describe all the binary systems composed of those elements, Fe–C [16], Fe–N [15], Ti–C [17], Ti–N [17] and Fe–Ti [18].

As a part of a long-term project to investigate the effects of carbide or nitride precipitates on steel properties on the atomic scale, the purpose of the present work is to develop the 2NN MEAM interatomic potentials for the Fe–Ti–C and Fe–Ti–N ternary systems. The previously developed potential parameters of all the sub-unary and binary systems were used without any modification, and a few ternary parameters were further determined. The reliability of the developed potentials was examined by computing the coherent interface properties between body-centered cubic (bcc) Fe and TiC or TiN and comparing them with available first-principles calculations. Since the experimental information or first-principles calculations for ternary systems necessary for the determination of ternary potential parameters are not always available, a systematic method to determine ternary parameters from the corresponding binary parameters is also proposed.

2. Interatomic potential

2.1. Potential formalism

In the MEAM, the total energy of a system is given by:

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

F_i is the embedding function for an atom i embedded in a background electron density $\bar{\rho}_i$, and S_{ij} and $\phi_{ij}(R_{ij})$ are the screening function and the pair interaction between atoms i and j separated by a distance R_{ij} . For energy calculations, the functional forms for F_i and ϕ_{ij} should be given. The background electron density at each atomic site is computed by combining several partial electron density terms for different angular contributions. A specific form is given to the embedding function F_i , but not to the pair interaction ϕ_{ij} . Instead, a reference structure where individual atoms are on the exact lattice points is defined and the total energy per atom of the reference structure is estimated from the zero-temperature universal equation of state by Rose et al. [19]. Then, the value of the pair interaction is evaluated from the known values of the total energy per atom and the embedding energy, as a function of the nearest-neighbor distance. In the original MEAM [12], only

first nearest-neighbor interactions are considered. Neglecting the second and more distant nearest-neighbor interactions is performed by the use of a strong, many-body screening function [20]. The consideration of the second nearest-neighbor interactions in the 2NN MEAM formalism is effected by adjusting the screening parameters, C_{\min} , so that the many-body screening becomes less severe. In addition, a radial cutoff function [20] is applied to reduce the calculation time. Details of the 2NN MEAM formalism have been published in the literature [10–18,20,21] and will not be repeated here. Only the part for many-body screening which becomes the key issue in determining ternary potential parameters will be briefly described again.

In the MEAM, the many-body screening function between atoms i and j , S_{ij} , is defined as the product of the screening factors, S_{ikj} , due to all other neighbor atoms k :

$$S_{ij} = \prod_{k \neq i, j} S_{ikj} \quad (2)$$

The screening factor S_{ikj} is computed using a simple geometric construction. Imagine an ellipse on an x, y plane, passing through atoms i, k and j , with the x -axis of the ellipse determined by atoms i and j (see Fig. 1a). The equation of the ellipse is given by:

$$x^2 + \frac{1}{C}y^2 = \left(\frac{1}{2}R_{ij}\right)^2 \quad (3)$$

For each k atom, the value of parameter C can be computed from relative distances among the three atoms. The basic idea for the screening is that, first, two limiting values are defined, C_{\max} and C_{\min} ($C_{\max} > C_{\min}$). Then, if the atom k is outside of the ellipse defined by C_{\max} , it is thought that the atom k does not have any effect on the interaction between atoms i and j . If the atom k is inside of the ellipse defined by C_{\min} , it is thought that the atom k completely screens the i – j interaction, and between C_{\max} and C_{\min} the screening changes gradually. The screening is affected by multiplying the screening function S_{ij} to the electron density and pair potential during the numerical procedure. The screening factor, S_{ikj} , is defined as a function of C as follows:

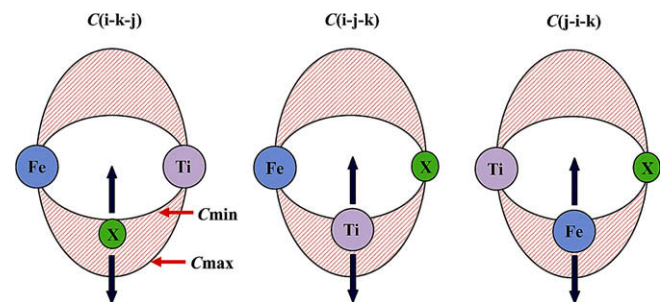


Fig. 1. A schematic illustration of the three different cases for the screening of interaction between two neighboring atoms of different types by a third element atom in ternary systems. The symbols, i, j and k , represent Fe, Ti and X (X = C, N), respectively.

$$S_{ikj} = f_c \left[\frac{C - C_{\min}}{C_{\max} - C_{\min}} \right] \quad (4)$$

where the smooth cutoff function is

$$f_c(x) = \begin{cases} 1 & x \geq 1 \\ [1 - (1 - x)^4]^2 & 0 < x < 1 \\ 0 & x \leq 0. \end{cases} \quad (5)$$

2.2. Ternary potential parameters

The MEAM potential parameter set for a ternary system is obtained by combining all sub-unary and binary parameters. All necessary unary and binary parameters for the Fe–Ti–C (or N) system are presented in Tables 1 and 2. In addition, three more ternary parameters for each of C_{\min} (i – k – j) and C_{\max} (i – k – j) are necessary.

As mentioned already, C_{\min} (i – k – j) and C_{\max} (i – k – j) parameters represent the degree of screening by a third element atom (k) to the interaction between two neighboring atoms (i and j) of different type. In ternary systems, the three additional cases shown in Fig. 1 should be considered, as well as the cases that occur in unary and binary systems. When no information on physical or thermodynamic properties of the ternary system is available for parameter optimization, a default assumed value should be given to each parameter. Such an assumption had to be made in the present study. Considering that Fe and Ti are relatively similar to each other compared to C (or N), it was assumed that the degree of screening by a C atom to the interaction between Fe and Ti atoms [C_{\min} and C_{\max} (Fe–C–Ti)] is an average between those to the Fe–Fe [C_{\min} and C_{\max} (Fe–C–Fe)] and Ti–Ti [C_{\min} and C_{\max} (Ti–C–Ti)] interactions. Similarly, the degree of screening by an Fe (or Ti) atom to the interaction between Ti (or Fe) and C atoms [C_{\min} and C_{\max} (Ti–Fe–C) or C_{\min} and C_{\max} (Fe–Ti–C)] was assumed to be an average between those by an Fe atom to the Fe–C [C_{\min} and C_{\max} (Fe–Fe–C)] and by a Ti atom to the Ti–C [C_{\min} and C_{\max} (Ti–Ti–C)] interactions. The same assumption was made for the determination of Fe–Ti–N ternary parameters. As a means to confirm the transferability of the above default assumption, comparisons with other ternary parameter sets obtained from different

assumptions were also made, as will be described in more detail later on.

3. Calculation of interface properties

The 2NN MEAM formalism includes up to the second nearest-neighbor interactions. Therefore, the radial cutoff distance during atomistic simulations should be at least larger than the second nearest-neighbor distance in the structures under consideration. In the present study, a value of 4.8 Å was chosen as the radial cutoff distance, which is larger than the second nearest-neighbor distance of hexagonal close-packed (hcp) Ti.

For the Fe–Ti–C and Fe–Ti–N systems, first-principles calculations [7,9] of the coherent interfacial energy between bcc Fe and NaCl-type TiC or TiN were available. As a means to evaluate the reliability of the present interatomic potential, the same property was calculated and compared with the higher-level calculations. Another set of first-principles calculations was also available for the same interface property in the form of the work of separation [3–5,22], and the same calculations were performed.

Calculation of interfacial energy is performed by computing the total energy of a super cell that involves an interface between the two phases (in this work, bcc Fe and TiC or TiN) and the summation of total energies of individual pure phase samples of the same size [23]. The total energy of the super cell is calculated by a molecular statics simulation applying a three-dimensional periodic boundary condition to remove any surface effects and allowing full relaxations of individual atom positions and sample dimensions. This energy is compared with the summation of total energies of individual pure phase samples, calculated maintaining the same lattice parameters with those of the super cell in the two directions parallel to the interface but allowing a relaxation into the direction perpendicular to the interface. Due to the periodic boundary condition, the super cell actually involves two interfaces. The interfacial energy σ is obtained from the following equation:

$$\sigma = [E_{\text{Fe/TiC(orN)}} - (E_{\text{bcc Fe}} + E_{\text{TiC(or N)}})]/2A \quad (6)$$

where A represents the area of the interface.

Table 1
2NN MEAM potential parameter sets for pure Fe, Ti, C and N.

	E_c	r_e	B	A	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	C_{\min}	C_{\max}	d
Fe ^a	4.29	2.48	1.73	0.56	4.15	1.00	1.00	1.00	2.60	1.80	−7.20	0.36	2.80	0.05
Ti ^b	4.87	2.92	1.10	0.66	2.70	1.00	3.00	1.00	6.80	−2.00	−12.0	1.00	1.44	0.00
C ^c	7.37	1.54	4.45	1.18	4.25	2.80	2.00	5.00	3.20	1.44	−4.48	1.41	2.80	0.00
N ^d	4.88	1.10	5.96*	1.80	2.75	4.00	4.00	4.00	0.05	1.00	0.00	2.00	2.80	0.00

The units of the cohesive energy E_c , equilibrium nearest-neighbor distance r_e and bulk modulus B are eV, Å and 10^{12} dyne cm^{-2} , respectively. The reference structures of Fe, Ti, C and N are bcc, hcp, diamond and dimer, respectively.

* This is an α value as defined in Ref. [15]. Bulk modulus B is not defined for a gaseous element.

^a Ref. [11].

^b Ref. [13].

^c Ref. [14].

^d Ref. [15].

Table 2

2NN MEAM potential parameter sets for the binary M–X (M = Fe, Ti and X = C, N, Ti) systems.

	Fe–C ^a	Fe–N ^b	Ti–C ^c	Ti–N ^c	Fe–Ti ^d
E_c	$0.75E_c^{\text{Fe}} + 0.25E_c^{\text{C}} + 0.95$	$0.5E_c^{\text{Fe}} + 0.5E_c^{\text{N}} + 0.7$	$0.5E_c^{\text{Ti}} + 0.5E_c^{\text{C}} - 0.78$	$0.5E_c^{\text{Ti}} + 0.5E_c^{\text{N}} - 1.74$	$0.5E_c^{\text{Fe}} + 0.5E_c^{\text{Ti}} - 0.22$
r_e	2.364	2.09	2.210	2.121	2.58
B	2.644	2.195	2.419	3.200	1.89
d	$0.75d^{\text{Fe}} + 0.25d^{\text{C}}$	$0.5d^{\text{Fe}} + 0.5d^{\text{N}}$	$0.5d^{\text{Ti}} + 0.5d^{\text{C}}$	$0.5d^{\text{Ti}} + 0.5d^{\text{N}}$	$0.5d^{\text{Fe}} + 0.5d^{\text{Ti}}$
$C_{\min}(\text{M–X–M})$	$0.36(=C_{\min}^{\text{Fe–Fe–Fe}})$	0.16	0.64	0.16	1.21
$C_{\min}(\text{X–M–X})$	0.16	0.16	0.64	0.09	0.78
$C_{\min}(\text{M–M–X})$	0.16	0.16	$[0.5(C_{\min}^{\text{Ti}})^{1/2} + 0.5(C_{\min}^{\text{C}})^{1/2}]^2$	0.81	$[0.5(C_{\min}^{\text{Fe}})^{1/2} + 0.5(C_{\min}^{\text{Ti}})^{1/2}]^2$
$C_{\min}(\text{M–X–X})$	0.16	$[0.5(C_{\min}^{\text{Fe}})^{1/2} + 0.5(C_{\min}^{\text{N}})^{1/2}]^2$	$[0.5(C_{\min}^{\text{Ti}})^{1/2} + 0.5(C_{\min}^{\text{C}})^{1/2}]^2$	$[0.5(C_{\min}^{\text{Ti}})^{1/2} + 0.5(C_{\min}^{\text{N}})^{1/2}]^2$	$[0.5(C_{\min}^{\text{Fe}})^{1/2} + 0.5(C_{\min}^{\text{Ti}})^{1/2}]^2$
$C_{\max}(\text{M–X–M})$	2.80	1.44	$1.44(=C_{\max}^{\text{Ti}})$	2.80	$2.80(=C_{\max}^{\text{Fe}})$
$C_{\max}(\text{X–M–X})$	1.44	2.80	$2.80(=C_{\max}^{\text{C}})$	$2.80(=C_{\max}^{\text{N}})$	2.80
$C_{\max}(\text{M–M–X})$	2.80	2.80	2.80	1.44	2.80
$C_{\max}(\text{M–X–X})$	2.80	2.80	2.80	2.80	2.80
ρ_0	$\rho_0^{\text{C}}/\rho_0^{\text{Fe}} = 6.0$	$\rho_0^{\text{N}}/\rho_0^{\text{Fe}} = 18$	$\rho_0^{\text{C}}/\rho_0^{\text{Ti}} = 6.0$	$\rho_0^{\text{N}}/\rho_0^{\text{Ti}} = 18$	$\rho_0^{\text{Ti}}/\rho_0^{\text{Fe}} = 1.0$

The units of the cohesive energy E_c , the equilibrium nearest-neighbor distance r_e and the bulk modulus B are eV, Å and 10^{12} dyne cm^{-2} , respectively. The reference structures of Fe–C, Fe–N, Ti–C, Ti–N and Fe–Ti are the L1₂ Fe₃C, NaCl-type (B1) FeN, TiC, TiN and CsCl-type (B2) FeTi, respectively.

^a Ref. [16].^b Ref. [15].^c Ref. [17].^d Ref. [18].

Between bcc Fe and TiC or TiN there exists a well-known coherent interface with the Baker–Nutting orientation relationship (see Fig. 2),

$$\{001\}_{\text{TiC(or N)}} \parallel \{001\}_{\text{Fe}}, \quad \langle 110 \rangle_{\text{TiC(or N)}} \parallel \langle 100 \rangle_{\text{Fe}}. \quad (7)$$

Based on the above orientation relationship, three different types of interfaces, with Fe atoms (a) on the top of C (or N) atoms, (b) on the top of Ti atoms and (c) in the middle of the Ti–C (or TiN) square (cave site), were considered (see Fig. 3) in order to determine the site preference of Fe atoms. The calculated interfacial energies for the three different interfaces between bcc Fe and NaCl-type TiC or TiN are presented in Table 3. The size of the super cell used for this calculation is $1.6 \text{ nm} \times 8.0 \text{ nm} \times 1.6 \text{ nm}$, with about 2000 atoms and with the longest dimension perpendicular

to the interface. The numbers of atoms in the Fe and TiC (or TiN) sides are set equal to each other as in the corresponding first-principles calculations [3–5,7,9,22]. As shown in Table 3, according to the present calculation, the most stable interface is the type (a) interface, where Fe atoms are interacting with C (or N) atoms across the interface. This is in accordance with an experiment (TEM) [24] and also with the first-principles calculation [3]. Therefore, the type (a) interface was chosen as the representative coherent interface, and further calculations of coherent interface properties in the present study were performed for this interface.

As a means to estimate the average interfacial energy of incoherent interfaces between bcc Fe and TiC (or TiN), bcc Fe samples with embedded spherical TiC (or TiN) phase were prepared. Using several such samples with different orientation relationships between the embedded TiC (or TiN) sphere and the matrix bcc Fe, the average interfacial energy of incoherent interfaces could be estimated. The results are presented in Table 3. The calculated incoherent interfacial energy is much higher than the coherent interfacial energy. This strong anisotropy of the interfacial energy must be the reason for the precipitation of thin plate-type TiC or TiN in steels [25].

The work of separation is the energy required to separate a super cell into two pure phase samples, creating a free surface in each sample. For the calculation of the work of separation, the same samples used for the calculation of interfacial energy are used. However, when calculating the total energy of individual pure phase samples, the side of each pure phase sample that composed the interface is left as a free surface, without applying the periodic boundary condition. Again, the same lattice parameters as those of the super cell in the two directions parallel to the interface

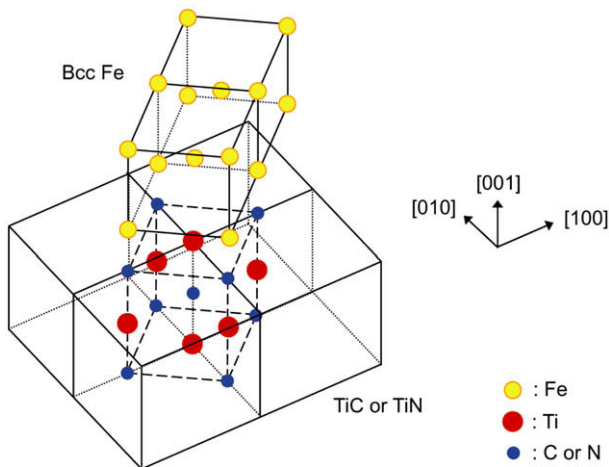


Fig. 2. The Baker–Nutting orientation relationship between bcc Fe and NaCl-type TiC or TiN.

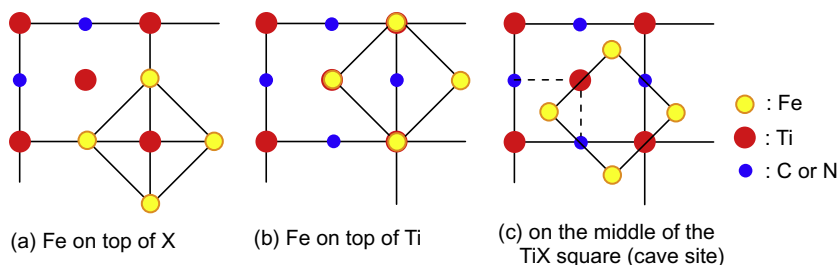


Fig. 3. A schematic illustration of some probable sites of Fe atoms at the Fe/TiX ($X = \text{C}, \text{N}$) interface. Red (large dark), blue (small dark) and yellow (light) circles indicate Ti, X and Fe atoms, respectively.

Table 3

Calculated interfacial energies for the three different types of coherent interfaces and an average interfacial energy of incoherent interfaces between bcc Fe and TiC or TiN.

Type	(a) Fe on C or N	(b) Fe on Ti	(c) Fe on the cave site	(d) Incoherent interfaces
Fe/TiC	0.302	3.633	1.108	2.130
Fe/TiN	0.175	Unstable (b) \rightarrow (c)	0.484	1.391

The unit of the interfacial energy is J m^{-2} . The values of (d) are an average of several calculations using different samples. For other notations, see Fig. 3.

are maintained. The work of separation is then obtained from the following equation:

$$W_{\text{se}} = \left[(E'_{\text{bcc Fe}} + E'_{\text{TiC(or N)}}) - E_{\text{Fe/TiC(or N)}} \right] / 2A. \quad (8)$$

In first-principles calculations [3–5,22], the work of separation is also obtained by allowing full relaxations of the sample size of pure phase samples. In this case, the resultant quantity is designated as the relaxed work of separation. The calculated (relaxed) work of separation for the coherent interface between bcc Fe and TiC or TiN is presented in Table 4, in comparison with available first-principles values.

Tables 3 and 4 show that the interface properties calculated using the present interatomic potentials are in acceptable agreement with all the first-principles calculations from different authors. This means that the present way of determining ternary potential parameters, taking an average of corresponding binary values, is a reasonable method for estimating ternary parameters. However, before making a final decision, as a means to confirm the transferability of the present default assumption, comparisons with other ternary parameter sets obtained from different assumptions were made. For ternary C_{max} or C_{min} parameters, instead of taking an average of corresponding binary values, the values could be taken from either binary system. For example, for the C (Fe–C–Ti), either C (Fe–C–Fe) or C (Ti–C–Ti) could be taken instead of their average. This gives three different assumed values for each of the three ternary C parameters, resulting in total of nine different parameter sets. These nine parameter sets, obtained from different assumptions, are summarized in Table 5. The set in the first row is by the present default assumption, used for the calculations of interface properties presented in Tables 3 and 4. The interface properties, the interfacial energy and the (relaxed) work of separation are calculated again using all nine parameter

Table 4

Calculated Interfacial energy and work of separation between bcc Fe and TiC or TiN, in comparison with first-principles calculations.

	Fe/TiC		Fe/TiN	
	MEAM	First principles	MEAM	First principles
Interfacial energy	0.302	0.263 ^a	0.175	0.343 ^d
Unrelaxed work of separation	4.81	3.988 ^b 3.83 ^c	3.47	3.79 ^e
Relaxed work of separation	2.42	2.56 ^b 2.52 ^c	2.74	–

The unit of the interfacial energy and work of separation is J m^{-2} .

^a Ref. [9].

^b Ref. [4].

^c Ref. [5].

^d Ref. [7].

^e Ref. [22].

sets, and are compared with first-principles calculations in Table 6. All nine parameter sets result in different interface property values for the Fe/TiC interface, while only the C_{max} (Fe–N–Ti) parameter has a significant effect on the Fe/TiN interface property. It is shown that the first parameter set (the default set) gives the best overall agreement with the first-principles calculations for both Fe/TiC and Fe/TiN interfaces. Based on this, the present default assumption (taking an average of corresponding binary parameters) is proposed as the first approximation for ternary C_{max} or C_{min} parameters when there is no information to use for the determination of ternary MEAM parameters.

As the present potential parameter set obtained from the default assumption showed better performance than any of the other parameter sets from different assumptions, the potential was further applied to calculate the misfit strain energy on the coherent Fe/TiC and Fe/TiN interfaces.

Table 5

Parameter sets of C_{\max} and C_{\min} for Fe–Ti–X (X = C, N) ternary systems that can be obtained from the combination of all assumptions to determine the ternary parameter from corresponding binary ones. Set A is by the present default assumption.

Type	C parameter		
	$C(i-k-j)$	$C(i-j-k)$	$C(j-i-k)$
(A)	$[0.5 (C^{\text{Fe-X-Fe}})^{1/2} + 0.5 (C^{\text{Ti-X-Ti}})^{1/2}]^2$	-----→ $[0.5 (C^{\text{Fe-Fe-X}})^{1/2} + 0.5 (C^{\text{Ti-Ti-X}})^{1/2}]^2$	
(B)	$[0.5 (C^{\text{Fe-X-Fe}})^{1/2} + 0.5 (C^{\text{Ti-X-Ti}})^{1/2}]^2$	Fe–X binary ($C^{\text{Fe-Fe-X}}$)	Ti–X binary ($C^{\text{Ti-Ti-X}}$)
(C)	$[0.5 (C^{\text{Fe-X-Fe}})^{1/2} + 0.5 (C^{\text{Ti-X-Ti}})^{1/2}]^2$	Ti–X binary ($C^{\text{Ti-Ti-X}}$)	Fe–X binary ($C^{\text{Fe-Fe-X}}$)
(D)	Ti–X binary ($C^{\text{Ti-X-Ti}}$)	-----→ $[0.5 (C^{\text{Fe-Fe-X}})^{1/2} + 0.5 (C^{\text{Ti-Ti-X}})^{1/2}]^2$	
(E)	Ti–X binary ($C^{\text{Ti-X-Ti}}$)	Fe–X binary ($C^{\text{Fe-Fe-X}}$)	Ti–X binary ($C^{\text{Ti-Ti-X}}$)
(F)	Ti–X binary ($C^{\text{Ti-X-Ti}}$)	Ti–X binary ($C^{\text{Ti-Ti-X}}$)	Fe–X binary ($C^{\text{Fe-Fe-X}}$)
(G)	Fe–X binary ($C^{\text{Fe-X-Fe}}$)	-----→ $[0.5 (C^{\text{Fe-Fe-X}})^{1/2} + 0.5 (C^{\text{Ti-Ti-X}})^{1/2}]^2$	
(H)	Fe–X binary ($C^{\text{Fe-X-Fe}}$)	Fe–X binary ($C^{\text{Fe-Fe-X}}$)	Ti–X binary ($C^{\text{Ti-Ti-X}}$)
(I)	Fe–X binary ($C^{\text{Fe-X-Fe}}$)	Ti–X binary ($C^{\text{Ti-Ti-X}}$)	Fe–X binary ($C^{\text{Fe-Fe-X}}$)

The symbols, i , j and k , represent Fe, Ti and X (X = C, N), respectively.

Table 6

Interfacial energy (E_{ifc}) and work of separation (W_{se}) for the coherent interface between bcc Fe and TiC or TiN, calculated using the nine ternary parameter sets presented in Table 5, in comparison with available first-principles calculations

Type	C_{\max}			C_{\min}			MEAM			First-principles
	$(i-k-j)$	$(i-j-k)$	$(j-i-k)$	$(i-k-j)$	$(i-j-k)$	$(j-i-k)$	E_{ifc}	W_{se}	Relaxed W_{se}	
<i>Fe/TiC</i>										
(A)	2.06	2.80	2.80	0.49	0.56	0.56	0.302	4.81	2.42	E_{ifc} : 0.263 ^a W_{se} : 3.988 ^b 3.83 ^c Relaxed W_{se} : 2.56 ^b 2.52 ^c
(B)	2.06	2.80	2.80	0.49	0.16	1.21	0.512	4.19	2.21	
(C)	2.06	2.80	2.80	0.49	1.21	0.16	0.355	4.80	2.37	
(D)	1.44	2.80	2.80	0.64	0.56	0.56	0.144	4.55	2.58	
(E)	1.44	2.80	2.80	0.64	0.16	1.21	0.378	4.78	2.34	
(F)	1.44	2.80	2.80	0.64	1.21	0.16	0.069	4.61	2.65	
(G)	2.80	2.80	2.80	0.36	0.56	0.56	0.612	4.32	2.11	
(H)	2.80	2.80	2.80	0.36	0.16	1.21	0.811	3.90	1.91	
(I)	2.80	2.80	2.80	0.36	1.21	0.16	0.648	4.05	2.07	
<i>Fe/TiN</i>										
(A)	2.06	2.06	2.06	0.16	0.42	0.42	0.175	3.47	2.74	E_{ifc} : 0.343 ^d W_{se} : 3.79 ^c
(B)	2.06	2.80	1.44	0.16	0.16	0.81	0.173	3.48	2.74	
(C)	2.06	1.44	2.80	0.16	0.81	0.16	0.176	3.47	2.74	
(D)	2.80	2.06	2.06	0.16	0.42	0.42	−0.105	3.75	3.02	
(E)	2.80	2.80	1.44	0.16	0.16	0.81	−0.107	3.75	3.02	
(F)	2.80	1.44	2.80	0.16	0.81	0.16	−0.104	3.75	3.02	
(G)	1.44	2.06	2.06	0.16	0.42	0.42	0.536	3.12	2.38	
(H)	1.44	2.80	1.44	0.16	0.16	0.81	0.534	3.12	2.38	
(I)	1.44	1.44	2.80	0.16	0.81	0.16	0.537	3.11	2.38	

The unit of the interfacial energy and the work of separation is J m^{-2} . The arrangement of ternary parameter sets is the same as that in Table 5. The symbols, i , j and k represent Fe, Ti and X (X = C, N), respectively.

^a Ref. [9].

^b Ref. [4].

^c Ref. [5].

^d Ref. [7].

^e Ref. [22].

First-principles calculations were also available for the same quantity [7,9]. Here, it was expected that the final size (lattice parameter) of the fully relaxed super cell would undergo a change depending on the ratio of the amounts (number of atoms) of Fe and TiC (or TiN). Therefore, the MEAM calculation was performed for super cells of various ratios, even though the super cell used in the first-principles calculations [7,9] involved an equal amount of Fe and TiC (or TiN). As expected, the final size of the

super cell varied depending on the fraction of Fe. Accordingly, the calculated misfit strain energy (per atom) in the individual phases also varied depending on the fraction of Fe in the super cell, as shown in Fig. 4. The strain energy (per atom) stored in TiC or TiN increases as the fraction of Fe in the super cell increases, while the opposite occurs for the strain energy in Fe. This can be easily understood because the final size of the super cell would get closer to the size of the pure Fe sample as the fraction of Fe in the

super cell increases, and the TiC or TiN would suffer an increasing amount of strain. On the other hand, the overall strain energy per atom for the whole super cell remains almost constant but decreases slightly as the fraction of Fe in the super cell increases over 70%, as also shown in Fig. 4.

In Fig. 4, the relevant first-principles results are also presented. Both the first-principles calculation and the present MEAM calculation show that the amount of misfit strain energy is larger in the Fe/TiC interface than in the Fe/TiN interface. This is because the amount of lattice mismatch between Fe and TiC is larger than that between Fe and TiN. However, the MEAM values for the Fe/TiC interface are even larger than the corresponding first-principles values, while those for the Fe/TiN interface show a good agreement with the first-principles values. This is because the lattice parameter of TiC is overestimated by about 2% by the MEAM [17], while TiN is reproduced accurately. It should also be noted here that, when the Fe fraction in the super cell is 50%, the Fe/TiC coherent interface is not stable according to the present MEAM. The bcc Fe near the interface transformed into an hcp structure at this level of misfit strain. The bcc Fe structure could only

be maintained when the Fe fraction in the super cell is larger than 53%. Therefore, all the calculations in Tables 3, 4 and 6 for the coherent Fe/TiC interface properties were actually carried out at a Fe fraction of 53%, not 50%.

Since it turned out that the calculated misfit strain energy is dependent on the sample constitution, i.e. the fraction of Fe in the super cell, it was necessary to examine whether other interface properties, the interfacial energy and work of separation, have a similar dependency. Fig. 5 thus shows the calculated interface energy and work of separation at various fractions of Fe in the super cell. The interfacial energy also shows a dependency on the sample constitution, decreasing with increasing fraction of Fe in the super cell. On the other hand, the work of separation is independent from the sample constitution. The present results indicate that one should be careful when reporting or using calculated coherent interfacial energy, paying attention to the constitution of the super cell used for the calculation. By reproducing the interface properties in reasonable agreement with relevant first-principles calculations, the present interatomic potential is believed to be applicable to atomistic simulations in order to investigate precipitation behavior or interactions with various defects

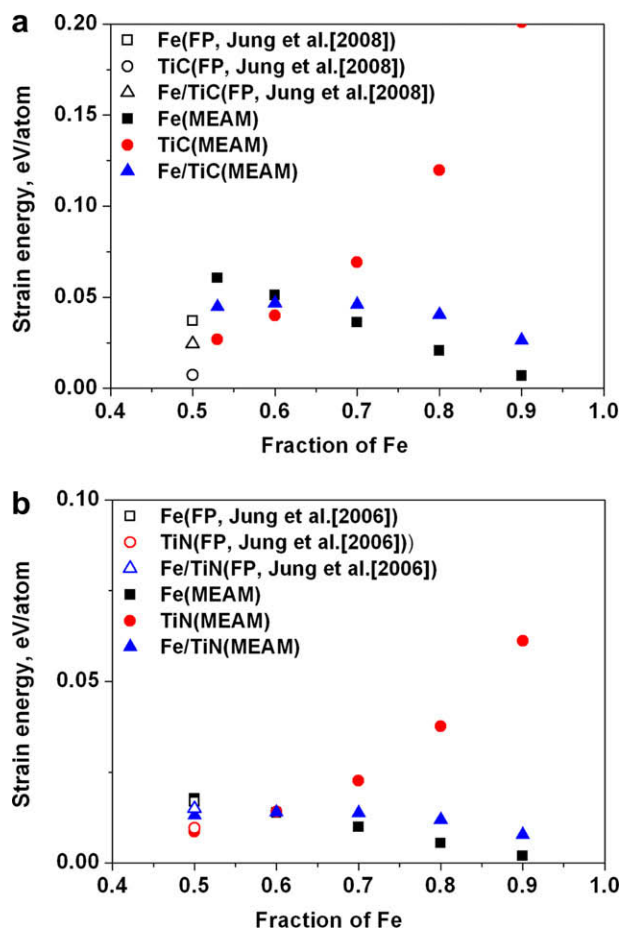


Fig. 4. Calculated misfit strain energy (per atom) in individual phases and in the whole supercell with various fraction of Fe for the coherent: (a) Fe/TiC and (b) Fe/TiN interfaces. Corresponding first-principles calculations [7,9] are also compared.

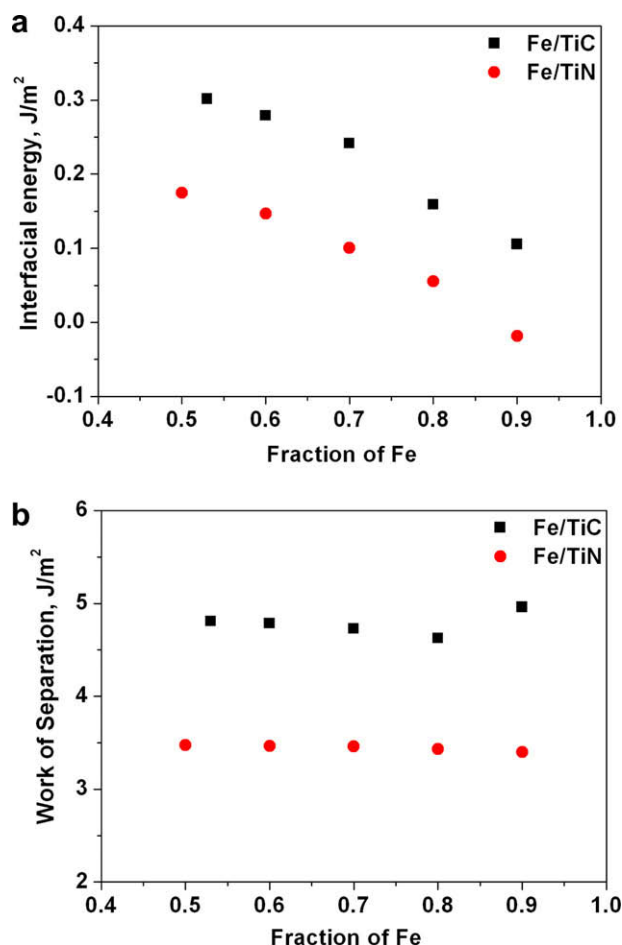


Fig. 5. Calculated: (a) interfacial energy and (b) work of separation for the coherent Fe/TiC and Fe/TiN interfaces with various fraction of Fe in the super cell.

of TiC and TiN in Fe matrix. However, one needs to be careful of the overestimation of lattice parameter of TiC by the present MEAM and the probable artifact that can result due to that overestimation.

4. Conclusion

It has been shown that the present 2NN MEAM interatomic potentials for the Fe–Ti–C and Fe–Ti–N systems predict the coherent interface properties (interfacial energy and work of separation) between bcc Fe and NaCl-type TiC or TiN in reasonable agreement with relevant first-principles calculations. It is also found that the interfacial energy varies depending on the relative amount (number of atoms) of individual phase layers in the super cell used for the calculation, while no significant size dependence is observed in the work of separation. The present way of determining ternary MEAM parameters (taking an average of corresponding binary values) is proposed as the first approximation when there is no information to use for the determination of ternary parameters. The present interatomic potentials can be further applied to atomistic simulations to investigate nucleation kinetics of TiC or TiN precipitates and their effects on mechanical properties in steels, once the overestimation of lattice parameter of TiC by the present MEAM and its probable effect on calculation results have been taken care of.

Acknowledgements

This work was supported by a grant from the Fundamental R&D Program for Core Technology of Materials

funded by the Ministry of Knowledge Economy, Republic of Korea.

References

- [1] Olson GB. *Science* 1997;277:1237.
- [2] Hartford J. *Phys Rev B* 2000;61:2221.
- [3] Shishidou T, Lee JH, Zhao YJ, Freeman AJ. *J Appl Phys* 2003;93:6876.
- [4] Arya A, Carter EA. *J Chem Phys* 2003;118:8982.
- [5] Lee JH, Shishidou T, Zhao YJ, Freeman AJ, Olson GB. *Philos Mag* 2005;85:3683.
- [6] Chung SH, Ha HP, Jung WS, Byun JY. *ISIJ Int* 2006;46:1523.
- [7] Chung SH, Jung WS, Byun JY. *Kor J Mater Res* 2006;16:473.
- [8] Jung WS, Chung SH, Ha HP, Byun JY. *Model Simul Mater Sci Eng* 2006;14:479.
- [9] Jung WS, Lee SC, Chung SH. *ISIJ Int* 2008;48:1280.
- [10] Lee BJ, Baskes MI. *Phys Rev B* 2000;62:8564.
- [11] Lee BJ, Baskes MI, Kim H, Cho YK. *Phys Rev B* 2001;64:184102.
- [12] Baskes MI. *Phys Rev B* 1992;46:2727.
- [13] Kim YM, Lee BJ, Baskes MI. *Phys Rev B* 2006;74:014101.
- [14] Lee BJ, Lee JW. *Calphad* 2005;29:7.
- [15] Lee BJ, Lee TH, Kim SJ. *Acta Mater* 2006;54:4597.
- [16] Lee BJ. *Acta Mater* 2006;54:701.
- [17] Kim YM, Lee BJ. *Acta Mater* 2008;56:3481.
- [18] Sa IY, Lee BJ. *Scripta Mater* 2008;59:595.
- [19] Rose JH, Smith JR, Guinea F, Ferrante J. *Phys Rev B* 1984;29:2963.
- [20] Baskes MI. *Mater Chem Phys* 1997;50:152.
- [21] Lee BJ, Shim JH, Baskes MI. *Phys Rev B* 2003;68:144112.
- [22] Lee JH, Freeman AJ, Olson GB. In: *American Physical Society (APS), Paris; 2004.*
- [23] Ågren J, Clavaguera-Mora MT, Costa e Silva A, Djurovic D, Gomez-Acebo T, Lee BJ, et al. *Calphad* 2007;31:53.
- [24] Chechenin NG, Bronsveld PM, Chezian A, Craus CB, Boerma DO, de Hosson JThM, et al. *Phys Stat Sol (a)* 2000;177:117.
- [25] Wei FG, Hara T, Tsuzaki K. *Metal Mater Trans B* 2004;35B:587.