Modified embedded-atom method interatomic potentials for the Nb-C, Nb-N, Fe-Nb-C, and Fe-Nb-N systems

Hyun-Kyu Kim
Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

Woo-Sang Jung
Materials Science and Technology Research Division, Korea Institute of Science and Technology, Seoul 136-791, Republic of Korea

Byeong-Joo Lee[a]
Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

Modified embedded-atom method (MEAM) interatomic potentials for Nb-C, Nb-N, Fe-Nb-C, and Fe-Nb-N systems have been developed based on the previously developed MEAM potentials for lower order systems. The potentials reproduce various fundamental physical properties (structural properties, elastic properties, thermal properties, and surface properties) of NbC and NbN, and interfacial energy between bcc Fe and NbC or NbN, in generally good agreement with higher-level calculations or experimental information. The applicability of the present potentials to atomic-level investigations to the precipitation behavior of complex-carbonitrides (Nb,Ti)(C,N) as well as NbC and NbN, and their effects on the mechanical properties of steels are also discussed.

I. INTRODUCTION

Niobium carbides and nitrides are important precipitates for strengthening steels. In order to obtain desired mechanical properties, it is necessary to understand the effect of precipitates on deformation behavior or microstructural evolution. For this, one needs to understand the interaction between precipitates and various defects such as dislocations or grain boundaries and to be able to control the size and shape of the precipitates. The size and shape of the precipitates are determined by the nucleation kinetics, which depends on matrix/precipitate interfacial energy and misfit strain energy.

All the above-mentioned properties originate from atomic level structures and are difficult to measure experimentally, but can be estimated relatively easily if atomistic simulation techniques are used. First-principles calculations provide the most reliable information on atomic-scale or sub-atomic scale properties. Indeed, many first-principles calculations have been devoted to the Nb-C (or N) and Fe-Nb-C (or N) systems.[1–19] However, those first-principles calculations are mainly for fundamental physical properties of the carbides or nitrides, or for the coherent interfacial energy between Fe matrix and carbides or nitrides. Due to the size (or number of atoms) limit, it is often not possible to inves-

tigate large-scale materials behaviors (e.g., interactions between precipitates and dislocations or grain boundaries) using only first principles. The alternative is to use (semi-)empirical interatomic potentials, which can deal with more than a million atoms. In this case, it is important that the interatomic potentials reproduce various fundamental physical properties of relevant materials systems correctly.

Even with the clear necessity for large-scale atomistic simulations, none has been done for the niobium carbide or nitride systems. This is because of the difficulty in developing (semi-)empirical interatomic potentials that can deal with all the elements, Fe, Nb, C, and N, and their alloys 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[20,21] by generalizing the MEAM.[22] The 2NN MEAM formalism has already been applied to develop interatomic potentials for the elements Fe,[21] Nb,[21] C,[23] and N,[25] and also for the Fe-C,[24] Fe-N,[25] and Fe-Nb[26] binary systems.

In addition to the previous works on the Ti-C, Ti-N,[27] Fe-Ti-C, and Fe-Ti-N[28] systems, 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-Nb-C and Fe-Nb-N ternary systems. The previously developed potential parameters of all the sub-unary and binary systems are used without any modification, and potentials for Nb-C and Nb-N binary systems are also newly developed. After combining all relevant unary and binary parameters, a few ternary parameters are further determined systematically for each ternary system, following the approach proposed in a previous work for the Fe-Ti-C and Fe-Ti-N systems.[28] The reliability of the developed potentials is then examined by computing fundamental physical properties of the Nb-C and Nb-N systems, the interfacial energy between bcc Fe and NbC or NbN, and comparing with available experimental data or first-principles calculations.

II. INTERATOMIC POTENTIAL

A. Potential formalisms

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

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

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 considering the directionality of bonding, that is, by combining several partial electron density terms for different angular contributions with weight factors $t^{(h)}(h = 1–3)$. Each partial electron density is a function of atomic configuration and atomic electron density. The atomic electron densities $\rho^{a(h)}$ ($h = 0–4$) are given as

$$\rho^{a(h)}(R) = \rho_0 \exp[-\beta^{(h)}(R/r_e - 1)] \quad , \qquad (2)$$

where ρ_0, the atomic electron density scaling factor, and $\beta^{(h)}$, the decay length, are adjustable parameters, and r_e is the nearest-neighbor distance in the equilibrium reference structure. 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 of Rose et al.[29] 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,[22] 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.[30] The consideration of the second nearest-neighbor interactions in the modified formalism is done by adjusting the screening parameters, C_{min}, so that the many-body screening becomes less severe. In addition, a radial cutoff function[30] is applied to reduce the calculation time. Details of the (2NN) MEAM formalism have been published elsewhere[20–22,30] and will not be repeated here.

In order to describe binary alloy systems, the pair interaction between different elements should be determined. For this, a similar technique to that used in determining the pair interaction for pure elements is applied to binary alloy systems. As for the Nb-C and Nb-N systems, NaCl-type NbC and NbN ordered structures are chosen as reference structures. In the NaCl-type NbC structure, for example, the total energy per atom (for 1/2Nb atom + 1/2C atom) is given as follows:

$$E_{NbC}^u(R) = \frac{1}{2} \left[F_{Nb}(\bar{\rho}_{Nb}) + F_C(\bar{\rho}_C) + Z_1 \varphi_{NbC}(R) \right.$$
$$\left. + \frac{Z_2}{2} (S_{Nb}\varphi_{NbNb}(aR) + S_C\varphi_{CC}(aR)) \right] \quad , \quad (3)$$

where Z_1 and Z_2 are the numbers of first and second nearest neighbors in the NaCl-type NbC structure, respectively. In the present case, Z_1 and Z_2 are 6 and 12, respectively. S_{Nb} and S_C are the screening functions for the second nearest neighbor interactions between Nb atoms and between C atoms, respectively, and a is the ratio between the second and first nearest-neighbor distances in the reference structure. The pair interaction between Nb and C (or N) can now be obtained in the following form:

$$\phi_{NbC}(R) = \frac{1}{Z_1} \left[2E_{NbC}^u(R) - F_{Nb}(\bar{\rho}_{Nb}) - F_C(\bar{\rho}_C) \right.$$
$$\left. - \frac{Z_2}{2} (S_{Nb}\phi_{NbNb}(aR) + S_C\phi_{CC}(aR)) \right] \quad . \quad (4)$$

The embedding functions F_{Nb} and F_C can be readily computed. The pair interactions φ_{NbNb} and φ_{CC} between the same types of atoms can also be computed from the descriptions of individual elements. To obtain $E_{NbC}^u(R)$, the universal equation of state[29] should be considered once again for the NaCl-type NbC as follows:

$$E^u(R) = -E_c(1 + a^* + da^{*3})e^{-a^*} \quad , \qquad (5)$$

where d is an adjustable parameter,

$$a^* = \alpha(R/r_e - 1) \quad , \qquad (6)$$

and

$$\alpha = \left(\frac{9B\Omega}{E_c} \right)^{1/2} \quad , \qquad (7)$$

where r_e is the equilibrium nearest-neighbor distance, E_c is the cohesive energy, B is the bulk modulus, and Ω is the equilibrium atomic volume of the reference structure. The parameters E_c, r_e (or Ω), B, and d of the NaCl-type NbC composing the universal equation of state are assumed or determined from experimental data or from high-level calculations. Then the pair interaction between Ti and C (or N) is determined as a function of the interatomic distance R.

B. Determination of potential parameters

The MEAM potential for a multicomponent alloy system is based on the MEAM for sub-unary and lower order alloy systems. In the present work for the Fe-Nb-C and Fe-Nb-N ternary systems, the MEAM parameters for pure elements and constituent binary systems were necessary. As mentioned already, the MEAM for pure Fe, Nb, C, N, and Fe-C, Fe-N, Fe-Nb binary systems, were available from Lee and coworkers.[21,23–26] Those potential parameters were taken in the present work without any modification. The MEAM potential parameters for pure elements are listed in Table I. Before completing the MEAM for ternary systems, the MEAM for the Nb-C and Nb-N binary systems needed to be developed.

As described in the previous section, the extension of the MEAM to a binary alloy system involves the determination of the pair interaction between different types of atoms. The main task is to estimate the potential parameters of the universal equation of state for the reference structure. Equations (5)–(7) show that the potential parameters are E_c, r_e (or Ω), B, and d. The first three are material properties if the reference structure is a real phase structure that exists on the phase diagram of the relevant system. Experimental data for that phase can be used directly. Otherwise, the parameter values should be optimized so that experimental information for other phases or high-level calculation results can be reproduced, if available, or assumptions should be made. The fourth parameter d is a model parameter. The value can be determined by fitting to

the $(\partial B/\partial P)$ value of the reference structure. When the reference structure is not a real phase, it is difficult to estimate a reasonable value of d for the alloy system. For such alloy systems, d is given an average value of those for pure elements.

In addition to the parameters for the universal equation of state, two more model parameters, $C_{\min}$ and $C_{\max}$, must be determined to describe alloy systems. As can be seen in Table I, each element has its own value of $C_{\min}$ and $C_{\max}$. $C_{\min}$ and $C_{\max}$ determine the extent of screening of an atom (k) to the interaction between two neighboring atoms (i and j). For pure elements, the three atoms are all the same type (i-j-k = A-A-A or B-B-B). However, in the case of binary alloys, one of the interacting atoms and/or the screening atoms can be different types (there are four cases: i-k-j = A-B-A, B-A-B, A-A-B, and A-B-B). Different $C_{\min}$ and $C_{\max}$ values may have to be given in each case. Another model parameter is the atomic electron density scaling factor ρ_0. For an equilibrium reference structure ($R = r_e$), the values of all atomic electron densities become ρ_0. This is an arbitrary value and does not have any effect on calculations for pure elements. This parameter is often omitted when describing the potential model for pure elements. However, for alloy systems, especially for systems where the composing elements have different coordination numbers, the scaling factor (relative difference) has a great effect on calculations.

The 13 model parameters discussed above, E_c, r_e, B, d, ρ_0, and four $C_{\min}$ and $C_{\max}$ parameters, must be determined to describe a binary alloy system. The optimization of the model parameters is performed by fitting to known physical properties of the alloy system. Both the Nb-C and Nb-N binary phase diagrams show the existence of two stable intermediate phases, the NaCl-type NbC (or NbN) and the hexagonal close-packed (hcp) Nb_2C (or Nb_2N). Since the NaCl-type carbide or nitride was the selected reference structure for individual systems, the E_c, r_e, and B parameter values could be determined directly from experimentally reported enthalpy of formation, lattice parameter, and bulk modulus of

TABLE I. 2NN MEAM potential parameter sets for elements, Fe, Nb, 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
Nb[a]	7.47	2.86	1.73	0.72	5.08	1.0	2.5	1.0	1.7	2.8	−1.6	0.36	2.80	0.00
C[b]	7.37	1.54	4.45	1.18	4.25	2.80	2.0	5.0	3.2	1.44	−4.48	1.41	2.80	0.00
N[c]	4.88	1.10	5.96*	1.80	2.75	4.00	4.0	4.0	0.05	1.00	0.0	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, Nb, C, and N are the bcc, bcc, diamond, and dimer, respectively.
*This is an α value as defined in Eq. (7). Bulk modulus B is not defined for a gaseous element.
[a]Ref. 21.
[b]Ref. 23.
[c]Ref. 25.

corresponding phases. A small adjustment of r_e and B values was necessary to maintain the structural stability of both NbC (or N) and Nb$_2$C (or N), and to reproduce the dilute heat of solution of C or N in bcc Nb. In addition to the above three parameters, some C_{min} and C_{max} parameters were given nondefault values to better describe the elastic constants of NbC (or N). The last model parameter that should be determined was the ratio between atomic electron density scaling factor ρ_0 of carbon (or nitrogen) and Nb. In previous works on the MEAM of Fe-Nb,[26] Fe-C,[24] and Fe-N[25] systems, the ratio ρ_0^{Nb}/ρ_0^{Fe}, ρ_0^C/ρ_0^{Fe}, and ρ_0^N/ρ_0^{Fe} were set to be 1, 6, and 18, respectively. This meant that the ratios ρ_0^C/ρ_0^{Nb} and ρ_0^N/ρ_0^{Nb} should be given the same values as in the Fe-C and Fe-N systems, 6 and 18, respectively. During the present optimization, it was confirmed that best overall results are obtained when the above values (6 and 18) are given to the ratio ρ_0^C/ρ_0^{Nb} and ρ_0^N/ρ_0^{Nb}, as has also been done in the work for the Fe-Ti-C and Fe-Ti-N systems.[28]

As already mentioned, the MEAM potential parameter set for a ternary system is obtained by combining all sub-unary and binary parameters. In addition, three more ternary parameters for each of C_{min}(i-k-j) and C_{max}(i-k-j) are necessary. In ternary systems, the 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. Considering that two elements, Fe and Nb, are relatively similar to each other compared to interstitial atoms such as C or N, it was assumed that the degree of screening by a C atom to the interaction between Fe and Nb atoms [C_{min} and C_{max}(Fe-C-Nb)] is an average between those to the Fe-Fe [C_{min} and C_{max}(Fe-C-Fe)] and Nb-Nb [C_{min} and C_{max}(Nb-C-Nb)] interactions. Similarly, the degree of screening by an Fe (or Nb) atom to the interaction between Nb (or Fe) and C atoms [C_{min} and C_{max}(Nb-Fe-C) or C_{min} and C_{max}(Fe-Nb-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 Nb atom to the Nb-C [C_{min} and C_{max}(Nb-Nb-C)] interactions. Actually, these assumptions had been introduced in the MEAM potential study of the Fe-Ti-C and Fe-Ti-N systems,[28] to skip the procedure where one has to determine ternary potential parameter values without enough amount of ternary information. Those assumptions resulted in reasonable descriptions of interfacial properties between the Fe matrix and TiC carbide or TiN nitride,[28] and were adapted in the present study for the Fe-Nb-C and Fe-Nb-N systems. By those assumptions, the ternary parameters could be automatically determined from potential parameters for constituent binary systems.

The finally determined MEAM parameter sets for the Nb-C and Nb-N binary systems and the Fe-Nb-C and Fe-Nb-N ternary systems are listed in Tables II and III.

TABLE II. 2NN MEAM potential parameter sets for the binary Nb-X (X = C or N) systems.

	Nb-C	Nb-N
E_c	$0.5E_c^{Nb} + 0.5E_c^C - 0.73$	$0.5E_c^{Nb} + 0.5E_c^N - 1.23$
r_e	2.280	2.1975
B	3.40	3.54
d	$0.5d^{Nb} + 0.5d^C$	$0.5d^{Nb} + 0.5d^N$
C_{min} (Nb-X-Nb)	0.49	$0.36 (= C_{min}^{Nb})$
C_{min} (X-Nb-X)	0.64	0.81
C_{min} (Nb-Nb-X)	2.00	$1.01 (= [0.5(C_{min}^{Nb})^{1/2} + 0.5(C_{min}^N)^{1/2}]^2)$
C_{min} (Nb-X-X)	2.00	$1.01 (= [0.5(C_{min}^{Nb})^{1/2} + 0.5(C_{min}^N)^{1/2}]^2)$
C_{max} (Nb-X-Nb)	1.44	2.00
C_{max} (X-Nb-X)	2.80	2.80
C_{max} (Nb-Nb-X)	2.80	2.80
C_{max} (Nb-X-X)	2.80	2.80
ρ_0	$\rho_0^C/\rho_0^{Nb} = 6$	$\rho_0^N/\rho_0^{Nb} = 18$

The units of the cohesive energy E_c, the equilibrium nearest-neighbor distance r_e, and bulk modulus B are eV, Å, and 10^{12} dyne/cm^2, respectively. The reference structure is NaCl-type NbX for both systems.

TABLE III. Parameter sets of C_{max} and C_{min} for Fe-Nb-X (X = C or N) ternary systems automatically determined from constituent binary parameters.

	Type	Fe-Nb-C	Fe-Nb-N	
C_{max}	C(Fe-X-Nb)	2.06	1.71	$[0.5(C^{Fe-X-Fe})^{1/2} + 0.5(C^{Nb-X-Nb})^{1/2}]^2$
	C(Fe-Nb-X)	2.80	2.80	$[0.5(C^{Fe-Fe-X})^{1/2} + 0.5(C^{Nb-Nb-X})^{1/2}]^2$
	C(Nb-Fe-X)	2.80	2.80	$[0.5(C^{Fe-Fe-X})^{1/2} + 0.5(C^{Nb-Nb-X})^{1/2}]^2$
C_{min}	C(Fe-X-Nb)	0.49	0.25	$[0.5(C^{Fe-X-Fe})^{1/2} + 0.5(C^{Nb-X-Nb})^{1/2}]^2$
	C(Fe-Nb-X)	0.82	0.49	$[0.5(C^{Fe-Fe-X})^{1/2} + 0.5(C^{Nb-Nb-X})^{1/2}]^2$
	C(Nb-Fe-X)	0.82	0.49	$[0.5(C^{Fe-Fe-X})^{1/2} + 0.5(C^{Nb-Nb-X})^{1/2}]^2$

III. CALCULATION OF PHYSICAL PROPERTIES

In this section, fundamental physical properties of the Nb-C, Nb-N, Fe-Nb-C, and Fe-Nb-N systems will be calculated using the present MEAM potentials shown in Tables I–III, and be compared with experimental information or higher-level calculations. The 2NN MEAM formalism includes up to 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. All calculations present here are performed with a radial cutoff distance of 4.5 Å which is between the second and third nearest-neighbor distances of the larger element Nb. If not designated, all MEAM values shown in this section are those calculated at 0 K.

The properties calculated in the present study can be divided into two groups. The first group is the fundamental

physical properties: lattice parameters, enthalpy of formation, and elastic constants of Nb-carbides or nitrides, and the dilute heat of solution of C or N in bcc Nb. Those properties are what is used for parameter optimization. The comparison between calculated and experimental values shows the quality of fitting. The second group is the properties with experimental information or higher-level calculation values, but that are not used for parameter optimization. The thermal expansion and surface energy of NbC (or N) and the coherent interfacial energy between bcc Fe and NbC (or N) belong to this group. Through comparisons with experimental data or higher-level calculations, the transferability of the present potential and its applicability to the investigation of precipitation behavior and effect of NbC (or N) precipitates on the mechanical properties of steels can be evaluated.

As mentioned above, the first property calculated using the present MEAM potential is the lattice parameters and enthalpy of formation of NbC (or N) and Nb_2C (or N). As shown in Table IV, those properties for NbN and Nb_2N are correctly reproduced. The lattice parameter of NbC is overestimated by about 2%, which should be kept in mind in future applications of this potential. The lattice parameter of NbC could be exactly fitted by selecting a correct value of r_e parameter. However, this value had to be adjusted to make the NaCl-type NbC structure mechanically stable. The lattice parameters of the Nb_2C are also overestimated to about the same extent. Further, using one E_c parameter value, the enthalpy of formation of both NbC and Nb_2C could not be reproduced simultaneously. In the present study, the E_c parameter value was selected so that the enthalpy

of formation of NbC is exactly reproduced since NbC is the practically important carbide in Nb-containing steels. The calculated elastic properties of NbC and NbN are compared with experimental data and first-principles calculations in Table V. The agreement between the MEAM calculation and experimental data looks generally good, when compared with the scattering range of first-principles calculations, except that C_{12} of NbN is overestimated. The calculated dilute heat of solution of carbon and nitrogen in bcc Nb are comparable with experimental data and/or thermodynamically assessed values by the CALPHAD method, as shown in Table VI.

As a means of examining the robustness of the present MEAM potential, the thermal expansion of NbC and NbN was calculated. This was also done to confirm that the carbide or nitride maintains its structure at finite temperatures without transforming into other structures or a collapse of the structure that happens frequently when using empirical potentials. As shown in Table VII, the present potential underestimates the thermal expansion of both compounds by around 30%. The melting points of NbC and NbN, roughly estimated by heating perfect crystalline samples using molecular dynamics, were both higher than 2000 K, and it was also confirmed that the NaCl-type B1 structure is maintained up to the melting temperature. Surface energy is a good test bed to evaluate the transferability of empirical interatomic potentials. The surface energy of (100), (110), and (111) surfaces of NbC and NbN according to the present potential is compared with first-principles calculations in Table VIII. It is shown that not only the absolute values but also the

TABLE IV. Lattice parameter and enthalpy of formation of NbX and Nb$_2X$ (X = C or N) calculated using the present 2NN MEAM potentials, in comparison with experimental data and/or first-principles calculations.

Type	Compounds	MEAM	Experimental data	First-principles calculation
Nb-C	NbC			
	Lattice constant, a (Å)	4.560	4.430,[a] 4.469,[b] 4.470,[c] 4.4707,[d] 4.471[e]	4.43,[f] 4.45,[g] 4.476,[h] 4.489,[i] 4.49[j]
	Enthalpy of formation (eV atom^{-1})	−0.730	−0.729 ± 0.013,[k] −0.731,[l] −0.729,[c] −0.701,[m] −0.721[n]	−0.585[p]
	Nb$_2$C			
	Lattice constant, a (Å)	3.218	3.119,[q] 3.122[b]	—
	c (Å)	5.104	4.959,[q] 4.964[b]	
	Enthalpy of formation (eV atom^{-1})	0.08	−0.674 ± 0.017,[k] −0.631,[m] −0.627[n]	—
Nb-N	NbN			
	Lattice constant, a (Å)	4.395	4.390,[c] 4.394,[r] 4.382,[s] 4.3913,[t] 4.379,[u] 4.392[v]	4.363,[f] 4.430,[j] 4.41,[i] 4.42,[w] 4.378[x]
	Enthalpy of formation (eV atom^{-1})	−1.23	−1.233 ± 0.017,[y] −1.22,[z] −1.175[aa]	—
	Nb$_2$N			
	Lattice constant, a (Å)	3.049	3.055,[bb] 3.056,[cc] 3.054[b]	—
	c (Å)	5.008	4.994,[bb] 4.996,[cc] 5.005[b]	
	Enthalpy of formation (eV atom^{-1})	−0.754	−0.97,[dd] −0.883,[ee] −0.867,[z,aa] −0.933[aa]	—

The reference states for the enthalpy of formation are bcc Nb and graphite C or gaseous N_2 at 1 atm.
[a]Ref. 31. [b]Ref. 32. [c]Ref. 33. [d]Ref. 34. [e]Ref. 37. [f]Ref. 12. [g]Ref. 18. [h]Ref. 1. [i]Ref. 6. [j]Ref. 12. [k]Ref. 35. [l]Ref. 38. [m]Ref. 39 thermodynamic assessment. [n]Ref. 40 thermodynamic assessment. [p]Ref. 11. [q]Ref. 36. [r]Ref. 41. [s]Ref. 42. [t]Ref. 43. [u]Ref. 8. [v]Ref. 44. [w]Ref. 13. [x]Ref. 19. [y]Ref. 45. [z]Ref. 46 thermodynamic assessment. [aa]Ref. 47 thermodynamic assessment. [bb]Ref. 48. [cc]Ref. 49. [dd]Ref. 50. [ee]Ref. 51.

TABLE V. Elastic properties of NaCl-type NbX (X = C or N) calculated using the present 2NN MEAM potentials, in comparison with experimental data and first-principles calculations.

	MEAM	Experimental data	First principles calculation
NbC			
B	3.40	2.96,[a] 3.02,[b] 3.40[c]	2.93,[d] 2.99,[e] 3.01,[f] 3.06,[g] 3.28,[h] 3.32,[i] 3.35,[j] 3.31,[k]
C_{11}	5.49	6.20[l]	5.46,[d] 6.27,[h] 6.4,[i] 6.67[k]
C_{12}	2.35	2.00[l]	1.67,[d] 1.79,[h] 1.8,[i] 1.63[k]
C_{44}	1.73	1.50[l]	2.24,[d] 2.20,[h] 1.4,[i] 1.61[k]
NbN			
B	3.54	2.92,[m] 3.20[c]	3.074,[d] 3.09,[f] 3.17,[o] 3.40,[p] 3.499,[h] 3.50,[q] 3.54[r]
C_{11}	5.79	6.08,[m] 5.56[n]	6.04,[h] 4.98,[d] 7.39[r]
C_{12}	2.42	1.34,[m] 1.52[n]	2.23,[h] 2.12,[d] 1.61[r]
C_{44}	1.68	1.17,[m] 1.25[n]	1.84,[h] 0.89,[d] 0.76[r]

The units of elastic constants B, C_{11}, C_{12}, C_{44} are 10^{12} dyne/cm^2.
[a]Ref. 32. [b]Ref. 52. [c]Ref. 33. [d]Ref. 12 GGA. [e]Ref. 3. [f]Ref. 1. [g]Ref. 6. [h]Ref. 12 LDA. [i]Ref. 18. [j]Ref. 4. [k]Ref. 7. [l]Ref. 53. [m]Ref. 54. [n]Ref. 55. [o]Ref. 13. [p]Ref. 5. [q]Ref. 15. [r]Ref. 8.

TABLE VI. Dilute heat of solutions of carbon and nitrogen in bcc Nb calculated using the present 2NN MEAM potentials, in comparison with experimental data and thermodynamic assessment.

In bcc Nb	MEAM	Experimental data
Dilute heat of solution of C (eV)	0.44	−0.22[a]
Dilute heat of solution of N (eV)	−1.71	−1.95,[b] −1.997[c]

[a]Ref. 56 thermodynamic assessment.
[b]Ref. 47 thermodynamic assessment.
[c]Ref. 50.

TABLE VII. Thermal linear expansion coefficients of NbC and NbN.

	NbC		NbN	
	MEAM	Experimental data	MEAM	Experimental data
Thermal linear expansion (at 293K)	4.5	6.6,[a] 7.2[b]	7.7	10.1[b]

The unit of thermal linear expansion is 10^{-6}/K.
[a]Ref. 57.
[b]Ref. 58.

TABLE VIII. Relaxed surface energy of low index surfaces of NbC and NbN calculated using the present (2NN) MEAM potentials, in comparison with first-principles calculations.

	Surface	MEAM	First principles calculation
NbC			
	(100)	2.46	2.81[a]
	(110)	2.65	—
	(111)	2.47	—
NbN			
	(100)	1.36	1.13[b]
	(110)	1.90	2.12[b]
	(111)	2.26	2.04–2.15[b]

The unit of the surface energy is J/m^2.
[a]Ref. 10.
[b]Ref. 9.

orientation dependency (anisotropy) of surface energy are reasonably reproduced for both NbC and NbN.

It has been shown that the present 2NN MEAM potentials for the Nb-C and Nb-N binary systems can reproduce most of the fundamental physical properties of the alloy systems considered. The potentials were combined with those for the Fe-C, Fe-N, and Fe-Nb binary systems to automatically generate ternary parameters (Table III) necessary to complete the potential parameter sets for the Fe-Nb-C and Fe-Nb-N ternary systems. As a means to confirm the applicability of the present ternary potentials to the atomic-level investigation of precipitation behavior of NbC or NbN in steels, the interfacial energy between bcc Fe and NaCl-type NbC or NbN was calculated.

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 NbC or NbN) and the summation of total energies of individual pure phase samples of the same size.[28] 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 conditions, the super cell actually involves two interfaces. The interfacial energy σ is obtained from the following equation:

$$\sigma = \left[E_{\text{Fe/NbC(or N)}} - \left(E_{\text{bcc Fe}} + E_{\text{NbC(or N)}} \right) \right] / 2A \quad , \quad (8)$$

where A represents the area of the interface.

Between bcc Fe and NbC or NbN there exists a well-known coherent interface with the Baker–Nutting orientation relationship.

$$\{001\}_{NbC(or\,N)} \| \{001\}_{Fe}, \quad <100>_{NbC(or\,N)} \| <110>_{Fe} \quad .$$

$$(9)$$

Based on the above orientation relationship, three different types of interfaces can be considered, with Fe atoms (i) on the top of C (or N) atoms, (ii) on the top of Nb atoms, and (iii) in the middle of the Nb–C (or NbN) square (cave site). In the case of Fe/TiC (or TiN) interface, all the experimental, first-principles and MEAM calculation indicated that the type (i) interface with Fe atoms interacting with C or N atoms is energetically the most stable.[28] The same type of interface was considered in the present study for the Fe/NbC (or NbN) interface.

The size of the super cell used for this calculation was 1.6 nm × 8.0 nm × 1.6 nm, with about 2000 atoms, and the numbers of atoms in the Fe and NbC (or N) sides were set equal to each other as in the corresponding first-principles calculations.[5,6] As mentioned already, the dimension of the super cell evolves to a natural size during the molecular statics relaxation. However, when the numbers of atoms in both sides were equal to each other, according to the present MEAM potential, the Fe part of the super cell underwent a phase transformation into an hcp structure during the relaxation. This was because of the excessive lattice mismatch between Fe and NbC (or N), and had also occurred when calculating the Fe/TiC interfacial energy.[28] As an alternative, in the present study, a fixed smaller value than the natural one was given to the super cell size along directions parallel to the interface and the relaxation was allowed only into the direction perpendicular to the interface, so that the transformation in the Fe part does not occur. Several super cell samples were prepared varying the sample size into directions parallel to the interface. Each sample yielded different values of overall internal stresses (or pressure). The interfacial energy calculated using each sample was plotted as a functional form of the internal pressure, extrapolated to the zero internal pressure as shown in Fig. 1, and the extrapolated value was finally selected as the target interfacial energy. To examine the reliability of the present estimation of the interfacial energy, the method was applied to the calculation of the Fe/TiN interfacial energy. Figure 2 shows Fe/TiN interfacial energy values obtained using super cell samples with nonrelaxed sample size along directions parallel to the interface (square symbols). The round symbol in Fig. 2 represents the interfacial energy obtained by a full relaxation of the super cell. It is shown that almost the same value as the one from fully relaxed sample is obtained when those values from nonrelaxed samples are interpolated to zero internal pressure.
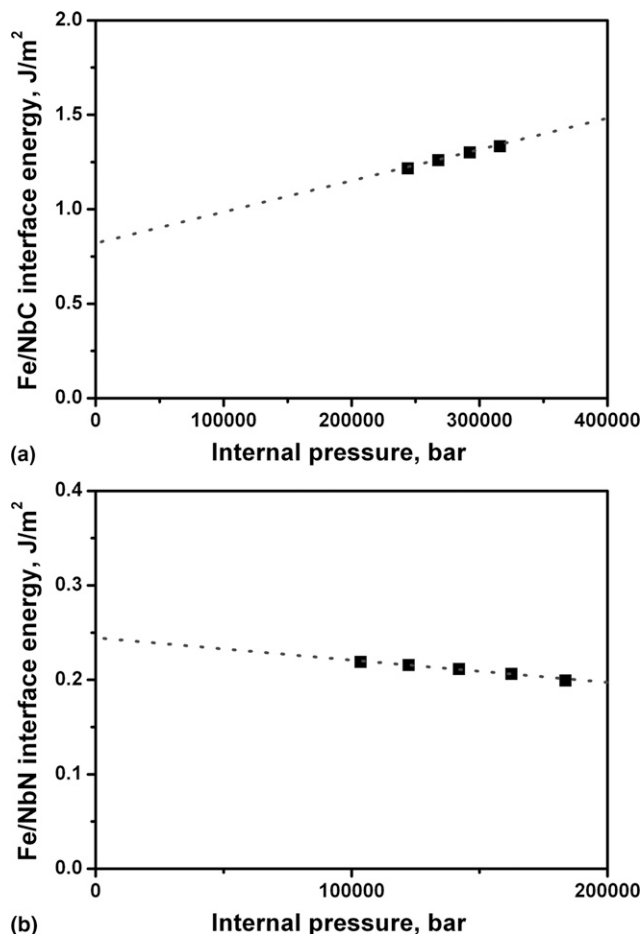

FIG. 1. Calculated interfacial energy for the coherent (a) Fe/NbC and (b) Fe/NbN interfaces at various arbitrary super cell sizes along directions parallel to the interface and resultant overall internal pressure in the super cell. The ideal interfacial energy is obtained by extrapolating the calculated interfacial energy to zero internal pressure.
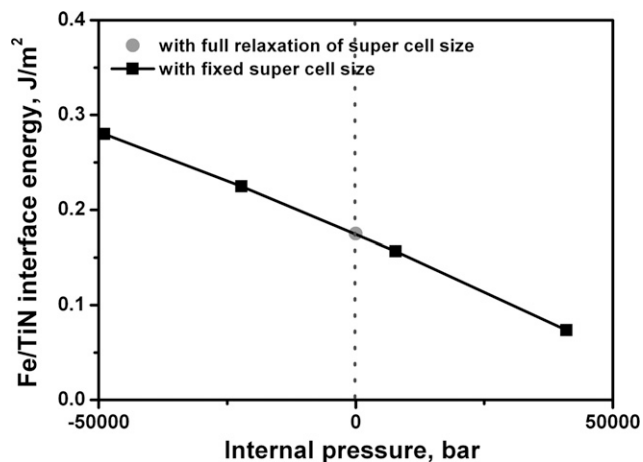

FIG. 2. Calculated interfacial energy for the coherent Fe/TiN interface at various arbitrary super cell sizes along directions parallel to the interface and resultant overall internal pressure in the super cell. The ideal interfacial energy obtained by interpolating the calculated interfacial energy to zero internal pressure coincides with the one (the round symbol) obtained by a full relaxation of the super cell.

TABLE IX. Calculated coherent interfacial energy between bcc Fe and NbX (X = C or N) with Baker-Nutting orientation relationship, in comparison with first-principles calculations and literature data. Values in parentheses are the average interfacial energy of incoherent interface.

Interface	MEAM (incoherent interface)	First principles calculation	Other estimation
Fe/NbC	0.817 (2.36)	−0.17[a]	0.3∼1.0[c]
Fe/NbN	0.245 (2.33)	−0.23[b]	0.23[d]

The unit of the interfacial energy is J/m^2.
[a]Ref. 6.
[b]Ref. 5.
[c]Ref. 59.
[d]Ref. 60.

The finally determined coherent interfacial energy between bcc Fe and NbC or NbN is presented in Table IX, in comparison with corresponding first-principles values[5,6] and those from other sources. The first-principles calculation yields negative values for the Fe/NbC and Fe/NbN interfacial energy, while the present MEAM yields positive values. The MEAM value for the Fe/NbC, 0.82 J/m^2, is inside a range of experimental values deduced from a nucleation and growth-kinetics modeling study,[59] and that for the Fe/NbN, 0.25 J/m^2, is in a very good agreement with a literature value used in a kinetic modeling study.[60] However, it should be mentioned here that the comparison between 0 K calculated values and finite temperature experimental values can only show that the MEAM potential provides the correct magnitude of these quantities. As a means to estimate the average interfacial energy of incoherent interfaces between bcc Fe and NbC (or NbN), a bcc Fe sample with embedded spherical NbC (or NbN) phase were prepared. Using several such samples with different orientation relationships between the embedded NbC (or NbN) sphere and the matrix bcc Fe, the average interfacial energy of incoherent interfaces could be estimated, as shown in parentheses in Table IX. The calculated incoherent interfacial energy is much higher than the coherent interfacial energy, although the anisotropy in the interfacial energy is less severe in the case of Fe/NbC. Similar results have also been obtained for the Fe/TiC interface,[28] and the strong anisotropy of the interfacial energy can be the reason for the precipitation of thin plate- or disk-type TiC or NbC in steels.[61–64]

The reasonable agreement between the present calculation and literature information on the Fe/NbC (or NbN) interfacial energy, and the reasonable description of elastic properties of relevant materials, NbC, NbN, and pure Fe, indicate the applicability of the present atomistic approach to the atomic-level investigation of precipitation behavior or interactions with various defects of NbC carbide or NbN nitride in an Fe matrix. However, one needs to avoid overestimation of the lattice parameter of

NbC by the present MEAM and the probable artifact that can result due to that overestimation.

Describing interatomic potentials of a wide range of elements using a common potential formalism and being able to deal with various alloy systems is easily the strongest point of the present (2NN) MEAM potential formalism. It should be noted here that the present MEAM potentials for the Fe-Nb-C and Fe-Nb-N systems can be easily combined with already published Fe-Ti-C and Fe-Ti-N potentials, and be applied to investigate the nucleation behavior of (Nb,Ti)(C,N) carbonitrides and their interaction with dislocations, grain boundaries, or other defects in steels.

IV. CONCLUSION

It has been shown that the present 2NN MEAM potentials for the Nb-C and Nb-N systems can reproduce various fundamental physical properties—structural properties (enthalpy of formation, lattice parameter, and dilute heat of solution), elastic properties (bulk modulus, elastic constants), thermal properties (thermal expansion and melting point), and surface energy of NbC and NbN—reasonably well. The interfacial energy between bcc Fe and NbC or NbN can also be reproduced in good agreement with literature values, using the simultaneously developed potentials for the Fe-Nb-C and Fe-Nb-N. Being combined with already developed MEAM potentials for the Fe-Ti-C and Fe-Ti-N systems, the present potentials can be applied to atomic-level investigations of the precipitation behavior of (Nb,Ti)(CN)-type carbonitrides and their effects on the deformation and mechanical properties of steels, once the overestimation of the lattice parameter of the MC-type carbides by the present MEAM and its probable effect on calculation results is taken care of.

ACKNOWLEDGMENT

REFERENCES

1. E.I. Isaev, S.I. Simak, I.A. Abrikosov, R. Ahuja, Yu.Kh. Vekilov, M.I. Katsnelson, A.I. Lichtenstein, and B. Johansson: Phonon related properties of transition metals, their carbides, and nitrides: A first-principles study. *J. Appl. Phys.* **101,** 123519 (2007).
2. E.I. Isaev, R. Ahuja, S.I. Simak, A.I. Lichtenstein, Y.K. Vekilov, B. Johansson, and I.A. Abrikosov: Anomalously enhanced super-conductivity and ab initio lattice dynamics in transition metal carbides and nitrides. *Phys. Rev. B* **72,** 064515 (2005).
3. K.B. Joshi and U. Paliwal: First-principles study of structural and bonding properties of vanadium carbide and niobium carbide. *Phys. Scr.* **80,** 055601 (2009).

4. F. Tran, R. Laskowski, P. Blaha, and K. Schwarz: Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. *Phys. Rev. B* **75,** 115131 (2007).

5. W-S. Jung, S-H. Chung, H-P. Ha, and J-Y. Byun: An ab initio study of the energetics for interfaces between group V transition metal nitrides and bcc iron. *Modell. Simul. Mater. Sci. Eng.* **14,** 479 (2006).

6. S-H. Chung, H-P. Ha, W-S. Jung, and J-Y. Byun: An ab initio study of the energetics for interfaces between group V transition metal carbides and bcc iron. *ISIJ Int.* **46,** 1523 (2006).

7. Z. Wu, X.J. Chen, V.V. Struzhkin, and R.E. Cohen: Trends in elasticity and electronic structure of transition-metal nitrides and carbides from first principles. *Phys. Rev. B* **71,** 214103 (2005).

8. X.J. Chen, V.V. Struzhkin, Z. Wu, M. Somayazulu, J. Qian, S. Kung, A.N. Christensen, Y. Zhao, R.E. Cohen, H.K. Mao, and R.J. Hemley: Hard superconducting nitrides. *Proc. Nat. Acad. Sci. U.S.A.* **102,** 3198 (2005).

9. I.M. Iskandarova, A.A. Knizhnik, B.V. Potapkin, A.A. Safonov, A.A. Bagatur'yants, and L.R.C. Fonseca: First-principles investigation of the electronic properties of niobium and molybdenum mononitride surfaces. *Surf. Sci.* **583,** 69 (2005).

10. H.W. Hugosson, O. Eriksson, U. Jansson, A.V. Ruban, P. Souvatzis, and I.A. Abrikosov: Surface energies and work functions of the transition metal carbides. *Surf. Sci.* **557,** 243 (2004).

11. H.W. Hugosson, O. Eriksson, U. Jansson, and B. Johansson: Phase stabilities and homogeneity ranges in 4*d*-transition-metal carbides: A theoretical study. *Phys. Rev. B* **63,** 134108 (2001).

12. T. Amriou, B. Bouhafs, H. Aourag, B. Khelifa, S. Bresson, and C. Mathieu: FP-LAPW investigations of electronic structure and bonding mechanism of NbC and NbN compounds. *Physica B* **325,** 46 (2003).

13. C. Stampfl, W. Mannstadt, R. Asahi, and A.J. Freeman: Electronic structure and physical properties of early transition metal mononitrides: Density-functional theory LDA, GGA, and screened-exchange LDA FLAPW calculations. *Phys. Rev. B* **63,** 155106 (2001).

14. K. Kobayashi: Electronic structure and physical properties of early transition metal mononitrides: Density-functional theory LDA, GGA, and screened-exchange LDA FLAPW calculations. *Jpn. J. Appl. Phys.* **39,** 4311 (2000).

15. G.L.W. Hart and B.M. Klein: Phonon and elastic instabilities in MoC and MoN. *Phys. Rev. B* **61,** 3151 (2000).

16. S. Öğüt and K.M. Rabe: Polymorphism and metastability in NbN: Structural predictions from first principles. *Phys. Rev. B* **52,** R8585 (1995).

17. A.F. Guillermet, J. Häglund, and G. Grimvall: Cohesive properties of 4*d*-transition-metal carbides and nitrides in the NaCl-type structure. *Phys. Rev. B* **45,** 11557 (1992).

18. J. Chen, L.L. Boyer, H. Krakauer, and M.J. Mehl: Elastic constants of NbC and MoN: Instability of B_1-MoN. *Phys. Rev. B* **37,** 3295 (1988).

19. D.A. Papaconstantopoulos, W.E. Pickett, B.M. Klein, and L.L. Boyer: Electronic properties of transition-metal nitrides: The group-V and group-VI nitrides VN, NbN, TaN, CrN, MoN, and WN. *Phys. Rev. B* **31,** 752 (1985).

20. B-J. Lee and M.I. Baskes: Second nearest-neighbor modified embedded-atom-method potential. *Phys. Rev. B* **62,** 8564 (2000).

21. B-J. Lee, M.I. Baskes, H. Kim, and Y.K. Cho: Second nearest-neighbor modified embedded atom method potentials for bcc transition metals. *Phys. Rev. B* **64,** 184102 (2001).

22. M.I. Baskes: Modified embedded-atom potentials for cubic materials and impurities. *Phys. Rev. B* **46,** 2727 (1992).

23. B-J. Lee and J.W. Lee: A modified embedded atom method interatomic potential for carbon. *Calphad* **29,** 7 (2005).

24. B-J. Lee: A modified embedded-atom method interatomic potential for the Fe–C system. *Acta Mater.* **54,** 701 (2006).

25. B-J. Lee, T-H. Lee, and S-J. Kim: A modified embedded-atom method interatomic potential for the Fe–N system: A comparative study with the Fe–C system. *Acta Mater.* **54,** 4597 (2006).

26. I.Y. Sa and B-J. Lee: Modified embedded-atom method interatomic potentials for the Fe–Nb and Fe–Ti binary systems. *Scr. Mater.* **59,** 595 (2008).

27. Y-M. Kim and B-J. Lee: Modified embedded-atom method interatomic potentials for the Ti–C and Ti–N binary systems. *Acta Mater.* **56,** 3481 (2008).

28. H-K. Kim, W-S. Jung, and B-J. Lee: Modified embedded-atom method interatomic potentials for the Fe–Ti–C and Fe–Ti–N ternary systems. *Acta Mater.* **57,** 3140 (2009).

29. J.H. Rose, J.R. Smith, F. Guinea, and J. Ferrante: Universal features of the equation of state of metals. *Phys. Rev. B* **29,** 2963 (1984).

30. M.I. Baskes: Determination of modified embedded atom method parameters for nickel. *Mater. Chem. Phys.* **50,** 152 (1997).

31. E. Rudy, F. Benesovsky, and K. Sedlatschek: A study of the Nb-Mo-C system. *Monatsh. Chem.* **92,** 841 (1961).

32. H.O. Pierson: *Handbook of Refractory Carbides and Nitrides: Properties, Characteristics, Processing and Applications* (Noyes Publications, Westwood, NJ, 1996).

33. L.E. Toth: *Transition Metal Carbides and Nitrides* (Academic Press, New York, 1971).

34. E.K. Storm: *Los Alamos Scientific Laboratory Report La-2942* (The Office of Technical Services, U.S. Department of Commerce, Washington, DC, 1964).

35. E.J. Huber, Jr., E.L. Head, C.E. Holley, Jr., E.K. Storms, and N.H. Krikorian: The heats of combustion of niobium carbides. *J. Phys. Chem.* **65,** 1846 (1961).

36. E.K. Storms and N.H. Krikorian: The niobium-niobium carbide system. *J. Phys. Chem.* **64,** 1471 (1960).

37. I.P. Parkin: Solid state metathesis reaction for metal borides, silicides, pnictides and chalcogenides: Ionic or elemental pathways. *Chem. Soc. Rev.* **25,** 199 (1996).

38. A. Teresiak and H. Kubsch: X-ray investigations of high-energy ball milled transition metal carbides. *Nanostruct. Mater.* **6,** 671 (1995).

39. W. Huang and M. Selleby: Thermodynamic assessment of the Nb-W-C system. *Z. Metallkd.* **88,** 55 (1997).

40. B-J. Lee: Thermodynamic assessment of the Fe-Nb-Ti-C-N system. *Metall. Mater. Trans. A* **32,** 2423 (2001).

41. A.N. Christensen: Preparation and structure of stoichiometric δ-NbN. *Acta Chem. Scand. Ser. A* **31,** 77 (1977).

42. G. Heger and O. Baumgartner: Crystal structure and lattice distortion of γ-NbN$_x$ and δ-NbN$_x$. *J. Phys. C: Solid State Phys.* **13,** 5833 (1980).

43. W. Lengauer and P. Ettmayer: Preparation and properties of compact cubic δ-NbN$_{1−x}$. *Monatsh. Chem.* **117,** 275 (1986).

44. G. Brauer and H. Kirner: High pressure synthesis of niobium nitrides and constitution of δ-NbN. *Z. Anorg. Allg. Chem.* **328,** 34 (1964).

45. A.D. Mah and N.L. Gellert: Heats of formation of niobium nitride, tantalum nitride and zirconium nitride from combustion calorimetry. *J. Am. Chem. Soc.* **78,** 3261 (1956).

46. M.W. Chase, Jr., C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald, and A.N. Syverud: JANAF thermodynamics tables, 3rd ed. *J. Phys. Chem. Ref. Data* **14**(Suppl. 1), 1616 (1985).

47. W. Huang: Thermodynamic assessment of the Nb-N system. *Metall. Mater. Trans. A* **27,** 3591 (1996).

48. T.A. Panaioti: Ion nitriding of tantalum and niobium alloys. *Met. Sci. Heat Treat.* **44,** 439 (2002).

49. A.N. Christensen: Preparation and crystal structure of β-Nb$_2$N and γ-NbN. *Acta Chem. Scand. Ser. A* **30,** 219 (1976).

50. J.R. Cost and C.A. Wert: Metal-gas equilibrium in the niobium-nitrogen terminal solid solution. *Acta Metall.* **11,** 231 (1963).

51. A.D. Mah: Heats of formation of niobium dioxide, niobium subnitride and tantalum subnitride. *J. Am. Chem. Soc.* **80,** 3872 (1958).

52. V.A. Gubanov, A.L. Ivanovsky, and V.P. Zhukov: *Electronic Structure of Refractory Carbides and Nitrides* (Cambridge University Press, Cambridge, UK, 1994).

53. W. Weber: Lattice dynamics of transition-metal carbides. *Phys. Rev. B* **8,** 5082 (1973).

54. A.N. Christensen, O.W. Dietrich, W. Kress, W.D. Teuchert, and R. Currat: Phonon anomalies in transition metal nitrides: δ-NbN. *Solid State Commun.* **31,** 795 (1979).

55. J.O. Kim, J.D. Achenbach, P.B. Mirkarimi, M. Shinn, and S.A. Barnett: Elastic constants of single-crystal transition-metal nitride films measured by line-focus acoustic microscopy. *J. Appl. Phys.* **72,** 1805 (1992).

56. B-J. Lee: Update of steel database. Unpublished work at KTH (1999).

57. A. Perecherla and W.S. Williams: Room-temperature thermal conductivity of cemented transition-metal carbides. *J. Am. Ceram. Soc.* **71,** 1130 (1988).

58. H. Holleck: Material selection for hard coatings. *J. Vac. Sci. Technol., A* **4,** 2661 (1986).

59. F. Perrard, A. Deschamps, and P. Maugis: Modelling the precipitation of NbC on dislocations in α-Fe. *Acta Mater.* **55,** 1255 (2007).

60. N. Fujita, H.K.D.H. Bhadeshia, and M. Kikuchi: Precipitation sequence in niobium-alloyed ferritic stainless steel. *Modell. Simul. Mater. Sci. Eng.* **12,** 273 (2004).

61. F. Perrard, P. Donnadieu, A. Deschamps, and P. Barges: TEM study of NbC heterogeneous precipitation in ferrite. *Philos. Mag.* **86,** 4271 (2006).

62. F.G. Wei, T. Hara, and K. Tsuzaki: High-resolution transmission-electron-microscopy study of crystallography and morphology of TiC precipitates in tempered steel. *Philos. Mag.* **84,** 1735 (2004).

63. K. Miyata, T. Omura, T. Kushida, and Y. Komizo: Coarsening kinetics of multicomponent MC-type carbides in high-strength low-alloy steels. *Metall. Mater. Trans. A* **34,** 1565 (2003).

64. E. Courtois, T. Epicier, and C. Scott: EELS study of niobium carbo-nitride nano-precipitates in ferrite. *Micron* **37,** 492 (2006).

J. Mater. Res., Vol. 25, No. 7, Jul 2010

1297