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Atomistic modeling of III–V nitrides: modified embedded-atom method interatomic potentials for GaN, InN and $\text{Ga}_{1-x}\text{In}_x\text{N}$

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Abstract

Modified embedded-atom method (MEAM) interatomic potentials for the Ga–N and In–N binary and Ga–In–N ternary systems have been developed based on the previously developed potentials for Ga, In and N. The potentials can describe various physical properties (structural, elastic and defect properties) of both zinc-blende and wurtzite-type GaN and InN as well as those of constituent elements, in good agreement with experimental data or high-level calculations. The potential can also describe the structural behavior of $\text{Ga}_{1-x}\text{In}_x\text{N}$ ternary nitrides reasonably well. The applicability of the potentials to atomistic investigations of atomic/nanoscale structural evolution in $\text{Ga}_{1-x}\text{In}_x\text{N}$ multi-component nitrides during the deposition of constituent element atoms is discussed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Due to large bandgaps and relatively low dielectric constants, III–V nitrides (GaN and InN) have attracted both scientific and technological interest as potential materials for optical and electronic devices such as high brightness, efficient blue and green light-emitting diodes, high-temperature–high-frequency field effect transistors and also ultraviolet and blue laser diodes [1–3]. The bandgap of GaN (3.4 eV) can be tailored by alloying with InN (1.9 eV) or AlN (6.2 eV), which allows control over the wavelength of emission [2–4]. These materials are used in electronic devices in the form of nanoscaled structures such as quantum dots (QDs) [5], nanowires [6] and nanorods [7]. Most of these nanoscaled structures evolve through self-assembled processes. For effective applications of these nanostructures to electronic devices, it is essential to understand the self-assembled phenomena and to be able to control the evolution of nanostructures. Those self-assembled phenomena are known

to be related to surface properties and local strain/stress distributions in nanostructures [8, 9]. However, it is not easy to directly measure those important properties for nanostructured materials by experimental methods. On the other hand, those nanoscaled properties can be investigated rather efficiently if atomistic simulation techniques are used.

The most accurate method to investigate the atomic-level behavior of nanostructured materials would be first-principles calculations. However, the number of atoms that can be dealt with by first-principles calculations is highly limited (to several hundreds). It should be noted here that the number of atoms in a quantum dot or wire of 10–20 nm size can reach several hundred thousand. Therefore, atomistic simulations based on (semi-)empirical interatomic potentials that can cover millions of atoms are strongly recommended for theoretical investigations of nanostructural evolutions.

Many (semi-)empirical interatomic potentials have been developed for GaN and/or InN: the tight-binding potential [10], Tersoff potential [11], Stillinger–Weber potential [12], analytical bond-order potential [13], the lattice inversion method potential [14] and Buckingham pair potentials [15–17].

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The GaN and InN nitrides exist in the form of zinc-blende and wurtzite-type structures. The $\text{Ga}_{1-x}\text{In}_x\text{N}$ films or QDs are fabricated by a co-deposition of individual atoms. Therefore, for atomistic simulations of deposition processes, an interatomic potential that can describe the behavior of individual pure elements as well as nitrides of the two structures is strongly required. Even though many interatomic potentials were developed as mentioned above, the potential that can describe pure elements and both types of nitrides simultaneously is not available yet, at least for the Ga–In–N ternary system.

In order to describe multi-component systems, it is essential to be able to describe various types of compounds and pure elements using a common mathematical formalism. From this point of view, the modified embedded-atom method (MEAM [18]) potential is highly applicable because it can cover a wide range of elements (fcc, bcc, hexagonal close-packed (hcp), diamond and even gaseous elements) using a common mathematical formalism and functional form. The MEAM was created by Baskes [18] by modifying the EAM [19, 20] to include the directionality of bonding. In the original MEAM [18], interactions among only first-nearest-neighbor atoms were considered. Recently, the MEAM was modified once again by Lee and Baskes [21, 22] to consider partially second-nearest-neighbor interactions and to overcome some critical shortcomings in the original MEAM. The generalized MEAM (second-nearest neighbor or 2NN MEAM) has been applied to a wide range of elements including bcc [22], fcc [23], hcp [24] metals, carbon [25], silicon [26], germanium [27], indium [28] and to binary systems between different types of elements [29–39].

The purpose of the present work is to provide an MEAM interatomic potential that can describe GaN, InN and $\text{Ga}_{1-x}\text{In}_x\text{N}$ nitrides of both zinc-blende and wurtzite types as well as all the elements, Ga, In and N, simultaneously. Binary potentials for the Ga–N, In–N and Ga–In binary systems are developed based on the previously developed MEAM potentials for pure Ga [40], In [28] and N [18] with a modification of the N potential. The binary potentials are combined to describe the ternary $\text{Ga}_{1-x}\text{In}_x\text{N}$ nitrides. In section 2, the formalism of the (2NN) MEAM and the procedure for the determination of potential parameters are briefly described. Comparisons between calculated and experimental physical and thermodynamic properties of GaN, InN nitrides and the Ga–In binary alloys are made in section 3. The applicability of the present potential to investigations of atomistic structural evolution in $\text{Ga}_{1-x}\text{In}_x\text{N}$ nitrides is also discussed in this section and section 4 is the conclusion.

2. Interatomic potential

2.1. Potential formalism

In the MEAM, the total energy of a system is given in the following form:

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

where F_i is the embedding function for an atom i embedded in a background electron density $\bar{\rho}_i$. 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 embedding function is given in the following form [18]:

$$F(\bar{\rho}) = A E_c \frac{\bar{\rho}}{\bar{\rho}^o} \ln \frac{\bar{\rho}}{\bar{\rho}^o} \quad (2)$$

where A is an adjustable parameter, E_c is the cohesive energy and $\bar{\rho}^o$ is the background electron density for the reference structure. The reference structure is a structure where individual atoms are on the exact lattice points without deviation. The background electron density $\bar{\rho}_i$ is composed of spherically symmetric partial electron density, $\rho_i^{(0)}$, and angular contributions, $\rho_i^{(1)}$, $\rho_i^{(2)}$ and $\rho_i^{(3)}$. Each partial electron density term has the following form [18]:

$$(\rho_i^{(0)})^2 = \left[\sum_{j \neq i} S_{ij} \rho_j^{a(0)}(R_{ij}) \right]^2, \quad (3a)$$

$$(\rho_i^{(1)})^2 = \sum_{\alpha} \left[\sum_{j \neq i} \frac{R_{ij}^{\alpha}}{R_{ij}} S_{ij} \rho_j^{a(1)}(R_{ij}) \right]^2, \quad (3b)$$

$$(\rho_i^{(2)})^2 = \sum_{\alpha, \beta} \left[\sum_{j \neq i} \frac{R_{ij}^{\alpha} R_{ij}^{\beta}}{R_{ij}^2} S_{ij} \rho_j^{a(2)}(R_{ij}) \right]^2 - \frac{1}{3} \left[\sum_{j \neq i} S_{ij} \rho_j^{a(2)}(R_{ij}) \right]^2, \quad (3c)$$

$$(\rho_i^{(3)})^2 = \sum_{\alpha, \beta, \gamma} \left[\sum_{j \neq i} \frac{R_{ij}^{\alpha} R_{ij}^{\beta} R_{ij}^{\gamma}}{R_{ij}^3} S_{ij} \rho_j^{a(3)}(R_{ij}) \right]^2 - \frac{3}{5} \sum_{\alpha} \left[\sum_{j \neq i} \frac{R_{ij}^{\alpha}}{R_{ij}} S_{ij} \rho_j^{a(3)}(R_{ij}) \right]^2. \quad (3d)$$

Here, $\rho_j^{a(h)}$ represent atomic electron densities from the j th atom at a distance R_{ij} from site i . R_{ij}^{α} is the α component of the distance vector between atoms j and i ($\alpha = x, y, z$). The way of combining the partial electron densities to give the total background electron density is not unique, and several expressions have been proposed [42]. Among them, the following form that can be widely used without numerical error is taken in the present work:

$$\bar{\rho}_i = \rho_i^{(0)} G(\Gamma) \quad (4)$$

where

$$G(\Gamma) = \frac{2}{1 + e^{-\Gamma}} \quad (5)$$

and

$$\Gamma = \sum_{h=1}^3 t_i^{(h)} \left[\frac{\rho_i^{(h)}}{\rho_i^{(0)}} \right]^2. \quad (6)$$

$t_i^{(h)}$ are adjustable parameters. The background electron density at each atomic site is computed by considering the directionality of bonding, that is, by combining several partial electron density terms for different angular contributions with weight factors $t_i^{(h)}$. The atomic electron density is given as

$$\rho^{a(h)}(R) = \rho_o \exp[-\beta^{(h)}(R/r_c - 1)], \quad (7)$$

where ρ_o the atomic electron density scaling factor and $\beta^{(h)}$ the decay lengths are adjustable parameters, and r_e is the nearest-neighbor distance in the equilibrium reference structure.

In the MEAM no specific functional expression is given directly to $\phi(R)$. Instead, the atomic energy (total energy per atom) is evaluated by some means as a function of nearest-neighbor distance. Then, the value of $\phi(R)$ is computed from known values of the total energy and the embedding energy as a function of nearest-neighbor distance. Let us consider a reference structure once again. Here, every atom has the same environment and the same energy. If up to second-nearest-neighbor interactions are considered, as is done in the second-nearest-neighbor MEAM [21, 22], the total energy per atom in a reference structure can be written as follows:

$$E^a(R) = F(\bar{\rho}^o(R)) + \frac{Z_1}{2}\phi(R) + \frac{Z_2S}{2}\phi(aR) \quad (8)$$

where Z_1 and Z_2 are the number of first-and second-nearest-neighbor atoms, respectively. S is the screening factor for second-nearest-neighbor interactions (the screening factor for first-nearest-neighbor interactions is 1) and a is the ratio between the second-and first-nearest-neighbor distances. It should be noted that for a given reference structure S and a are constants, and the total energy and the embedding energy become functions of only nearest-neighbor distance R . On the other hand, the energy per atom for a reference structure can be obtained from the zero-temperature universal equation of state by Rose *et al* [41] as a function of nearest-neighbor distance R :

$$E^u(R) = -E_c(1 + a^* + da^{*3})e^{-a^*} \quad (9)$$

where d is an adjustable parameter

$$a^* = \alpha(R/r_e - 1) \quad (10)$$

and

$$\alpha = \left(\frac{9B\Omega}{E_c}\right)^{1/2}. \quad (11)$$

$E^u(R)$ is the universal function for a uniform expansion or contraction in the reference structure. B is the bulk modulus and Ω is the equilibrium atomic volume of the reference structure. The pair potential between two atoms separated by a distance R , $\phi(R)$, is now obtained by equating equations (8) and (9) as follows [21, 22]:

$$\phi(R) = \psi(R) + \sum_{n=1} (-1)^n \left(\frac{Z_2S}{Z_1}\right)^n \psi(a^n R). \quad (12)$$

where

$$\psi(R) = \phi(R) + \frac{Z_2S}{Z_1}\phi(aR). \quad (13)$$

Here, the summation is performed until a correct value of atomic energy is obtained for the equilibrium reference structure.

The use of the many-body screening [42] is one of the main differences between the MEAM and other empirical potentials. 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 :

$$S_{ij} = \prod_{k \neq i,j} S_{ikj}. \quad (14)$$

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 . The equation of the ellipse is given by

$$x^2 + \frac{1}{C}y^2 = \left(\frac{1}{2}R_{ij}\right)^2. \quad (15)$$

For each k atom, the value of parameter C can be computed from relative distances among the three atoms, i, j and k , as follows:

$$C = \frac{2(X_{ik} + X_{kj}) - (X_{ik} - X_{kj})^2 - 1}{1 - (X_{ik} - X_{kj})^2} \quad (16)$$

where $X_{ik} = (R_{ik}/R_{ij})^2$ and $X_{kj} = (R_{kj}/R_{ij})^2$. The screening factor, S_{ikj} , is defined as a function of C as follows:

$$S_{ikj} = f_c \left[\frac{C - C_{\min}}{C_{\max} - C_{\min}} \right] \quad (17)$$

where C_{\min} and C_{\max} are the limiting values of C determining the extent of screening and the smooth cutoff function is

$$f_c(x) = \begin{cases} 1 & x \geq 1 \\ [1 - (1 - x)^4]^2 & 0 < x < 1 \\ 0 & x \leq 0. \end{cases} \quad (18)$$

The basic idea for the screening is that: first define two limiting values, 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 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. In the numerical procedure of simulation the electron density and pair potential are multiplied by the screening function S_{ij} , as in done in equation (1) and equations (3a)–(3d). In addition to the many-body screening function, a radial cutoff function which is given by $f_c[(r_c - r)/\Delta r]$, where r_c is the cutoff distance and Δr (0.1 Å) is the cutoff region, is also applied to the atomic electron density and pair potential [42] for computational convenience.

To describe an alloy system, the pair interaction between different elements should be determined. For this, a similar technique that is used to determine the pair interaction for pure elements is applied to binary alloy systems. For the Ga–N system, for example, a zinc-blende-type GaN ordered structure was chosen as the reference structure. In the zinc-blende-type GaN structure, the total energy per atom (for 1/2 Ga atom+1/2 N atom) is given as follows:

$$E_{\text{GaN}}^u(R) = \frac{1}{2} \left[F_{\text{Ga}}(\bar{\rho}_{\text{Ga}}) + F_{\text{N}}(\bar{\rho}_{\text{N}}) + Z_1 \phi_{\text{GaN}}(R) + \frac{Z_2}{2} (S_{\text{Ga}} \phi_{\text{GaGa}}(aR) + S_{\text{N}} \phi_{\text{NN}}(aR)) \right], \quad (19)$$

Table 1. MEAM potential parameter sets of Ga, In and N. (Note: the units of cohesive energy E_c , equilibrium nearest-neighbor distance r_e and the bulk modulus B are eV, Å and 10^{12} dyn cm $^{-2}$, respectively. The reference structures of Ga, In and N are fcc, fcc and dimer, respectively.)

	E_c	r_e	B	A	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	C_{\min}	d
Ga	2.90	3.003	0.527	0.97	4.80	3.10	6.00	0.50	2.72	2.06	-4.00	1.4	0.097
In	2.51	3.328	0.433	1.00	5.06	5.50	5.46	2.00	3.00	3.10	2.50	1.5	0.050
N	4.88	1.100	5.960 ^a	1.80	2.20	1.70	1.65	4.00	0.05	1.00	0.00	2.0	0.0

^a This is an α value as defined in [33]. Bulk modulus B is not defined for a gaseous element.

where Z_1 and Z_2 are the numbers of first- and second-nearest neighbors in the zinc-blende-type GaN structure, respectively. In the present case, Z_1 and Z_2 are 4 and 12, respectively. S_{Ga} and S_{N} are the screening functions for the second-nearest-neighbor interactions between Ga atoms and between N atoms, respectively, and a is the ratio between the second- and first-nearest-neighbor distances in the reference structure. The pair interaction between Ga and N can now be obtained in the following form:

$$\phi_{\text{GaN}}(R) = \frac{1}{Z_1} \left[2E_{\text{GaN}}^{\text{u}}(R) - F_{\text{Ga}}(\bar{\rho}_{\text{Ga}}) - F_{\text{N}}(\bar{\rho}_{\text{N}}) - \frac{Z_2}{2} (S_{\text{Ga}}\phi_{\text{GaGa}}(aR) + S_{\text{N}}\phi_{\text{NN}}(aR)) \right]. \quad (20)$$

The embedding functions F_{Ga} and F_{N} can be readily computed. The pair interactions ϕ_{GaGa} and ϕ_{NN} between the same types of atoms can also be computed from the descriptions of individual elements. To obtain $E_{\text{GaN}}^{\text{u}}(R)$, the universal equation of state [41] should be considered again for the zinc-blende-type GaN with equations (3a)–(3d). The parameters E_c , r_e (or Ω), B and d in the universal equation of state are determined from relevant experimental data or from high-level calculations. The pair interaction between Ga and N is then determined as a function of the interatomic distance R .

2.2. Determination of potential parameters for binary systems

The MEAM for an alloy system is based on the MEAM potentials for the constituent elements. In the present work, the MEAM parameters for gallium and indium were taken from Baskes *et al* [40] and Do *et al* [28], respectively. For nitrogen, potential parameters from the original MEAM were available [18]. The MEAM parameters for nitrogen were determined by fitting to the cohesive energy, nearest-neighbor distance of the N_2 dimer and the equilibrium shape of the N_3 trimer. Because the number of data used for the determination of parameters was smaller than the number of parameters, some parameters were left undetermined. During the present work, it was found that the original MEAM parameters for nitrogen cannot be used without any modification to develop Ga–N and In–N binary potentials. Therefore, the MEAM potential for nitrogen was modified so that it can better describe the binary systems, maintaining the good agreement with experimental information on pure nitrogen already obtained. The new potential reproduces the cohesive energy and nearest-neighbor distance of the N_2 dimer equally well and it was also confirmed that all the nitrogen atoms exist in forms of the N_2 dimer during molecular dynamics runs at finite temperatures

(room temperature, for example). The MEAM potential parameters for pure gallium, indium and nitrogen are presented in table 1. Here, it should be mentioned that the parameter set for nitrogen in table 1 cannot be the unique and final one for nitrogen. It can only be one of the probable parameter sets that can reproduce minimum experimental information on N_2 gas (the cohesive energy and atomic distance of the N_2 dimer). It is believed that many more binary nitride systems should be assessed based on the MEAM formalism before a unique and final parameter set for nitrogen can be determined.

As described in section 2.1, the extension of the MEAM to binary alloy systems 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 (9)–(11) 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 in nature. 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. For such alloy systems, d is given an average value of those for pure constituent elements.

In addition to the parameters for the universal equation of state, two more model parameter sets must be determined to describe an alloy system. One is the C_{\min} values. As can be seen in table 1, each element has its own value of C_{\min} . C_{\min} determines 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 ($i-k-j = \text{A-A-A}$ or B-B-B). However, in the case of alloys, one of the interacting atoms and/or the screening atom can be different types (there are four cases: $i-k-j = \text{A-B-A}$, B-A-B , A-A-B and A-B-B). Different C_{\min} values may have to be given in each case. The other model parameter is the atomic electron density scaling factors ρ_o for individual elements. For an equilibrium reference structure ($R = r_e$), the values of all atomic electron densities become ρ_o . 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 large effect on calculations.

Table 2. MEAM potential parameter sets for the Ga–N, In–N and Ga–In binary systems, and source for the determination of each value. (Note: 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} dyn cm $^{-2}$, respectively. The reference structures of Ga–N, In–N and Ga–In are zinc blende, zinc blende and NaCl-type B1, respectively.)

Parameter	Ga–N	In–N	Ga–In
E_c	$0.5E_c^{\text{Ga}} + 0.5E_c^{\text{N}} - 0.560$ Enthalpy of formation of GaN	$0.5E_c^{\text{In}} + 0.5E_c^{\text{N}} - 0.1650$ Enthalpy of formation of InN	$0.5E_c^{\text{Ga}} + 0.5E_c^{\text{In}} + 0.1355$ Enthalpy of mixing of Ga–In
r_e	1.94 Lattice parameter of GaN	2.1564 Lattice parameter of InN	2.8276 ($0.5\Omega^{\text{Ga}} + 0.5\Omega^{\text{In}}$) Assumption
B	2.00 Bulk modulus of GaN	1.380 Bulk modulus of InN	$0.5B^{\text{Ga}} + 0.5B^{\text{In}}$ Assumption
d	0.0 For fitting $\partial B/\partial P$ of GaN	0.0 For fitting $\partial B/\partial P$ of InN	$0.5d^{\text{Ga}} + 0.5d^{\text{In}}$ Assumption
$C_{\min}(i-j-i)$	C_{\min}^{Ga} Assumption	C_{\min}^{In} Assumption	C_{\min}^{Ga} Assumption
$C_{\min}(j-i-j)$	C_{\min}^{N} Assumption	C_{\min}^{N} Assumption	0.78 Enthalpy of mixing
$C_{\min}(i-i-j)$	$(0.5(C_{\min}^{\text{Ga}})^{1/2} + 0.5(C_{\min}^{\text{N}})^{1/2})^2$ Assumption	$(0.5(C_{\min}^{\text{In}})^{1/2} + 0.5(C_{\min}^{\text{N}})^{1/2})^2$ Assumption	$(0.5(C_{\min}^{\text{Ga}})^{1/2} + 0.5(C_{\min}^{\text{In}})^{1/2})^2$ Assumption
$C_{\min}(i-j-j)$	2.00 Structural stability (wurtzite)	2.00 Structural stability (wurtzite)	2.30 Enthalpy of mixing of Ga–In
ρ_0	$\rho_0^{\text{N}}/\rho_0^{\text{Ga}} = 27$ Elastic constants of GaN	$\rho_0^{\text{N}}/\rho_0^{\text{In}} = 27$ Elastic constants of InN	$\rho_0^{\text{In}}/\rho_0^{\text{Ga}} = 1$ Enthalpy of mixing of Ga–In

The above model parameters, E_c , r_e , B , d , C_{\min} and ρ_0 , 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.

In the case of the Ga–N and In–N binary systems, the nitrides GaN and InN of the zinc blende structure were selected as the reference structure. Since those two zinc-blende-type nitrides exist in nature, the heat of formation, lattice parameter, bulk modulus and even the ($\partial B/\partial P$) value necessary to determine the values of E_c , r_e , B and d parameters were available experimentally or at least from first-principles calculations. Therefore, those parameters could be determined directly from the available relevant data. The elastic constants for the zinc-blende-type GaN and InN were also available from experiments and/or first-principles calculations, and could be used for the optimization of the C_{\min} and ρ_0 values. However, the C_{\min} parameters were found not to have any effect on the elastic constants. Therefore, most of the C_{\min} parameters were given a default assumed value. Only the parameters, C_{\min} (Ga–N–N) and C_{\min} (In–N–N), that have effects on the structural stability of wurtzite structure were given a non-default value. The only binary potential parameter that could be adjusted to fit the elastic constants was the ρ_0 values (the ratio between ρ_0^{Ga} and ρ_0^{N} or between ρ_0^{In} and ρ_0^{N}). This was not enough to fit all the elastic constants of zinc-blende-type and wurtzite-type nitrides simultaneously. Some potential parameters for pure nitrogen had to be modified as mentioned earlier, in order to obtain good overall agreements with all the known elastic properties.

There is no stable intermetallic compound in the Ga–In binary system. The only experimental information that could be used for parameter optimization was the enthalpy of mixing for the liquid Ga–In alloys. Since there was no realistic compound that could be used as the reference structure, an NaCl-type (FCC B1) GaIn compound was arbitrarily selected as the reference structure. The E_c parameter could be

determined together with some C_{\min} parameters, so that the enthalpy of mixing for the liquid is best reproduced. During this process, it was found that the same values could be given for the ρ_0^{Ga} and ρ_0^{In} . However, r_e and B parameters could not be determined since no relevant information was available. On the other hand, in a previous work on the MEAM potential development of the Fe–Pt [28] binary system, it had been found that the lattice parameter and bulk modulus of the reference structure, approximated by taking a weighted average of the atomic volume and bulk modulus for constituent elements, are close to first-principles or experimental values. Therefore, in the present work, the nearest-neighbor distance r_e and the bulk modulus B of the reference structure were approximated as a weighted average (1:1) of those for pure Ga and In (assuming that $\Omega_{\text{GaIn}} = 0.5\Omega_{\text{Ga}} + 0.5\Omega_{\text{In}}$ and $B_{\text{GaIn}} = 0.5B_{\text{Ga}} + 0.5B_{\text{In}}$). The validity of those assumptions was confirmed later on by performing a first-principles calculation on the corresponding quantities. Due to the same reason (lack of information), an average value of those for pure elements was also given to the d parameter.

Table 2 shows the finally determined MEAM potential parameter sets for the Ga–N, In–N and Ga–In binary systems. It should be mentioned here that actually one more parameter group C_{\max} (one for each element and four for each binary system) is necessary in addition to the parameters listed in tables 1 and 2. In the present work for the Ga–In–N system, all the C_{\max} parameters were given a default value, 2.80.

2.3. Determination of potential parameters for ternary system

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 Ga–In–N system are presented in tables 1 and 2. In addition, three more ternary parameters, C_{\min} (Ga–N–In), C_{\min} (Ga–In–N) and C_{\min} (In–Ga–N), are necessary.

Table 3. MEAM parameter sets for the Ga–In–N ternary system and source for the determination of each value.

Parameter	Selected value	Source
C_{\min} (Ga–N–In)	$1.45[(0.5(C_{\min}^{\text{Ga–N–Ga}})^{1/2} + 0.5(C_{\min}^{\text{In–N–In}})^{1/2})^2]$	Assumption
C_{\min} (Ga–In–N)	$1.71[(0.5(C_{\min}^{\text{Ga–Ga–N}})^{1/2} + 0.5(C_{\min}^{\text{In–In–N}})^{1/2})^2]$	Assumption
C_{\min} (In–Ga–N)	$1.71[(0.5(C_{\min}^{\text{In–In–N}})^{1/2} + 0.5(C_{\min}^{\text{Ga–Ga–N}})^{1/2})^2]$	Assumption

Table 4. Calculated physical properties of GaN using the MEAM potential, in comparison with experimental data, first-principles calculations and other calculations. (Note: values listed are the cohesive energy E_c (eV), the lattice parameter a and c (Å), internal structural parameter u , elastic constants (10^{12} dyn cm $^{-2}$ or 100 GPa), bulk modulus B (10^{12} dyn cm $^{-2}$ or 100 GPa) and $\partial B/\partial P$.)

GaN	Exp.	FP	Tight-binding ^b	Tersoff ^c	Stillinger–Weber ^d	Analytical bond-order ^e	Lattice inversion ^f	Buckingham pair potential ^a				
								Zapol	Chisholm	Purton	MEAM	
Zinc-blende												
E_c	4.45–4.48 ^g	4.1–5.45 ^h		4.32		4.53						4.45
a	4.49–4.54 ⁱ	4.30–4.50 ^j		4.50		4.50	4.50	4.53		4.52		4.48
C_{11}	2.64 ^k	2.93–2.96 ^l	3.99	2.59		2.87	3.07	3.00		2.89		2.87
C_{12}	1.53 ^k	1.54–1.59 ^l	1.73	1.55		1.69	1.85	1.91		1.70		1.56
C_{44}	0.68 ^k	1.55–2.06 ^l	1.61	1.89		1.28	1.76	1.60		1.67		1.48
B	1.85–2.45 ^m	1.73–2.40 ⁿ	2.49	1.90		2.08	2.25					2.00
$\partial B/\partial P$	3.2–4.3 ^o	2.66–4.6 ^p		4.61		4.14						4.55
Wurtzite												
E_c	4.45–4.48 ^g	4.1 ^q				4.53						4.45
a	3.160–3.192 ^r	3.04–3.16 ^s			3.32	3.18	3.20	3.23	3.20	3.22		3.17
c	5.125–5.196 ^t	4.97–5.14 ^s			5.16	5.19	5.11	5.16	5.14	5.15		5.17
u	0.377 ^l	0.375–0.378 ^s			0.39	0.38	0.38	0.39				0.37
C_{11}	2.96–3.90 ^u	3.50–3.96 ^v			3.68	3.47	3.99	3.86	4.10	3.79		3.51
C_{12}	1.30–1.60 ^u	0.94–1.44 ^v			1.38	1.54	1.64	1.60	1.61	1.37		1.48
C_{13}	0.70–1.58 ^u	0.67–1.04 ^v			1.27	1.23	1.36	1.41	1.42	1.20		1.01
C_{33}	2.09–3.98 ^u	3.92–4.05 ^v			3.79	3.81	3.84	3.91	4.13	3.78		3.97
C_{44}	0.24–1.09 ^u	0.91–1.18 ^v			0.99	0.81	1.19	1.15	1.23	1.20		0.93
C_{66}	0.83–1.34 ^u	1.15–1.37 ^v			1.15	0.98	1.17	1.13	1.25			1.01
B	1.73–2.45 ^w	1.79–2.40 ^x			2.10	2.08	2.27		2.36			2.00
$\partial B/\partial P$	3.2–4.3 ^y	2.92–4.5 ^z										4.55

^a Reference [15–17]; ^b Reference [10]; ^c Reference [11]; ^d Reference [12]; ^e Reference [13]; ^f Reference [14]; ^g Reference [43, 44];

^h Reference [69–72]; ⁱ Reference [45–49]; ^j Reference [44, 58, 69–77]; ^k Reference [49]; ^l Reference [72, 77, 78]; ^m Reference [49–52];

ⁿ Reference [44, 58, 69–72, 74, 77, 79, 80]; ^o Reference [51, 52]; ^p Reference [44, 70, 72, 74, 77, 79]; ^q Reference [69]; ^r Reference [53–60];

^s Reference [69, 73, 74, 76]; ^t Reference [56]; ^u Reference [60–68]; ^v Reference [77, 78, 81, 82]; ^w Reference [50–52, 61, 63, 65];

^x Reference [58, 69, 74–80, 83]; ^y Reference [50–52]; ^z Reference [70, 74, 77, 79, 83].

As mentioned already, $C_{\min}(i-k-j)$ parameters represent the degree of screening by a third element atom (k) to the interaction between two neighboring atoms (i and j) of different types. If 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 case. Considering that Ga and In are relatively similar to each other compared to N, it was assumed that the degree of screening by an N atom to the interaction between Ga and In atoms [$C_{\min}(\text{Ga–N–In})$] is an average between those to the Ga–Ga [$C_{\min}(\text{Ga–N–Ga})$] and In–In [$C_{\min}(\text{In–N–In})$] interactions. Similarly, the degree of screening by a Ga (or In) atom to the interaction between In (or Ga) and N atoms [$C_{\min}(\text{In–Ga–N})$ or $C_{\min}(\text{Ga–In–N})$] was assumed to be an average between those by a Ga atom to the Ga–N [$C_{\min}(\text{Ga–Ga–N})$] and by an In atom to the In–N [$C_{\min}(\text{In–In–N})$] interactions. This assumption has also been made in a previous work on the MEAM potential development for the Fe–Ti–C and Fe–Ti–N ternary systems [39] and was found to yield the best result among

various probable assumptions. The finally determined ternary potential parameters are presented in table 3.

3. Calculation of physical properties

The MEAM potential developed by the above procedure was used to compute fundamental physical properties of the Ga–N, In–N binary and Ga–In–N ternary nitride systems in order to evaluate its reliability and transferability. All calculations were carried out using a radial cutoff distance of 4.0 Å which is between the second- and third-nearest-neighbor distances of zinc-blende-type nitrides.

Tables 4 and 5 show the calculated cohesive energy, lattice parameters and elastic constants of both zinc-blende and wurtzite-type GaN and InN, respectively. All calculations are carried out at 0 K allowing full relaxation of individual atoms. Relevant experimental data, first-principles calculations and other empirical atomistic calculations are presented for comparison. All empirical atomistic calculation results are comparable with relevant experimental data or first-principles calculations. It is also shown that the present MEAM describes

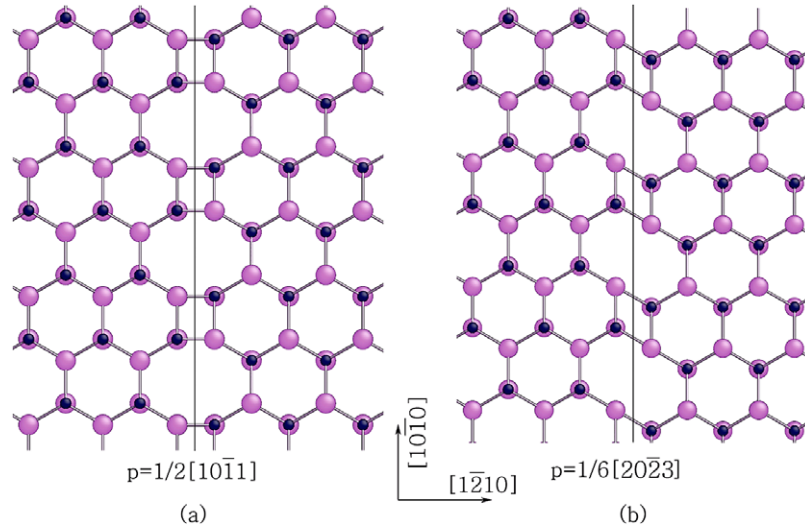


Figure 1. Schematic illustrations of the $(\bar{1}2)10$ prismatic stacking fault in wurtzite GaN. Atomic positions have been projected onto the (0001) plane. (a) Drum type [97]. (b) Amelinckx type [98].

Table 5. Calculated physical properties of InN using the MEAM parameters, in comparison with experimental data, first-principles calculations and other empirical calculations. (Note: values listed are the cohesive energy E_c (eV/atom), the lattice parameter a and c (Å), internal structural parameter u , elastic constants (10^{12} dyn cm^{-2} or 100 GPa), bulk modulus B (10^{12} dyn cm^{-2} or 100 GPa) and $\partial B/\partial P$.)

InN	Exp.	FP	Tight-binding ^b	Tersoff ^c	Lattice inversion ^d	Buckingham pair potential ^a		
						Chisholm	Purton	MEAM
Zinc-blende								
E_c	3.86 ^e			4.36				3.86
a	4.961–5.03 ^f	4.92–4.98 ^g		4.95	4.92		4.98	4.98
C_{11}	1.72 ^h	1.84–1.87 ⁱ	2.58	1.87	2.04		1.54	1.85
C_{12}	1.19 ^h	1.16–1.25 ⁱ	1.15	1.20	1.02		0.99	1.14
C_{44}	0.37 ^h	0.86–1.77 ⁱ	1.03	1.48	1.03		1.01	0.66
B	1.36 ^h	1.37–1.61 ^j	1.63	1.43	1.37			1.38
$\partial B/\partial P$		3.9–4.4 ^k		4.67				4.70
Wurtzite								
E_c	3.86 ^e							3.86
a	3.54–3.60 ^l	3.50–3.54 ^m			3.51	3.54	3.56	3.52
c	5.69–5.76 ^l	5.54–5.71 ^m			5.56	5.69	5.63	5.75
u		0.38–0.39 ^m			0.38			0.37
C_{11}	1.90–2.23 ⁿ	2.23–2.71 ^o			2.51	2.98	2.06	2.10
C_{12}	1.04–1.15 ⁿ	1.15–1.24 ^o			0.89	1.07	0.83	1.09
C_{13}	0.92–1.21 ⁿ	0.92–0.94 ^o			0.83	1.09	0.73	0.94
C_{33}	1.82–2.24 ⁿ	2.00–2.24 ^o			2.28	2.51	2.02	2.25
C_{44}	0.10–0.48 ⁿ	0.46–0.48 ^o			0.82	0.89	0.65	0.46
C_{66}		0.74 ^p			0.81			0.51
B	1.25–1.39 ^q	1.25–1.65 ^r			1.37	1.65		1.38
$\partial B/\partial P$	12.7 ^s	3.4–3.8 ^t , 8.1 ^u						4.70

^a Reference [16, 17]; ^b Reference [10]; ^c Reference [11]; ^d Reference [14]; ^e Reference [84]; ^f Reference [43, 48, 85];

^g Reference [73, 75–77, 90]; ^h Reference [48]; ⁱ Reference [76–78]; ^j Reference [75–77, 90]; ^k Reference [77, 90]; ^l Reference [86–88];

^m Reference [73, 76, 77]; ⁿ Reference [68, 89]; ^o Reference [77, 78]; ^p Reference [77]; ^q Reference [88, 89]; ^r Reference [75–78];

^s Reference [51]; ^t Reference [77, 83, 90]; ^u Reference [75].

the fundamental physical properties of both zinc-blende and wurtzite-type GaN and InN equally well compared to any other potentials. Important here is that the present MEAM is the only potential that can describe pure elements, Ga, In and N, as well as the nitrides, simultaneously. The present authors are aware of that the wurtzite-type nitrides are slightly more stable in nature [2, 73]. However, according to the present MEAM, the cohesive energy of the zinc-blende-type

and wurtzite-type nitrides is not different from each other. This is because the MEAM counts only up to second-nearest-neighbor interactions where individual atoms in both structures have the same environment. The structure of nitrides during deposition is known to be determined by the crystal structure of substrates (zinc-blende on cubic substrate, wurtzite on hexagonal substrate [2]). This means that the difference in the stability of both structures must be small. Therefore, the

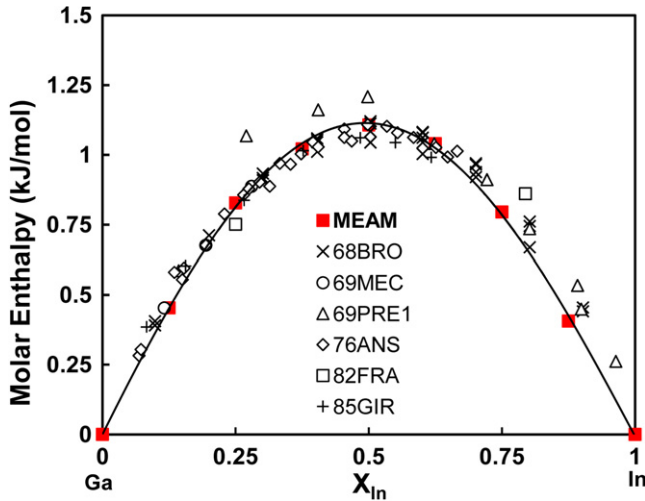


Figure 2. Calculated enthalpy of mixing for the liquid Ga–In alloys, in comparison with experimental data compiled by Anderson and Ansara [99]. The filled squares are the present MEAM calculation and other symbols are experimental data [100–105].

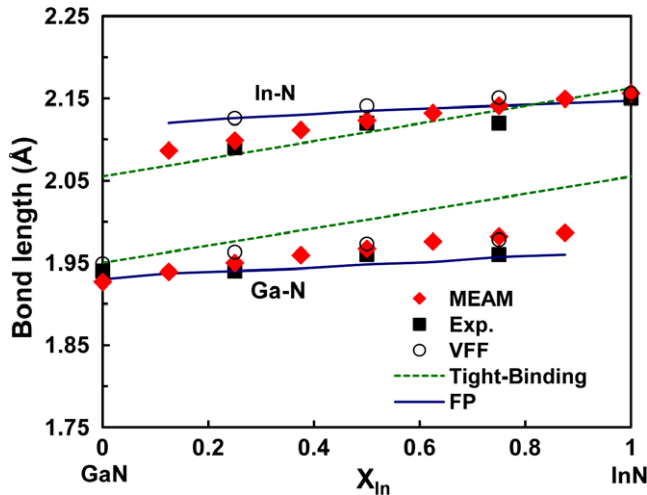


Figure 3. Average bond-length of Ga–N and In–N bonding in $\text{Ga}_{1-x}\text{In}_x\text{N}$ versus composition x , in comparison with experimental data [110] and other calculations [10, 111, 112].

calculated equal cohesive energy of both structures would not cause any problem, and it is believed that the present potential can be applied to atomistic simulations on both zinc-blende and wurtzite-type nitrides. It should be mentioned here that calculations of cohesive energy of other artificial nitrides (such as B1, L10 and B2 type GaN or InN structures) with the same composition were carried out and it was confirmed that the zinc blende and wurtzite are the most stable structures.

In addition to the bulk properties mentioned above, point defect and planar defect properties were calculated for comparison with other (high-level) calculations. For the point defect property, the formation energy of a Schottky defect, and Frenkel defects by individual elements in the zinc-blende structure, were calculated. Experimental data or first-principles data were not available for those quantities. The MEAM results are compared with other empirical calculations

Table 6. Calculated point defect formation energy (eV) for zinc-blende-type GaN and InN, in comparison with other empirical calculations.

		Zapol ^a	Chisholm ^b	MEAM
GaN	Schottky	4.8	4.47	7.30
	Cation Frenkel	6.9	7.42	4.80
	Anion Frenkel	6.1	6.66	10.2
InN	Schottky		3.39	2.02
	Cation Frenkel		7.43	3.28
	Anion Frenkel		4.76	5.69

^a Buckingham pair potential [15].

^b Buckingham pair potential [16].

Table 7. Calculated surface formation energy (eV/atom) for various surfaces, In comparison with the first-principles calculations.

			Northrup ^a	Filippetti ^b	MEAM
GaN	Wurtzite	(10 $\bar{1}0$)	0.975	0.99	1.104
		(11 $\bar{2}0$)	0.875	—	1.004
	Zinc-blende	(110)	—	0.97	1.070
		(110)	—	—	—
InN	Wurtzite	(10 $\bar{1}0$)	—	0.86	0.739
		(11 $\bar{2}0$)	—	—	0.724
	Zinc-blende	(110)	—	0.84	0.739
		(110)	—	—	—

^a First-principles calculation [91].

^b First-principles calculation [92].

Table 8. Calculated prismatic stacking fault energy (meV Å⁻²), in comparison with first-principles calculations and other empirical calculations.

		Northrup ^a	Ruterana ^b	Kioseoglou ^c	MEAM
GaN	Amelinckx	123	78	226	232
	Drum	72	22	144	80
InN	Amelinckx	—	65	—	63
	Drum	—	21	—	46

^a First-principles calculation [95].

^b Stillinger–Weber potential [96].

^c Stillinger–Weber potential [12].

using Buckingham pair potentials in table 6. The defect formation energy values using the two different potentials are comparable, but show an opposite tendency for the relative size of Frenkel defect formation energy by Ga (or In) and N, which should be clarified by high-level calculations later on. As a representative planar defect property, the surface energy of a few surfaces of wurtzite and zinc-blende structures was calculated. The MEAM results are in good agreement with first-principles values as shown in table 7. In addition to the surface energy, the MEAM was employed for calculation of the formation energy of prismatic stacking faults. Two different types of (1 $\bar{2}$ 10) prismatic stacking faults (see figure 1) have been observed experimentally in epitaxial nitride film [93, 94]. The MEAM results are compared with first-principles calculations and other empirical atomistic calculations in table 8. All calculations show a qualitative agreement in that the structure proposed by Drum [97] is more stable than that by Amelinckx [98].

The experimental information available for the Ga–In binary system is the enthalpy of mixing of the liquid. The calculated enthalpy of mixing of the Ga–In liquid alloys is

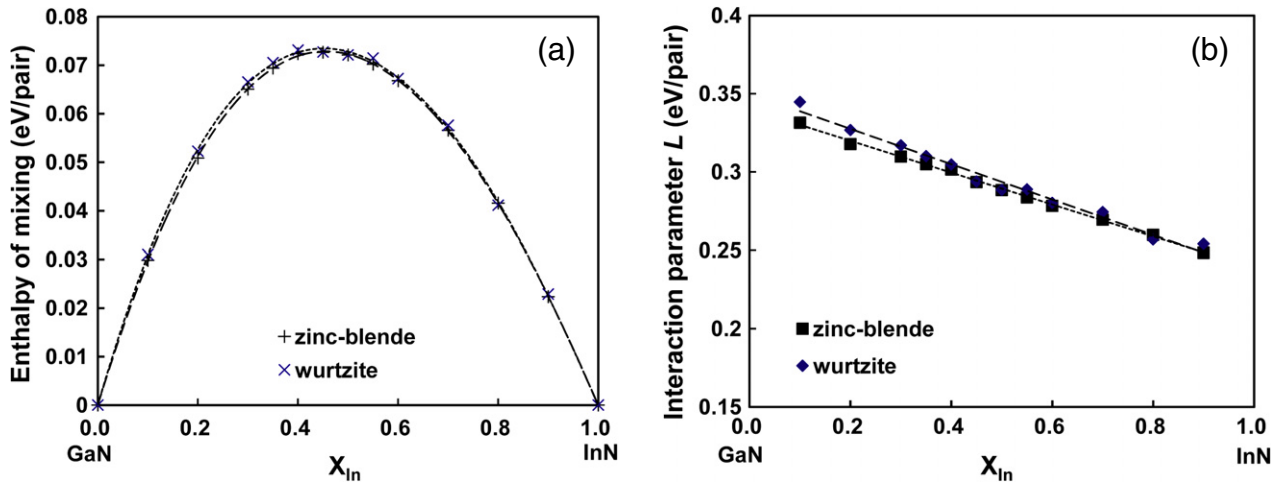


Figure 4. (a) Enthalpy of mixing and (b) interaction parameter L for $\text{Ga}_{1-x}\text{In}_x\text{N}$ as a function of composition x , calculated using the present MEAM potential at 0 K.

Table 9. Lattice parameter a (Å) and bulk modulus B (10^{12} dyn cm^{-2} or 100 GPa) of the NaCl-type GaIn, by first-principles calculations (LDA and GGA) and MEAM.

	First-principles calculation		
	LDA	GGA	MEAM
a	5.617	5.824	5.655
B	0.528	0.376	0.480

presented in figure 2, in comparison with experimental data compiled by Anderson and Ansara [99]. The experimental data are those measured in a temperature range of 383–1230 K. Since no temperature dependence exists in the experimental data, an arbitrary temperature of 650 K, which is above the melting points of both MEAM Ga and In [28, 40], was selected for the present calculation. As mentioned already, the nearest-neighbor distance re and the bulk modulus B of the reference structure for the Ga–In binary system (NaCl-type GaIn) were approximated as a weighted average of those for pure Ga and In. As a further means to confirm the validity of the present approximation, a first-principles calculation was performed for the lattice parameter and bulk modulus of the NaCl-type GaIn compound based on the local density approximation (LDA) and the generalized gradient approximation (GGA) using the VASP-PAW [106–109]. The results are presented in table 9, in comparison with the present MEAM calculation. The present MEAM values are between those by the LDA and GGA calculations.

By combining all the potential parameters in tables 1–3, the atomistic calculations can now be extended to the Ga–In–N ternary system. As the first example of the application of the present MEAM to the ternary system, the In–N and Ga–N bond length in the ternary $\text{Ga}_{1-x}\text{In}_x\text{N}$ nitride was calculated as a function of the composition, x . As a candidate optoelectronic device material, alloying between GaN and InN is used to tune bandgaps for desired wavelengths of the emitted light. Because of the large lattice mismatch ($\sim 11\%$) between InN and GaN, understanding the bond-length variation of the In–N and

Ga–N bonds with the change in composition is important and many theoretical calculations were also performed at various levels. In figure 3, the MEAM calculation is compared with experimental data [110], a first-principles calculation [112] and other semi-empirical calculations [10, 111]. The MEAM shows an equally good agreement with experimental data when compared to the higher-level calculations.

In the $\text{Ga}_{1-x}\text{In}_x\text{N}$ alloy nitrides, a phase separation into Ga-rich and In-rich nitrides has been observed experimentally [113–115]. Since the phase separation would disturb the pre-designed homogeneous bond length and tuning of the bandgap, it is also important to know the phase separation behavior in a wide composition and temperature range. A number of theoretical studies on the thermodynamic property of the mixture between GaN and InN were performed using various calculation methods, such as first-principles, valence force-field and empirical potentials. The calculations provide information on the enthalpy of mixing and interaction parameter between GaN and InN, and the shape, critical temperature and composition of the miscibility gap for the $\text{Ga}_{1-x}\text{In}_x\text{N}$ alloy nitrides. Similar calculations were performed using the present MEAM potential for comparison with the previous calculations at various levels. Figures 4(a) and (b) show the enthalpy of mixing ΔH_m and interaction parameter L [$\Delta H_m = Lx(1-x)$] of the $\text{Ga}_{1-x}\text{In}_x\text{N}$ alloy nitrides of both zinc-blende and wurtzite structures, calculated at 0 K using the present MEAM potential. Assuming that the amount of excess entropy of mixing is negligible, the phase diagram of the GaN–InN quasi-binary system can be calculated using a CALPHAD technique [116, 117] as shown in figure 5. The critical composition and temperature of the $\text{Ga}_{1-x}\text{In}_x\text{N}$ alloy nitrides are 0.39 and 1782 K, respectively, for the zinc-blende structure and are 0.38 and 1819 K, respectively, for the wurtzite structure. All the calculated thermodynamic properties concerning the miscibility gap are compared with those from other calculations in table 10.

It has been shown that the present MEAM interatomic potential reproduces the structural, elastic and defect properties of both zinc-blende and wurtzite-type GaN and InN nitrides

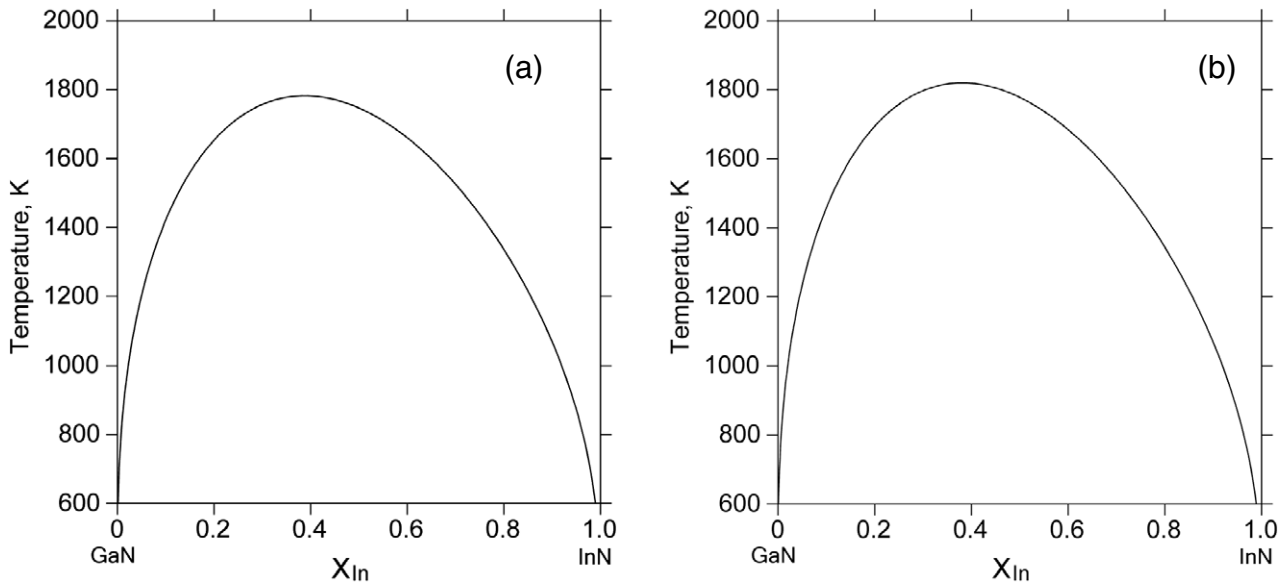


Figure 5. Calculated miscibility gap for the (a) zinc-blende and (b) wurtzite-type $Ga_{1-x}In_xN$, by the CALPHAD technique [116, 117] using the calculated interaction parameter.

Table 10. Miscibility gap data of the $In_xGa_{1-x}N$ ternary nitride by various calculations. (Note: values listed are the critical composition x_c , the enthalpy of mixing ΔH_m (eV/anion-cation pair), interaction parameter L (eV/anion-cation pair) and critical temperature T_c (K).)

	Teles ^a	Ho ^b	Saito ^c	Matsuoka ^d	Purton ^e	Other calc.	MEAM
Structure	ZB	ZB	WZ	WZ	ZB (WZ)	—	ZB (WZ)
Miscibility gap	Asymmetric	Symmetric	Asymmetric	Symmetric	Asymmetric	—	Asymmetric
x_c	~0.42	0.5	0.39	0.5	~0.3 (~0.27)	—	0.39 (0.38)
ΔH_m (eV/pair)	0.053	0.065	0.068	—	0.084 (0.076)	—	0.073 (0.073)
L (eV/pair)	—	0.26	$-0.0915x + 0.3215$	0.463	—	—	$-0.102x + 0.340$ $(-0.113x + 0.350)$
T_c (K)	1295	1523	1690	2689	1725 ± 13	1950 ^f 1620 ^g 1550 ^h 2457 ⁱ	1782 (1819)

^a First-principles calculation [112]; ^b modified valence-force-field model [118]; ^c valence-force-field method [119];

^d delta-lattice-parameter method [120]; ^e Buckingham pair potential [17]; ^f first-principles calculation [121]; ^g first-principles calculation [122]; ^h valence-force-field method [123]; ⁱ delta-lattice-parameter model [115].

in good agreement with experimental information or higher-level calculations. The atomistic structural behavior in the $Ga_{1-x}In_xN$ alloy nitrides is also reproduced reasonably well. As already mentioned, self-assembled structural phenomena are closely related to surface properties and local strain/stress distributions in nanostructures. Since those alloy properties are well reproduced by the present MEAM potential in addition to the fundamental physical properties of individual elements, it is believed that the present potential can be applied to the investigation of the atomistic and nanostructural evolution in $Ga_{1-x}In_xN$ nitrides during the deposition process.

4. Conclusions

An interatomic potential set of the Ga-In-N ternary system, that can reproduce reasonably well the fundamental physical properties of constituent elements, binary and ternary nitrides simultaneously, is now available. The potential is suitable for atomistic investigation of atomic/nanoscale structural

evolution in $Ga_{1-x}In_xN$ multi-component nitrides during the deposition of constituent element atoms. The potential can be easily extended to higher-order multi-component systems by combining with already developed MEAM potentials for a wide range of elements and alloys.

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