

Molecular simulation study of the structural properties in $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys: Comparison between Valence Force Field and Tersoff potential models

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Abstract

The thermodynamic and structural properties of compound semiconductor alloys have been generally modelled using either the Valence Force Field model or the Tersoff potential model. This work compares the properties, such as lattice constant and bond length, of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloy as predicted by Monte Carlo simulations in the semigrand isothermal isobaric ensemble using both the potential models, with experimental data. The lattice constants are expected to follow the Vegard's law at any given temperature. Valence Force Field model predicts bond length data which follows the experimentally determined values at 300 K; whereas the Tersoff model forecasts that the virtual crystal approximation will be followed. The VFF model, with its experimentally determined parameters, is found to be better for modelling the alloy at room temperature. The Tersoff model, with its fitted parameters, on the other hand predicts the effect of temperature on the microscopic structure of the alloy better. The parameters of the Tersoff potential characterizing the In–Ga interactions can be further improved to predict bond lengths more accurately.

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1. Introduction

Compound semiconductor alloys are used in the fabrication of many useful optoelectronic devices [1]. The $\text{In}_x\text{Ga}_{1-x}\text{As}$ system is studied here as a representative example of III–V compound semiconductor alloys. These alloys are of technological importance as they find extensive application in the manufacture of electronic devices. The energy band gap of the alloy ranges from 0.33 eV for InAs to 1.43 eV for GaAs [2]. By mixing the two binary compounds, the properties of the resulting ternary alloy can be tuned to intermediate values. While the energy band gap is tuned with composition, the lattice constant also changes causing

a lattice mismatch with the substrate on which the alloy is grown and the quality of the crystal grown may suffer. Prediction of properties using molecular simulations will allow the selection of the substrate with matching lattice constant or one with the least mismatch reducing the need for experimentation with the material itself. Knowledge of the linear thermal expansion coefficient (α_T) is important as many semiconductor devices consist of permanently joined layers of different materials. In this paper, we therefore endeavour to model the structure of this alloy using two different empirical potential models and compare the simulation results with experimental data where available. The effect of changes in composition and temperature on the microscopic structural properties is also considered. The main objective of this study is to establish the conditions where the physical properties predicted by molecular simulations in conjunction with the potential models are valid.

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Ho and Stringfellow [3,4] first used the Valence Force Field (VFF) model, also known as the Keating model [5], to study the solution thermodynamics of InGaN and other III–V alloys. Takayama et al. [6,7] have since refined the molecular model and have determined the miscibility characteristics and microstructure of other ternary and quaternary compound semiconductor alloys using the energy minimization approach of Ho and Stringfellow [3,4]. Adhikari and Kofke [8,9] used the molecular simulation approach to predict the miscibility diagram and local composition using the Valence Force Field (VFF) model for the InGaN, InAlN, GaAlN and InGaAlN alloys.

Tersoff developed another empirical potential to model covalent systems such as silicon, germanium, SiGeC [10–12]. The Tersoff model has a longer range than the VFF model and this range can be adjusted. Unlike the VFF model, which is limited to modelling crystals with tetrahedral structure allowing only small distortions, the Tersoff model allows for more significant deformations. The potential was found by Tersoff to predict the properties of Si with various polymorphous forms with good accuracy and was also found to have transferability. However, the potential function was found by Tersoff to be not long-ranged enough to describe Si melts successfully. This model was extended to III–V systems such as InGaAlAs by other authors by calculating the various fitting parameters. The growth of the InGaAs alloy has been studied by Ashu et al. using the molecular dynamics approach in 1995 [13] and modifications to the potential were introduced by Nakamura et al. in 2000 [14]. Nakamura et al. pointed out that the bonds in InGaAs alloy have some ionic character and introduced an additional Coulombic term. Tersoff applied his form of the potential function to SiC in the rocksalt (NaCl) structure, which has a considerable ionic character and observed the lattice constant and cohesive energy to be a reasonable approximation (slight underestimation) of the experimental data; whereas for the cubic structure, the results were in excellent agreement as compared to experimental values. The III–V alloys crystallize in the cubic zinc-blende structure and the hexagonal wurtzite structures, which have similar tetragonal nearest-neighbour arrangements. As Tersoff has noted, in the short-range of the potential, the difference in energy between the two structures is minor. Thus, for purposes of the present study, the cubic zinc-blende structure is considered and the improvement in accuracy provided by the introduction of the Coulombic term does not merit the reduction in computational speed that the additional calculations will cause. Ashu et al. utilized the potential in the form used in this study and successfully determined the critical thickness for the formation and extension of interface misfit dislocations. Molecular dynamics has also been used to predict structural and thermodynamic properties of binary alloys such as BAs [15], GaN [16] and AlN [17]. The structural and thermodynamic properties of InAs and GaAs have also been predicted successfully using Monte Carlo methods by Adhikari and Kumar [18].

This paper is organized to include in Section 2 a description of the two potential models used, viz., VFF and Tersoff potential energy functions (PEF). The details of the simulation method used are presented in Section 3. In Section 4, the simulation results and an analysis of the same has been made. The conclusions follow in the last Section 5.

2. Potential models

Molecular simulation techniques allow us to understand the atomistic interactions which result in observable macroscopic properties. The interatomic interaction forces are best modelled by first principles calculations involving the solution of quantum mechanical equations for subatomic particles. However, such calculations are computationally expensive even when modelling a small number of atoms in vacuum. Thus, empirical potential energy functions have been developed to model the interatomic interactions. The potential models considered in this study are believed to be realistic in modelling the interactions present in the compound semiconductor alloys. The aim of this paper is to predict the properties with highest accuracy achievable for the conditions considered using these potential models and then compare the same with literature data. The two potential models considered are further described in detail as follows.

2.1. Valence Force Field model

The VFF potential models the microscopic strain energy, E_m , which arises when a solid solution is formed by mixing two binary alloys (in this case, InAs and GaAs) of different lattice constants. The resulting bond stretching and bond bending are accounted for in this model which is described in Eq. (1).

$$E_m = \frac{3}{8} \sum_{i=1}^4 \alpha_i \frac{(d_i^2 - d_{i0}^2)^2}{d_{i0}^2} + \frac{6}{8} \sum_{i=1}^4 \sum_{j=i+1}^4 \frac{\beta_i + \beta_j}{2} \left(\frac{(\vec{d}_i \vec{d}_j + d_{i0} d_{j0} / 3)^2}{d_{i0} d_{j0}} \right) \quad (1)$$

where d_i is the distance between the central atom As and a corner atom In or Ga in the tetrahedron, d_{i0} is the equilibrium bond length in the binary compound InAs or GaAs, α is the bond stretching force constant and β is the bond bending force. The parameters [6,7] used in this study are given in Table 1.

Table 1
Parameters for the Valence Force Field model (Refs. [6,7])

System	d_0 (Å)	α (N/m)	β (N/m)
GaAs	5.6533	41.99	8.95
InAs	6.0584	35.18	5.50

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