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A first principles study of high Bi content in GaSbBi supercell structures for optoelectronic applications

Utsa Das[a,b,*], S. Dhar[a]

[a] Department of Electronic Science, University of Calcutta, 92, A.P.C. Road, Kolkata, 700009, India
[b] Department of Electronics, The Bhawanipur Education Society College, Kolkata, 700020, India

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ABSTRACT

We report the study of structural and optical properties of high Bi content in GaSb supercell leading to the formation of 2x2x1 and 1x2x2 $GaSb_{0.875}Bi_{0.125}$ supercell structures. This calculation has been performed using the density functional theory (DFT) formalism of Full Potential Linear Augmented Plane Wave (FP-LAPW) method employing WIEN2K package. The minimum volume, bulk modulus, differential pressure and the total energy for both the structures have been investigated under equilibrium conditions. Calculation of optical properties includes absorption, reflection, refraction, extinction co-efficient and the energy losses in both the supercell structures. Phenomenally both the structures are highly stable although the 2x2x1 supercell has a higher compressive flexibility as well as higher total minimum energy in comparison to the 1x2x2 supercell structure. Moreover, the calculated lattice parameters indicate both the structures to be of Zinc Blende in nature. The refractive index and the extinction coefficient values are observed to be higher for 2x2x1 than 1x2x2 supercell structure in the considered incident photon energy range. Significantly, the characteristic curve of refractive index and extinction co-efficient are retraced by the real and imaginary part of the dielectric for both the structures. The optical band gap and maximum optical conductivity has been found to be higher for the 1x2x2 supercell structure in comparison to its counterpart. The reflection and the energy loss characteristic curve are found to be contradictory to one another. The reflectivity coefficient maintains almost a constant value along the incident photon energy range for both the structures; although, the 2x2x1 supercell structure obtains a higher value than the 1x2x2 supercell structure and the vice-versa phenomenon is observed for the energy loss characteristic curve. At higher values of incident photon energy, both the structures attains its distinct plasma frequency values.

1. Introduction

Among various III-V compounds, GaSb has a very distinct property of its spin-orbit splitting energy being almost equal to its band gap [1]. This property is likely to reduce the Auger recombination losses in laser diodes made out of the material. Partial incorporation of Bi in GaSb has been successfully performed by several research groups employing different epitaxial growth techniques [2–5]. It has been observed that due to the large atomic size of Bi atoms, GaSbBi has a tendency to have Bi segregation over the surface. Thus, maintaining a high crystalline quality of such an alloy at a lower growth temperature is rather demanding, although the post growth annealing method has been observed to upgrade the quality of GaSbBi alloys for lower Bi contents [6].

* Corresponding author at: Department of Electronic Science, University of Calcutta, 92, A.P.C. Road, Kolkata, 700009, India.
E-mail address: udelc_rs@cauniv.ac.in (U. Das).

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A maximum of 9.6% Bi incorporation with a high crystalline quality of the alloy was reported by Rajpalke et al. [7] during growth by molecular beam epitaxy (MBE) technique. Recently, Delorme et al. [8] reported successful incorporation of upto 14% Bi by varying the MBE growth temperature. The structural properties were calculated and a smooth, droplet free surface was observed upto 11.4% Bi incorporation.

In this paper, we investigate the effects of high content of Bi (> 12%) in GaSb supercells. The primary focus is to study the structural and optical properties of 2x2x1 and 1x2x2 $GaSb_{0.875}Bi_{0.125}$ supercell structures.

2. Computational details

This computation has been performed using the Full Potential Linear Augmented Plane Wave (FP-LAPW) method based on Density Functional Theory (DFT), employing WIEN2K package [9]. The Generalized Gradient Approximation (GGA) parameterized by Perdew-Burke-Ernzerhof (PBE) has been utilized for the calculation of exchange-correlation potential [10]. The valence states of Ga, Sb and Bi states are $3d^{10}4s^24p^1$, $4d^{10}5s^25p^3$ and $5d^{10}6s^26p^3$, respectively. The basis sets comprising s, p, d and f orbitals have been used for both the cation and the anion atoms for all the compounds. A multiplicity of both 2x2x1 and 1x2x2 of the elementary GaSb [11] supercell leads to the formation of 32 atoms supercell structure. A mesh consisting of 50 k points has been considered in the irreducible wedge of the Brillouin zone. Bulk GaSb has a Zinc Blende structure with F-43 m space group symmetry, but in this calculation we have selected a P_1 symmetry to make it a surface super cell structure. In this supercell structure, a systematic replacement of Sb atoms by Bi atoms leads to the formation of $GaSb_{0.875}Bi_{0.125}$ alloy supercell. In the interstitial region of both the structures, a plane wave cut-off parameter, $R_{max}K_{max} = 7$ has been constantly maintained. Inside the atomic spheres, a maximum value of angular momentum, $l_{max} = 10$, has been maintained constant for expansion of the wave functions. The separation between the valence and the core energy states has been considered to be -6.0 Ry. The calculation has been iterated until the total energies are converged below 10^{-5}Ry with respect to the Brillouin zone integration. The relativistic effect of spin-orbit (SO) calculation is included in this calculation. The impact of this effect is scaled according to the atomic number of the atom [12]. Thereby the alloy containing fairly heavy element (i.e., Bi), SO coupling is a non-negligible effect. Thus we include SO while employing PBE-GGA to account for the exchange correlation effects.

3. Results and discussions

3.1. Structural properties

Fig. 1 (a) and (b) represent a multiplicity value of 2x2x1 and 1x2x2 of the elementary GaSb supercell structure comprising of 32 atoms. The co-ordinate system in both the figures represents spacial formation of the supercell structures. The blue mark along the z-

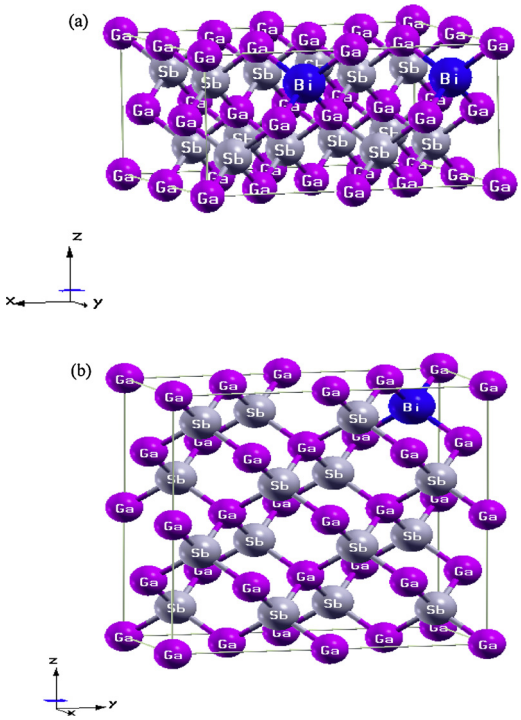

Fig. 1. Lattice Structure of (a) 2x2x1 and (b) 1x2x2 $GaSb_{0.875}Bi_{0.125}$ supercell structure.