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Theoretical study on the electronic and optical properties of bulk and surface (001) $In_xGa_{1-x}As$

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ABSTRACT

The optical properties of surface and bulk $In_xGa_{1-x}As$ materials are compared systematically first time in this paper. The band structures, density of states and optical properties including dielectric function, reflectivity, absorption coefficient, loss function and refractive index of bulk and surface $In_xGa_{1-x}As$ materials are investigated by first-principles based on plane-wave pseudo-potentials method within the LDA approximation. The results agree well with the available theoretical and experimental studies and indicate that the electronic and optical properties of bulk and surface $In_xGa_{1-x}As$ materials are much different, and the results show that the considered optical properties of the both materials vary with increasing indium composition in an opposite way. The calculations show that the optical properties of surface $In_{0.75}Ga_{0.25}As$ material are unexpected to be far from the other two indium compositions of surface $In_xGa_{1-x}As$ materials while the optical properties of bulk $In_xGa_{1-x}As$ materials vary with increasing indium composition in an expected regular way.

1. Introduction

Ternary $In_xGa_{1-x}As$ compound semiconductor as photoelectric material have been widely studied for a variety of optoelectronic devices, such as detectors and lasers [1–4], surfaces solar cells [5], modulators [6]. As we know, the physical properties of $In_xGa_{1-x}As$ material will change with x, composition of indium in $In_xGa_{1-x}As$. Many experimental and theoretical groups have conducted abundant of research about the effect of indium composition on the properties of $In_xGa_{1-x}As$. R.P. Mirin et al. used molecular beam epitaxy method to grow $In_{0.3}Ga_{0.7}As$ small islands on the GaAs substrate, and the experimental results show that at room temperature the full width at half maximum of 1.3 μm photoluminescence was only about 28 *meV* [7]. WANG.L et al. studied the stress accumulation in the $In_xGa_{1-x}As$ layer of $InAs/In_xGa_{1-x}As$ material system, in which he found that the stress will lead to the critical thickness change sharply with different indium composition, and the critical thickness is 1.08 ML when x is 0.25 [8]. M. Hadjab et al. have calculated a series of results about optical properties of $In_xGa_{1-x}As$ material by using first-principle methods [9]. However, all above studies are just concentrated on either bulk $In_xGa_{1-x}As$ or surface $In_xGa_{1-x}As$ [9–16], the differences of properties between bulk and surface $In_xGa_{1-x}As$ are not compared systematically. The purpose of this paper is going to deeply investigate and compare both of bulk and surface structures of $In_xGa_{1-x}As$ by first-principle methods, which would be beneficial to the further understanding of the ternary alloy material.

2. Theoretical model and calculation method

The calculation is accomplished by using Cambridge Serial Total Energy Package (CASTEP) program which based on the density functional theory (DFT) within the local density approximation (LDA), and all the results are performed by plan-wave pseudopotential method, in which coulomb potential energy caused by electron–ion interaction is described using pseudo-potential concept. Orbitals of gallium ($3d^{10}4s^24p^1$), indium ($4d^{10}5s^25p^1$) and arsenic ($4s^24p^3$) are treated as valence electrons [14]. The model of $In_xGa_{1-x}As$ bulk structure is built by replacing the gallium atoms with indium atoms in the zinc-blend bulk GaAs structure, while the $In_xGa_{1-x}As$ surface (001) structure is built by cleaving the (001) surface of GaAs and replacing corresponding gallium atoms with indium atoms, and 7 layers are used to calculate the

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properties. Different indium composition $In_xGa_{1-x}As$ structures in both models are obtained by replacing different numbers of Ga atoms. Both structures with different indium ingredients are shown by Figs. 1 and 2. (a),(b),(c) is correspond to x = 0.25,0.5,0.75 respectively. The dangling bonds at the bottom of the $In_{0.25}Ga_{0.75}As$ surface (001) structure are saturated by hydrogen atoms while a 10 Å vacuum layer is created above the top layer, and 4 layers near the bottom are constrained. It means that the bulk material lattice constant equal to the lattice constant of GaAs. Before calculation, the convergence test is completed and the cut energy is set at 380eV in both structures, while the k-point density is respectively set as $2 \times 5 \times 5$ in bulk structure and $5 \times 5 \times 1$ in surface structure. For two structures, the convergence accuracy is set as: the maximum displacement of the atom is less than 0.001 Å, and the maximum stress of the atom is set to 0.05Gpa, the energy change on each atom is no more than $1.0e^{-5}$ eV, and the maximum force is 0.03 eV/Å.

3. Results and discussion

3.1. Electronic structure

The electronic band structures and optical properties of both structures of $In_xGa_{1-x}As$ are calculated when x is changed as 0.25,0.5,0.75. For the band gap, both structures under all indium proportions are lower than experimental values [14], it is a common phenomenon in the calculation with density functional theory when LDA is used, however, the conduction bands can be aligned with the experimental results by scissors operator. However, lower band gap has no effect on the analysis in this paper. On one hand, the band structure and density of states are accurately calculated by CASTEP [9], on the other hand, the purpose of this paper is to compare the physical properties of the two structures under different indium composition. Here the band structures only for both bulk and surface $In_{0.5}Ga_{0.5}As$ alloy are given in Fig. 3 (a),(b). The band gap of the surface $In_{0.5}Ga_{0.5}As$ is 0.161eV, which is close to the results in literature [16]. The band gap of bulk $In_{0.5}Ga_{0.5}As$ is 0.431eV and is in compliance with the results [9]. Both of the values found to be less than the experimental results [17].

Whether it is the bulk $In_{0.5}Ga_{0.5}As$ or surface $In_{0.5}Ga_{0.5}As$, the maximum value of valence band and the minimum value of conduction band are set in the same location in the space K, which means both of the structures are direct band gap semiconductor. However, according to the calculated results, the bands of surface $In_{0.5}Ga_{0.5}As$ structure is flatter than that of the bulk $In_{0.5}Ga_{0.5}As$ structure, which indicates the effective mass of electrons near the surface are heavier so as to the movement of electrons is restricted [18]. Consequently, the surface-localized electronic states are appeared because of the dangle bonds caused by the broken of periodicity of crystal structure [19–21].

For a further analysis, the density of states of bulk and surface $In_xGa_{1-x}As$ are plotted in Fig. 4. The sub plot(a) and (b) shows the total density of states of both $In_xGa_{1-x}As$ structures, and sub plot(c),(d),(e),(f) show the s,p,d orbitals partial density of states (PDOS) of both structures with x = 0.5.According to the results of subplot (a) and (b), it is remarkable that there is a large variation of the total density of states (TDOS) between surface and bulk $In_xGa_{1-x}As$ structures. There are some more obvious small peaks found in the TDOS of surface $In_xGa_{1-x}As$ structures which indicates the electrons near to the surface are more localized than the bulk ones, which is corresponding to the differences of energy band structures of the two kinds of material. Combining the TDOS and PDOS(x = 0.5) of both structures, it can be found that the states situated near −15eV are contributed by gallium 3d and indium 4d orbitals. The results also show that the states near 7eV are formed by hybridization between In/Ga s and arsenic p orbitals. By carefully comparing the PDOS of surface and bulk structures for x = 0.5, it also can be found that the electrons in the surface structure is more localized which indicates again that the periodicity of the crystal at surface is destroyed would lead to the property of material be seriously affected.

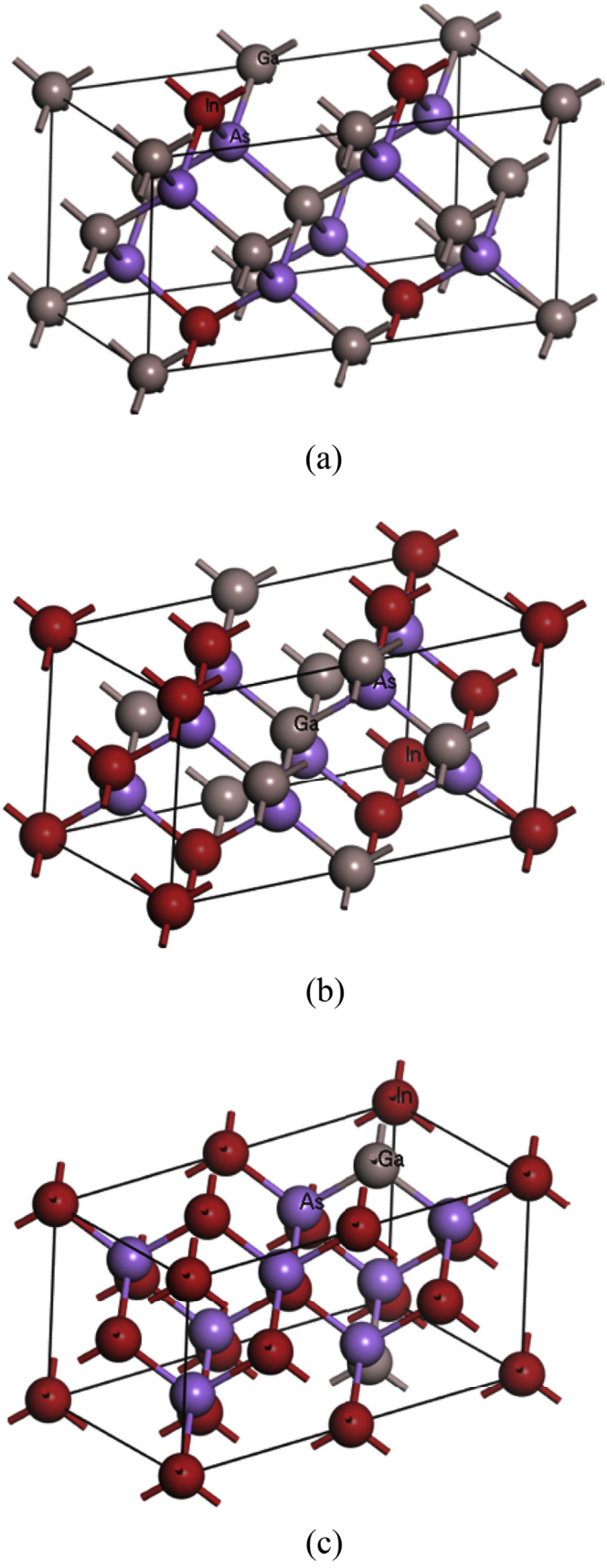

Fig. 1. Bulk structure of 16-atom $In_xGa_{1-x}As$.