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A first principle study of band structure of III-nitride compounds

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Abstract

The band structure of both phases, zinc-blende and wurtzite, of aluminum nitride, indium nitride and gallium nitride has been studied using computational methods. The study has been done using first principle full-potential linearized augmented plane wave (FP-LAPW) method, within the framework of density functional theory (DFT). For the exchange correlation potential, generalized gradient approximation (GGA) and an alternative form of GGA proposed by Engel and Vosko (GGA-EV) have been used. Results obtained for band structure of these compounds have been compared with experimental results as well as other first principle computations. Our results show a significant improvement over other theoretical work and are closer to the experimental data.

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1. Introduction

Electronic band structure of semiconductors plays a key role in determining their properties and applications in various devices such as lasers, detectors, integrated circuits, etc. Compound semiconductors have attracted an increasing deal of interest in new applications. Many of the nitride compound semiconductors have wide variety of applications. III–V compounds, specially the III-nitride semiconductors such as AlN, GaN and InN materials are of current interest for their potential in optoelectronic and high power/temperature electronic devices including light emitting diodes, laser diodes [1,2] solar blind photo detectors [3] and heterostructure field effect transistors [4,5]. These compounds show considerable resistance to corrosion in aqueous solutions [6–8] and it is therefore useful to know the band gap of these nitride compounds.

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Group III-nitrides crystallize in zinc-blende (ZB) and wurtzite (WZ) structures. The space group of ZB structure nitrides is $F\bar{4}3m$ and contains four molecules in its unit cube like that of zinc sulfide and is developed on a face-centered lattice. Where as WZ structure nitrides have their space group C6mc with two molecules in hexagonal unit cell like zinc-oxide [9]. The nitride compounds are usually considered as wide-band gap materials. However recent measurements [10–14] suggest that the band gap of InN is smaller (~0.8 eV [15]) than commonly accepted (~1.9 eV [16]) band gap obtained to interpret experimental data [2]. The low band gap values of two phases of InN have become a test to identify the general chemical trends of semiconductor band gaps [17,18]. Small band gap value of InN is particularly useful as it will provide an extra dimension in the application of this compound. As a small band gap material, InN and its III-nitride alloys could be suitable for low future-generation solar cells. Main attention in recent years on group III nitrides particularly GaN and AlN is due to the fact that in addition to wide band gap, they also have a high thermal conductivity and large bulk modulus. Significant role of nitrogen in these compounds is in the formation of their physical properties similar to other wide band gap semiconductors such as diamond [19]. An in-depth study of III-Nitride compounds based on first principle should therefore provide very useful information.

In our present work we have undertaken first principle study of the electronic properties of AlN, GaN and InN using full-potential linearized augmented plane wave (FP-LAPW) method. We first calculate optimized value of internal parameter u, using experimental lattice parameters. We then calculate the band structure of both phases (ZB and WZ) of aluminum nitride, gallium nitride and indium nitride within the framework of density functional theory (DFT). For the exchange correlation potential, two approximations have been used; generalized gradient approximations (GGA) [20] and an alternative form of GGA proposed by Engel and Vosko (GGA-EV) [21]. Dufek et al. [22] successfully applied this form of GGA (GGA-EV) to a wide range of solids. Akbarzadeh and Mokhatari [19,23] also calculated the band structure of II–V nitrides using GGA-EV and obtained good results. In this paper, we have calculated the electronic band structure of III-N compounds using GGA and GGA-EV. Results obtained for band structure for both approximations are compared with experimental data and other theoretical work. Our results with GGA-EV are a significant improvement over the earlier theoretical studies.

2. Computational methods

Electronic configuration of AlN, GaN and InN is **Al**: Ne $3s^2 3p^1$, **Ga**: Ar $3d^{10} 4s^2 4p^1$, **In**: Kr $4d^{10} 5s^2 5p^1$ and **N**: He $2s^2 2p^3$. In our computational work, we distinguish between the inner-shell electrons of Al ($1s^2 2s^2 2p^6$), Ga ($1s^2 2s^2 2p^6 3s^2 3p^6$), In ($1s^2 2s^2 2p^6 3s^2 3p^6$ $3d^{10} 4s^2 4p^6$), N ($1s^2$) and the valence band electrons of the Al ($3s^2 3p^1$), Ga ($3d^{10} 4s^2 4p^1$), In ($4d^{10} 5s^2 5p^1$) and N ($2s^2 2p^3$). Atoms in WZ structure of AlN, GaN and InN are in (2b) positions as R (≡Al, Ga, In): (0, 0, 0), $(\frac{1}{3},\frac{2}{3},\frac{1}{2})$; X (≡N): (0, 0, u), $(\frac{1}{3},\frac{1}{2},\frac{1}{2}+u)$. Here '$u$' the internal parameter, is the relative displacement between R and X sub lattices along the c direction [9]. In ZB structure, atoms are in FCC positions as R (0, 0, 0); X $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$.

In order to compute electronic band structure of III-Nitrides, we have employed WIEN2k [24,25]. This approach allows one to map exactly the many body problem of an electron gas to a set of single particles moving in an effective local potential. The corresponding Kohn-Sham (KS) equations are solved iteratively till self-consistency is reached. The FP-LAPW is well-known method of solving KS single particle equations. In this method, the primitive cell with simple cubic symmetry is divided into non-overlapped atomic spheres and interstitial regions, where the KS wave functions, charge density and potential are treated differently in both regions of the unit cell. Inside the non-overlapping spheres of radius R_{MT} around each atom, spherical harmonic expansion is used and in the remaining space of the unit cell the plane wave basis set is chosen. R_{MT} values for Al and N in both ZB–AlN and WZ–AlN structures are taken