Band structure and band gap of Aluminium nitride in Zincblend phase

S. J. MOUSAVI*, A. BAKHSHINEZHAD[a]
Department of Physics, Rasht Branch, Islamic Azad University, Rasht, Iran
[a]Department of Electronic, sowmesara Branch, Islamic Azad University, sowmesara, Iran

Aluminium nitride is the largest-band gap nitride semiconductor and it is suitable for high-temperature electronics and opto-electronic applications. It is characterized by high temperature stability, (melting temperature ~3000 °C), high elastic stiffness and excellent thermal conductivity. In this paper we have studied the Zincblend (ZB) phase of AlN which has cubic structure with first principles methods. Electronic and structural properties of AlN have been studied in the framework of density functional theory (DFT). Bulk modules, band structures and total and partial density of states (DOS) of ZB aluminum nitride have been calculated using the self-consistent FP-LAPW method. The results are in good agreement with experiment. The equilibrium lattice parameter has been calculated about 4.35 (°A). Our calculated value for the direct band gap of AlN is 3.9 eV.

(Received June 19, 2012; accepted September 20, 2012)

Keywords: ZnS, Band structure

1. Introduction

Recent studies and developments about electrical and optical properties of materials have generated considerable practical interest in the optical and electronic structures of Aluminium Nitrides (AlN). This material is the largest band gap nitride semiconductor in its wurtzite (wz) phase. AlN has been crystallizes in the wurtzite (hexagonal) structure with ($P6_3mc$) space group [1,2 {ref1}]. The zincblend (ZB) is the other phase of AlN with cubic crystal structure. The wurtzite III-V nitrides are wide band gap materials with direct optical transition characterized by high iconicity, high bond strength and good thermal conductivity.

Aside from technological application, the electronic structure of AlN is also of fundamental interest. While a number of theoretical calculations of band structure exist, the experimental work available for comparison has been limited in either energy range or energy resolution. Extant experimental studies are mostly on thin films due to the difficulty of growing high –purity bulk crystal of AlN.

The aim of this work is to examine the electronic properties and band structure of Zincblend phase of Aluminium Nitride.

2. Method of calculations

The band structure and electronic properties of Aluminium Nitride have been calculated by self consistent scheme by solving kohn-sham equations. Using a full potential linearized augmented plane wave method in the framework of density functional theory along with the generalized gradient approximation (GGA).

The electronic configuration of AlN is Al: Ne 3s2 3p1 and N: He 2s2 2p3. We have distinguished the Al (1s2 2s2 2p6) and N (1s2) inner shell electrons from the valence band electrons of the Al (3s2 3p1) and N(2s2 2p3) shells. In Zincblend phase of AlN structure the Al and N are in FCC positions as follows: Al (0, 0, 0) and N (0.25, 0.25, 0.25). The lattice parameter for ZB AlN or cubic AlN (cAlN) taken from [4 ref 1] as a= 4.37A°. The Calculation was performed with 400 k-points and RKmax=7 (R is smallest muffintin radius and Kmax is the cut-off wave vector of the plane wave basis set) for the convergence in terms of the energy are achieved. The values of other parameters are Gmax= 14 a_0^{-1} (Gmax is the magnitude of largest vector in charge density Fourier expansion or the plane wave cut off and the a0 is the bohr radius), RMT(Al) =1.6 au., RMT(N) =1.5 au. (RMT is the muffin-tin radius). The iteration was halted when the difference charge density was less than 0.0001 e.a_0^{-3} between steps as convergence criterion. The core cut off energy, which defines the separation of core and valence state, was chosen as -8 Ry.

3. Results and discussion

Fig. 1 shows the crystal structure of AlN in Zincblend system.

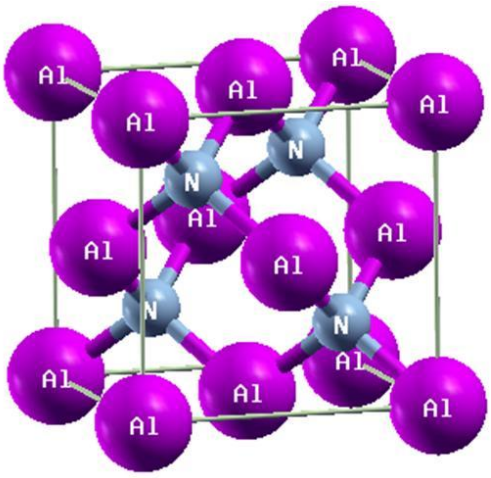

Fig. 1. AlN crystal structure in Zincblend system.

After optimization of $R_{MT}K_{max}$ and cut off energy, lattice constant are optimized. Optimizations of lattice constant have performed by minimization of volume respect to energy of lattice.

Fig. 2 shows the variation of energy respect to volume of lattice in cubic AlN structure.

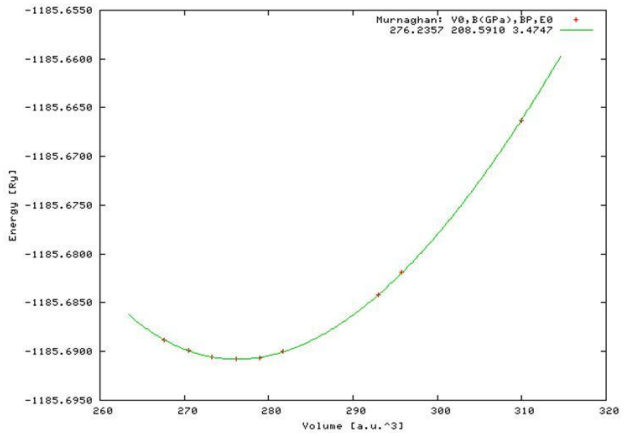

Fig. 2. Variation of energy respect to volume on c AlN.

We have calculated the lattice constant of cubic AlN about 4.35 A^o. This value seems to be accurate when compared with the available experimental value 4.38 A^o [1].

Fig. 3 shows the calculated total density of state (DOS) of cubic AlN.

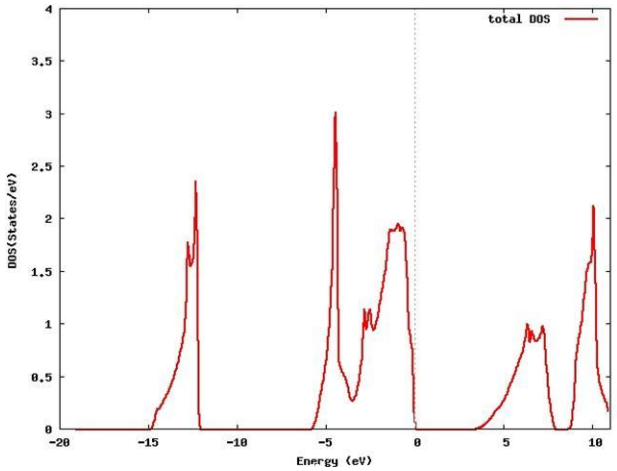

Fig. 3. Total density of state of cubic AlN.

Three regions should be recognized in total DOS on c AlN, conduction band (CB), upper valence band (UVB) and lower valence band (LVB). The width of the UVB is about 6.5 eV and for LVB about 2.5 eV. The LVB has one peak which is located at around 12.5 eV. UVB has two peaks at -5 and -2 eV. These peaks are the sources of electrons that can make transitions to the conduction band. The region between the upper and lower valence bands is referred to as the iconicity gap and upper valence band is separated from conduction band by a 3.9 eV gap which is called band gap.

Fig. 4 shows the partial DOS of AL atoms in cubic AlN structure.

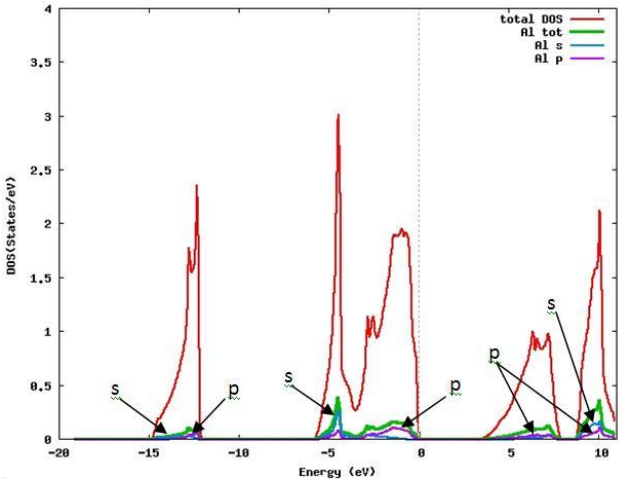

Fig. 4. Partial DOS of Al atoms in cubic AlN structure.

The lower valence bands, upper valence bands and conduction bands of Al atoms are composed of a small mixing from the 3s and 3p orbital of Al atoms.

Fig. 5 shows the partial DOS of N atoms in cubic AlN structure.

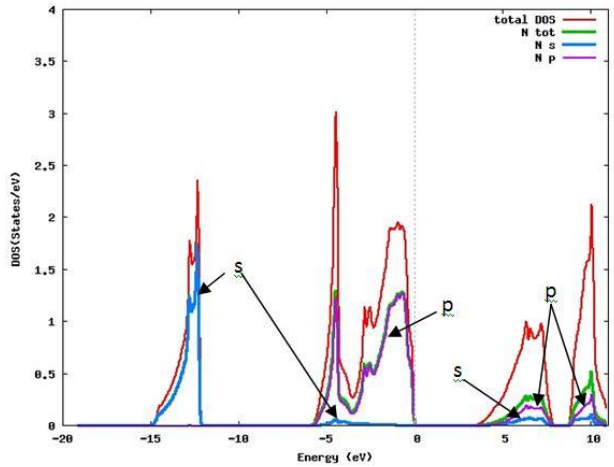

Fig. 5. Partial DOS of N atoms in cubic AlN structure.

The lower valence bands (LVB) of N atoms are composed of the 2s orbital and the upper valence bands consist mostly of the 2p orbital. N-2s and n-2p states contribute mainly to the conduction band of density of state.

With comparison of Figs. 4 and 5, we can see that electronic states below the Fermi level of AlN dominated by N states.

Fig. 6 shows the electronic density of c AlN in (110) plane. The bonds between Al and N atoms are ionic.

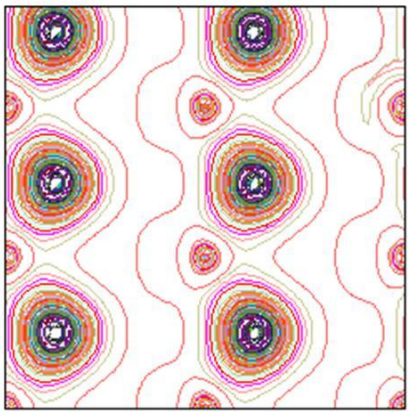

Fig. 6. Electronic density of c AlN in (110) plane.

In Fig. 7 the electronic density of AlN has been shown in three dimensions.

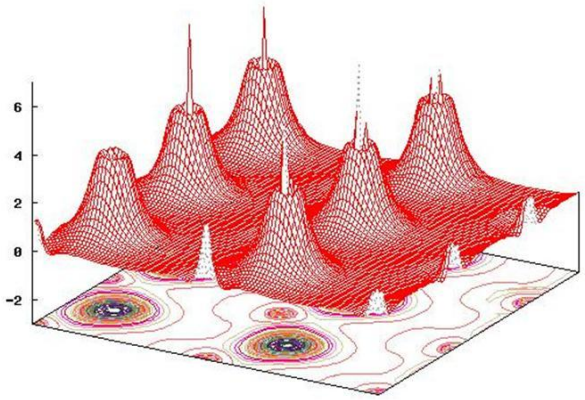

Fig. 7. Electronic density of c AlN in three dimensions.

4. Conclusion

Electronic structure of cubic Aluminum Nitride have been studied by density functional theory using of full potential augmented plan wave and by local density approximation method. The crystal structure of c AlN has been optimized and total and partial density of state has been calculated. The band gap of AlN in cubic phase has been calculated about 3.9 eV which is semiconductor. Electron density of AlN shows that the bonds between Al and N atoms must be covalent.

References

[1] I. Petrov, E. Mojab, R. C. Powell, J. E. Greene, L. Hultman, J. E. Sundgren, Appl. Phys. Lett. **60**, 2491 (1992).
[2] M. J. Paisley, R. F. Davis, J. Cryst. Growth. **127**, 136 (1993).
[3] K. Schwarz, P. Blaha, Computational Material Science **28**, 259 (2003).
[4] R. Parr, W. Yang, Oxford University Press. New York, (1989).

*Corresponding author: j_mousavi@iaurasht.ac.ir