The First Principle Studies Of Band Structure Calculations Of $MgAl_2O_4$ and 2H-SiC Using Pseudopotential Approaches

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Abstract— **We have studied the band structure properties of 2H-SiC in crystal structure and $MgAl_2O_4$ in close-packed face-centered structure. In our calculations we have adopted a pseudopotential approach based on the Density Functional Theory (DFT). We have calculated the band structure and density of state (DOS). The result shows that the electronic band structure and density of state data for 2H-SiC and $MgAl_2O_4$ are comparable with their experimental calculations.**

Keywords-*: Crystal structure; Density functional theory.*

I. INTRODUCTION

a) 2H-SiC

SiC is the only 4-4 compound known to form stable long-range ordered structures [1]. Over 200 polytypes have been observed. One form of polytype 3C is cubic, exhibing the zinc blend structure. Another form, 2H, has the wurtzite structure (space group $p6_3mc$). All other poly types have either a hexagonal unit cell (with c/a>2) or a rhombohedral unit cell [2]. In all polytypes, every atom is tetrahedrally surrounded by four atoms of the other species. For 2H-SiC (wurtzite) the repeat unit is AB.
In all SiC polytypes, the chemical bonds between the Si and C atoms are the same.Wide band gap, high breakdown field, high thermal conductivity and low thermal expansion make silicon carbide a very interesting material for high temperature and high ferequency electronics [3,4].

b) $MgAl_2O_4$

In spinel structure (sometimes called garnet structure) is named after the mineral spinel ($MgAl_2O_4$); the general composition is AB_2O_4. The spinel structure has a close-packed face- centered cubic structure of space group (Fd3m, number 227).
In this paper, we report a calculation which is used to model band structure in hexagonal SiC and close-packed face-centered cubic spinel. Details of the employed model and the results of bans structure is interpreted in section II.

II. MODEL DETAILS AND RESULTS

First principle or ab-initio approaches provide a method for modeling systems based soley on their atomic coordinates and Z number of different atoms. These techniques rely on the fact that there should be one unique charge density or distribution which describes the ground state of system. This reduces the problem of solving for the electronic structure of a system from a 3N dimevsional problem to one that only depends on the charge density. A number of approaches have been developed to properly reduce a system to the minimum energy electronic configuration and abinit includes several of these [5]. First principle codes such as abinit have proved useful topics ranging from the composition of the planetary core to electrical properties of single molecules [6].
Our calculations are performed within the local density approximation(LDA) to the density functional theory (DFT) as implemented in the plane-wave pseudopotential ABINIT package [5] to ensure good numerical convergence, the plane-wave energy cut off is set to be 30 Ha and the brillouin zone integration is performed with 6×6×6 **K**-meshpoints. The norm-conserving pseudopotentials generated by OPIUM program are tested against the all electron full-potential linearized augmented plane –wave method [6].The orbitals of Mg $3s^2$, Al $3s^2$ $3p^1$, and O $2s^2$ $2p^4$ in $MgAl_2O_4$ and Si $3s^2$ $3p^2$,and C $2s^2$ $2p^2$ in 2H-SiC are explicity included az valance electrons.