Research Journal of Physical Sciences ISSN 2320–4796
Vol. **2(4),** 1-5, July **(2014)** *Res. J. Physical Sci.*

Electronic and Structural Properties of the Silicon and Germanium Carbides

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Available online at: www.isca.in
Received 6th May 2014, revised 10th June 2014, accepted 1st July 2014

Abstract

We calculated theoretically the electronic and structural properties of SiC and GeC employing the density functional theorem (DFT) full potential - linearized augmented plane wave (FP-LAPW) method. The exchange-correlation potentials are calculated using the revised generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof (PBEsol). Properties calculated include: energy band gap, lattice constant, bulk modulus and the pressure derivative of bulk modulus. The results are compared with experimental values and available results from previous theoretical studies.

Keywords: Full potential linearized augmented plane wave, density functional theory, generalized gradient approximation, and exchange correlation.

Introduction

Group IV-IV semiconductors SiC and GeC have great technological promise. The distinctive physical properties of SiC such as its mechanical, chemical and thermal stability makes it very important[1]. These beneficial characteristics can be seen in areas of high thermal conductivity, high breakdown electric field and high maximum current density which are needed in producing high temperature (300°C) and high power electronic devices. Thus it is preferred to elemental silicon in making power switches, microwave devices, etc. Its anti-oxidation and anti-corrosion properties are utilized in extreme harsh working environments such as under strong acid, alkali and high temperature conditions.

GeC on the other hand has interesting elastic properties and important photo voltaic properties. These important physico-chemical properties can only be explained by studying the electronic structure of these compounds in detail. Therefore, over the years, many studies have been carried out to determine experimentally the band structure of semiconductors including group IV-IV compounds. This work, presents self-consistent electronic band structure calculations of SiC and GeC in the zinc blende structure using the full potential linearized augmented plane waves (FP-LAPW) approach in the framework of the density functional theory[2,3]. The revised Perdew-Burke-Ernzerhof generalized gradient approximation PBEsol GGA is used to calculate the exchange correlation term[4]. We compare our results with experimental measurements where possible and with other first principles calculations.

Method of Calculation

In this work, we utilize the FP-LAPW method which is based on the density functional theory and is considered as a very accurate technique for doing electronic structure computations for crystals[2,3]. The method solves the Kohn Sham equations yielding the ground state density, total energy and Kohn Sham eigenvalues of a many body system by making use of a basis set which is specially adapted to the problem.

The FP-LAPW method, partitions space into an interstitial region and non-overlapping muffin-tin spheres centred at the atomic sites. It then uses different basis sets in the two sections. Within the spheres the basis set is described by a linear combination of radial functions times spherical harmonics while in between the spheres a plane wave is used.

All calculations were performed self consistently without shape approximations in the charge densities or potentials. The exchange and correlation potential energy is calculated within the generalized gradient approximation using the scheme of Perdew et al PBEsol which is a revised version of Perdew-Burke-Ernzerhof generalized gradient approximation PBE96 GGA[4, 5]. Our calculations are performed for SiC and GeC in the zinc blende structure with two atoms per unit cell. The Si and Ge atoms are positioned at (0, 0, 0) a while the C atom is at (0.25,0.25,0.25) a in each of the compounds. The experimental values of the lattice constants were used for the calculations which are 4.36Å for SiC and 4.45Å for GeC. The values of the sphere radii used are Si, Ge, C are 1.8, 2.0 and 1.6 au.

The implementation of the FP-LAPW was carried out using the WIEN2K code[6]. The Brillouin zone (BZ) integration was done with 116k points in the irreducible part of the BZ. The core states are separated from the valence states by an energy cut-off of -6.0 Rydberg. The valence states were treated scalar relativistically while the full relativistic approach was adopted for the core states. The values of the sphere radii, the nearest neighbor distance, optimized $R_{MT}K_{max}$ and the number of plane waves used in our calculation are shown in table 1.

Results and Discussion

The ground state bulk properties of SiC and GeC were calculated without spin-orbit interaction by computing the total energy at five different volumes around experimental volume and fitted to the Murnaghan equation of state[7]. From the fitting we obtained the equilibrium lattice constant a, the bulk modulus B and the pressure derivative of bulk modulus B′. In table 2 the values obtained at equilibrium in the zinc blende phase are displayed and compared with those obtained from other calculations.

Our results for the lattice constant 4.362Å and 4.568 Å for SiC and GeC respectively using GGA PBEsol for the exchange correlation energy compare favourably with experimental values of 4.36Å and 4.56Å. It gives a better result than the values of 4.34Å and 4.54Å by Khenata using the PBE96 GGA[8].

The energy band structures for SiC and GeC along the principal symmetry directions W-L-Λ-Γ-Δ-X-Z-W-K are shown in figure 1 and 2. The zero of the energy scale shows the position of the Fermi level. The vertical lines show positions of symmetry. The computations were executed using the experimental values of their lattice constants for ease of comparison with experimental results and other calculated data. The general profiles of the band structure are found to be similar for the two compounds and are in agreement with previous study by Remediakis and Kaxiras within the framework of density functional theory in the local density approximation (LDA) [9, 10]. For both compounds the conduction band minimum occurred at X while the valence band maximum is at Γ showing that both compounds are indirect band gap semiconductors. The results for energy band gaps are displayed in table 3. The obtained band gap of 1.24eV and 1.59eV for SiC and GeC respectively agree very well with the values of 1.25ev (SiC) and 1.52eV (GeC) Khenata *et al* using PBE 96GGA[8]. However, as usual with the GGA, the fundamental band gaps are underestimated when compared with experiment. The band gap for SiC for which experimental value is available is found to be underestimated by 49%. This trend has been observed by earlier workers with GGA.

In order to expatiate on the electronic band structure, the total and partial density of states (DOS) for both compounds was also calculated using the PBEsol GGA. These are displayed in figure 3 and 4. The prominent features again are similar to findings of Khenata R.[8]. The features below the Fermi level can be seen to be primarily due to C while in the conduction band the anions, Si and Ge play more dominant roles.

Table-1
The number of plane waves (PW), nearest neighbour distance (NN), muffin-tin radii (RMT), and $R_{MT}K_{max}$ values used for the zinc blende calculations.

				RMT(au)			
Structural Parameters	**PW**	**NN(au)**	**$R_{MT}K_{max}$**	**Atom 1**	**Atom 2**	**k-points**	
SiC	245	3.56768	9.00	2.0	1.6	72	
GeC	258	3.64133	9.00	1.8	1.6	72	

Table-2
Structural parameters of SiC and GeC

SiC	Present Work	Other Calculations	Experiment
a(Å)	4.362	4.30[1],4.34[8],4.40[13],4.33[17]	4.36[14]
B(Mbar)	2.215	2.25[1],2.28[8]	2.25[15]
B′	3.9118	3.90[1], 3.94[16]	
GeC	Present Work	Other Calculations	Experiment
a(Å)	4.568	4.431[1],4.61[13],4.54[8],4.526[17]	4.56[18]
B(Mbar)	1.872	1.88[1], 2.03[8]	2.25[9]
B′	3.925	3.45[1], 3.73[8]	

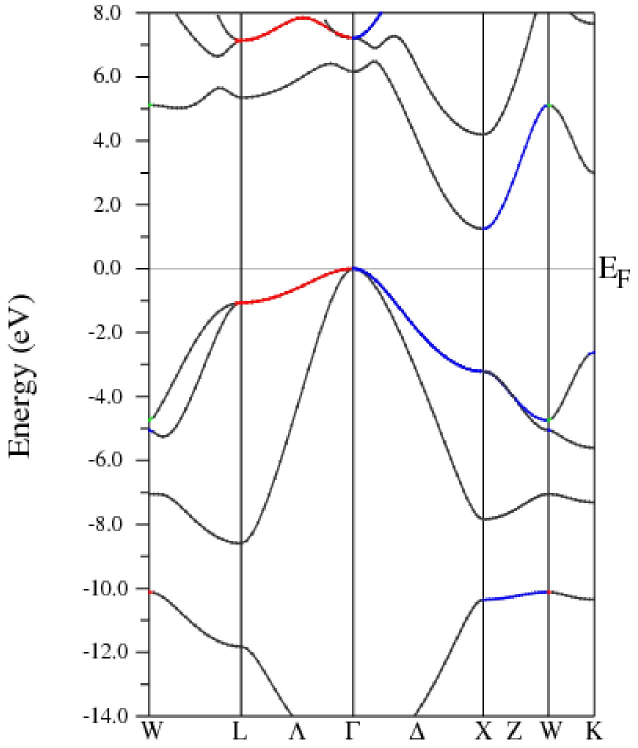

Figure-1
Electronic structure of SiC

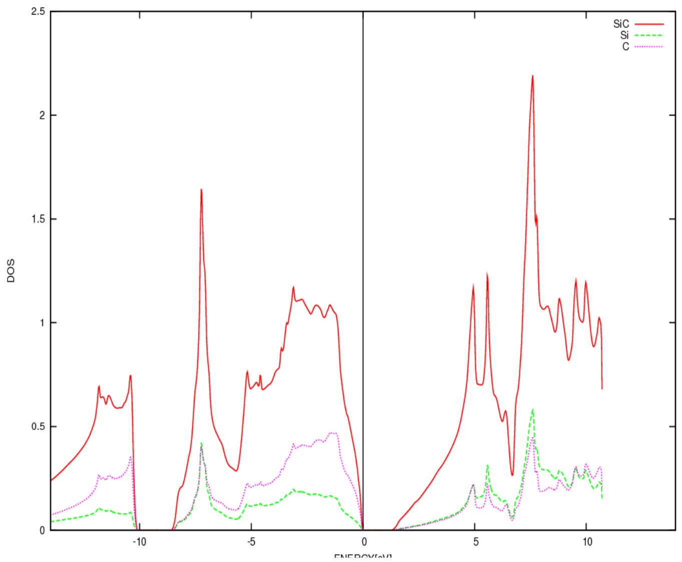

Figure-3
Density of states of SiC, Si and C

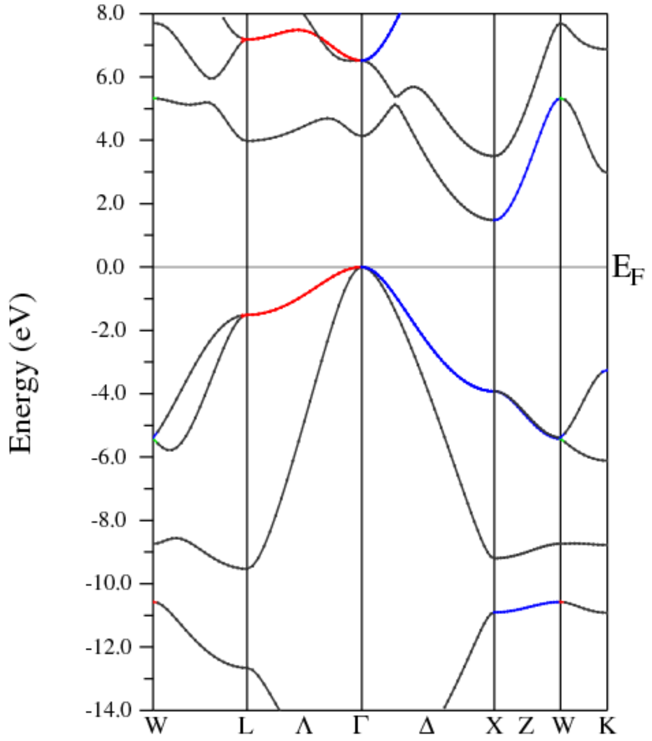

Figure-2
Electronic structure of GeC

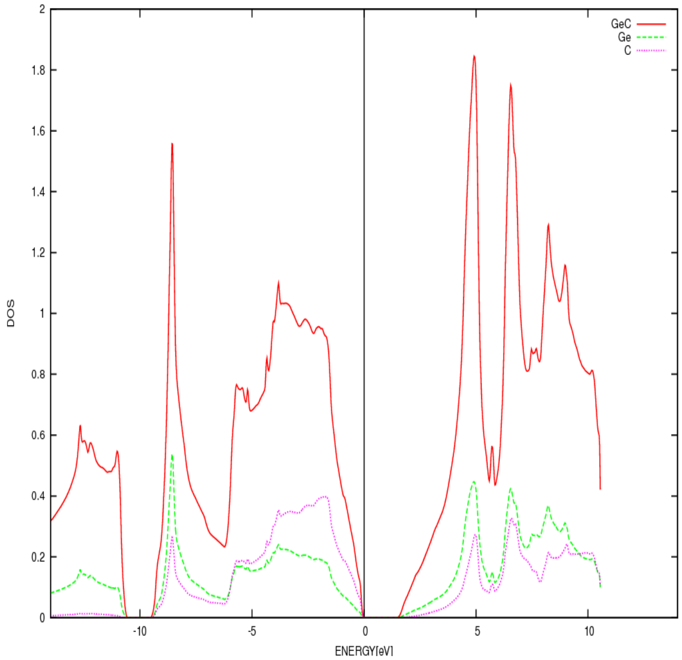

Figure-4
Density of states of GeC, Ge and C

Table-3
Energy band gaps (eV) for SiC and GeC

	Present Work	**Experiment**	**Other calculated values**
SiC	1.24	2.42[12]	1.25[8], 1.60[13], 1.22[16]
GeC	1.59		1.52[8], 2.50[13], 1.40[16]

Conclusion

In this paper, we have used the FP-LAPW method to carry out a complimentary study of the electronic and structural properties of SiC and GeC. The results are compared with both experimental values and results from other works. The use of PBEsol for the exchange-correlation potential gave good structural parameters in excellent agreement with experiment and similar to what was obtained in an earlier work using PBE96 GGA[8] using PBE96 GGA. For the electronic structure the overall band profile for the two compounds are similar and is in agreement with previous band structure results. However the calculated band gap for SiC for which experimental result is available is grossly underestimated. We can therefore conclude that the while the PBEsol GGA gives good structural values for SiC and GeC, it still underestimates the band gaps.

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