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Electronic Properties of Zirconium Carbide by using Full-Potential Linearized Augmented Plane Wave Method (FP-LAPW):A first principle study

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Abstract

In this paper, we have study the density of state (DOS) and band structures of Zirconium Carbide by using full-potential linearized augmented plane wave method (FP-LAPW) base on density functional theory (DFT) within generalized gradient approximation (GGA). We have calculated the optimized lattice constant of ZrC and used it to find the DOS and the band structures. The results shows ZrC to be metallic.

Keywords: *Density of state (DOS), band structures, DFT, FP-LAPW, GGA.*

1. Introduction

Zirconium carbide (ZrC) belongs transition metal (TM) carbide with f.c.c. structure. Transition metal carbides have attracted growing attention because of their scientific and technological interest. Zirconium carbide is extremely hard and crystallize in stable rock-salt-like structures. Further, it is corrosion resistant and has very high melting points. These properties indicate strong covalent bonding [1] between the carbon *s–p* and the transition metal *d* orbitals. This compound shows conductivities comparable with those of the pure transition metals. ZrC is an important technological material, having large number of applications such as nuclear fuel particles coatings, field emitter coatings, or thermo-photovoltaic radiator coatings. Study of electronic band structures and density of states is required for detail investigation in view of its high potential in technological applications [2].

In this paper we will present a theoretical study of the electronic properties of ZrC by using the density functional theory (DFT) as given by Kohn and Sham *et al*. [3].

2. Methods

The calculations of Density functional electronic band were carried out for ZrC, using full potential linearized augmented plane wave method (FP-LAPW) as implemented in the WIEN2k code [4]. The exchange and correlation effects were treated using the generalized gradient approximation (GGA) as parameterized by Perdew and Wang [5]. The core states were treated fully relativistically and the valence states were treated semi-relativistically.

In this calculation, the angular momenta inside the muffin-tin spheres is l_{max} = 9, R_{MT} * K_{max} = 7 and G_{max} = 12. R_{MT}* K_{max} determines the number of basis functions, where K_{MAX} is the energy plane wave cut-off, and R_{MT} is the smallest of all atomic sphere radii. An energy cut-off of -6.0 Ry. is taken to separate the core states from the valence states. For ZrC, the experimental lattice constant used is 4.6828 Å, R_{MT} = 2.43 a.u. for ZrC and for C R_{MT} = 1.99 a.u. The number of special k points used for the calculation is 10000 in the entire Brillouin zone. The Bravais lattice is face-centered cubic belonging to space group Fm-3m and the basis consists of one ZrC atom.

3. Results and Discussion

3.1 Density of states

We have calculated the total and partial density of states (DOS) of ZrC as well as the energy band structures. Fig. 1 shows the total density of states of ZrC, Zr and C respectively. We find from this plot that maxima in total DOS of ZrC occurs at 2.402 eV below the Fermi level (E_F=0). Similarly the plot also shows that the maxima in total DOS of Zr and C also occurs at 2.402 eV below the Fermi level which is coinciding with the occurrence in maxima of total DOS for ZrC. In the conduction region, the first maxima in the total DOS of ZrC occurs at 5.453 eV above the Fermi level. Similarly the first maxima in total DOS of Zr and C also occurs at 5.453 eV and 5.44 eV respectively above the Fermi level. The Second maxima in total DOS of ZrC, occurs at 7.859 eV. The contribution to second maxima in total DOS of Zr and C atoms in conduction region is negligible. The third peak in total DOS for ZrC, Z and C are very small in height and hence are neglected.

In Fig. 2, we have shown the total and partial DOS plots of Zr atom. We find from this plot that the maxima in partial DOS of Zr occurs at 2.402 eV eV below the Fermi level in the valence band which is contributed by *d*-state electrons. The contribution of *p*-state electrons is very less compared to contribution by *d*-state electrons. The contribution of *s*-state electrons is very small and

hence neglected. In the conduction band, the first maxima takes place at 5.465 eV above the Fermi level. This maxima is also the contribution by the *d*-state electrons. The Second and third maxima in the partial DOS plot of Zr occur at 7.865 eV and 10.0 eV which arises due to the contribution by the *d*-state electrons respectively above the Fermi level. Contribution to partial DOS by *s* and *p*-state electron is negligible which is evident from the low peak of DOS.

In Fig. 3, we have shown the partial DOS plot of C atom. From this plot we find that the maxima in DOS occurs at 2.402 eV below the Fermi level in the valence band which is contributed by *p*-state electrons. The contribution of *s* and *d*-state electrons are negligible in the valence band. In the conduction band, very less amount of contribution is coming from the *s* and *p* state electrons. The maxima in partial DOS plot of C atom occur at 5.065 eV and 10.0 eV above the Fermi level. These maxima are contributed by the *p*-state electrons of C. The maxima occurs at 7.865 eV is contributed by *s*-state electros of C atom. Contribution to partial DOS by *d*- state electrons is negligible which is evident from the partial DOS plot of C atom.

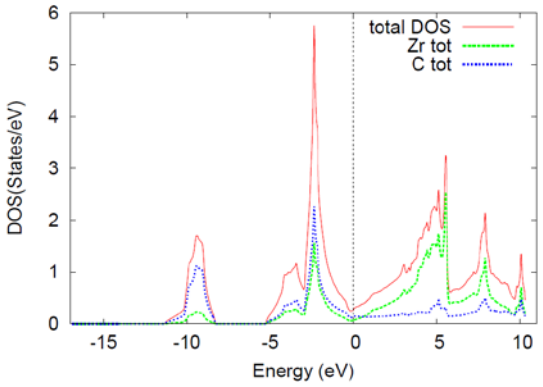

Fig. 1 Plot of Total DOS for ZrC, Zr and C. Fermi level is at 0.

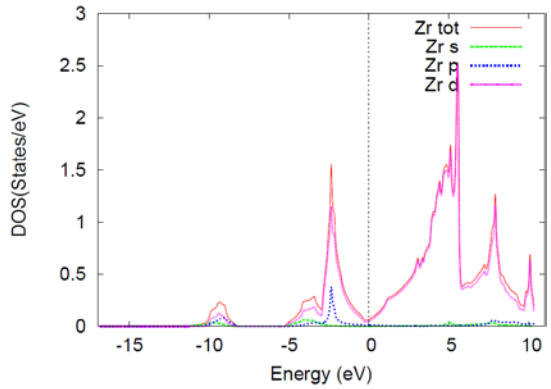

Fig. 2 Plot of total DOS and partial DOS of Zr.

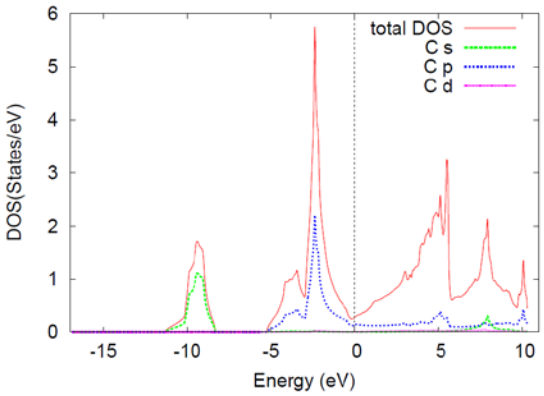

Fig. 3 Plot of total DOS and partial DOS of C.

3.2 Band structures

The band structures plot of ZrC is shown in Fig. 4. It has five high symmetry points indicated by W, L Γ, X and K with origin as Γ . These points are connected by lines labeled as Λ, Δ and Z which shows path through the Brillouin zone along which the energy of the electrons is calculated. They are infact high symmetry directions. The DOS plot shown in Fig. 1, 2 and 3 supplements the band structures of the system. The lowest lying bands are due to *s*-states of C atom from below the core states. The second bands which lie at -5.45 eV and -2.402 eV are the energy bands of ZrC due to its *s* and *p* state electrons. Peaks occur at -2.39 eV and -2.76 at W point are p-state of C atom and *p* and *d*-state of Zr. From the plots of band structures we find that all the energy bands shows the behaviour of electrons in metals. Hence, ZrC exhibit metallic nature.

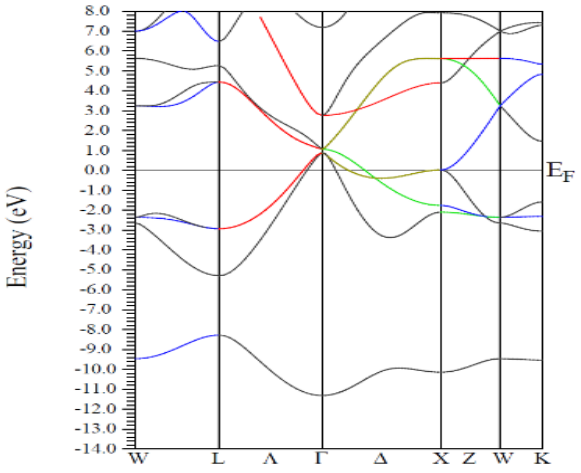

Fig. 4. Band structure plot for fcc ZrC.

4. Conclusions

From the study total and partial DOS of Zr and C, we find that the main contribution to the maxima in total DOS of ZrC is due to the electrons transition from the *d*-state of Zr atom and *p*-state of C atom. Further we also find from the band diagrams in Fig. 4 that the band lines are similar to the behavior of electrons in a metal. This is interesting to note here that ZrC is also a photosensitive material which had been also studied by Thapa *et al*. [7] in photo field emission study [7].

Acknowledgments

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References

[1] L. E. Toth, Transition Metal Carbides and Nitrides, New York: Academic Press, 1971.

[2] M. Mrovec, D. N. Manh, D. G. Pettifor and V. Vitek, “Bond-order potentials with analytic environment-dependent tight-binding integrals: application to BCC molybdenum”, Mat. Res. Soc. Symp. Proc., 653, 2001, Z6.3.1- Z6.3.6.

[3] W. Kohn & L. J. Sham, “Self-consistent equations including exchange and correlation effects”, Phys. Rev., A, 140, 1965, 1133-1138.

[4] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka & J. Luitz, “An augmented plane wave plus local orbitals program for calculating crystal properties, in: WIEN2K”, Vienna Universitat of Technology, Vienna, 2001.

[5] J. P. Perdew, S. Burke and M. Ernzerhof “Generalized gradient approximation made simple”, Phys. Rev. Lett., **77**, 1996, 3865-3868.

[6] M. Posternak, H. Krakauer, A. J. Freeman and D. D. Koelling, “Self-consistent electronic structure of surfaces: Surface states and surface resonances on W (001)”, Phys. Rev., B, 21, 1980, 5601-5612.

[7] Ram Kumar Thapa, L. Nirmala Devi, Benjamin Vanlalruata, Rebecca Lalngaihawmi, Amit Shankar, Sandeep Chhteri, Dibya Prakash Rai and M.P. Ghimire, “Laser Assisted Field Emission Study in Zirconium Carbide”, 2015 International Conference on Electrical and Electronics: Techniques and Applications (EETA 2015) ISBN: 978-1-60595-276-5 (Phuket, Thailand, 23-24 August 2015).