http://sciencevision.info

Research Note

Sci Vis 10 (2), 57-61
April-June, 2010
ISSN 0975-6175

DOS and band structures calculations of transition metals (W and Nb) using FP-LAPW method

R. K. Thapa[1]*, M. P. Ghimire[1], Rosangliana[2], Sandeep[1] and Lalmuanpuia[1]

[1] Department of Physics, Mizoram University, Aizawl 796009, India
[2] Department of Physics, Govt. Zirtiri Residential Science College, Aizawl 796001, India

Received 3 April 2010 | Revised 7 April 2010 | Accepted 9 April 2010

ABSTRACT

The paper describes a technique to determine the density of states (DOS) and band structures results of W and Nb by using FP-LAPW method in the framework of density functional theory (DFT), within generalized gradient approximation (GGA). We have calculated the optimized lattice constants of both W and Nb and used them to find the DOS and band structures. Our study indicates that DOS of W and Nb are similar in character. The DOS of Nb at the Fermi level is quite large as compared to W. These are indicative of good conductivity. The contribution to DOS and band structures is due to d state electrons of W and Nb. Our study indicates that W and Nb are metallic in character.

Key words: DFT; GGA; FP-LAPW; DOS; band structure.

INTRODUCTION

Transition-metals have been the object of much research for some time because of their unusual physical properties.[1] As a refractory metal, tungsten (W) and niobium (Nb) is an excellent material for experimental studies on well -characterized surfaces because clean annealed facets can readily be prepared by flashing to white heat.[2] Stimulated by the availability of high quality experimental data showing a rich variety of features, W (100) has been widely adopted as a prototype for theoretical studies of the electronic structures of metal-vacuum interfaces. Moreover, the electronic structure of the tungsten-vacuum interface is of great practical importance, as thermionic emission from a heated tungsten filament is widely used in electronic devices. Study of electronic band structure and density of states is very much required for detail investigation of these properties in view of its high potential in technological applications.[3]

In this paper we will present a theoretical study of the electronic properties of these materials by using the density functional theory (DFT) as given by Hohenberg and Sham *et al*.[4]

METHODS

Corresponding author: R. K. Thapa
Phone. +91-0389-2328044 Fax. +91-0389-2330522
E-mail: r.k.thapa@gmail.com

Density functional electronic band calculations were carried out for W and Nb, using full potential linearized augmented plane wave method (FP-LAPW) as implemented in the WIEN2k code.[5] The exchange and correlation effects were treated using the generalized gradient approximation (GGA) as parametrized by Perdew and Wang.[6] The core states were treated fully relativistically and the valence states were treated semi-relativistically.

For the calculations, the angular momenta inside the muffin-tin spheres is L_{max} = 10, R_{MT}* K_{MAX} = 8 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 -9.0 Ry. is taken to separate the core states from the valence states. For W, the experimental lattice constant used is 3.159 Å, R_{MT}= 2.44 a.u. For Nb, the experimental lattice constant used is 3.32 Å, R_{MT}= 2.5 a.u. 20 special k points (equivalent to 500 k points in the entire Brillouin zone) were used in both calculations. The Bravais lattice is body-centered cubic; the basis consists of one W and Nb atom each.

RESULTS AND DISCUSSION

In the transition metals, it is well known that the s-p and d bands overlap so that both are partially occupied. This leads to strong hybridization effects, particularly in those energy ranges where the s-p and d bands are degenerate.[7]

Density of sStates (DOS)

We have calculated and compared the DOS results of W and Nb as shown in Figure 1 and Figure 2. The DOS is an integral over the full Brillouin zone. In case of W, peaks occur at -3.8 eV and -2.0 eV in the valence region and 3.2 eV in the conduction region. These peaks are contributed by d- states of W.[8] Sharp peak implies that there are many k vectors having the same eigen value. The d states decomposes into d-eg and d-t_{2g} states which changes the behaviour considerably at E_F. d-t_{2g} contributes to total DOS in the valence region and d-eg to the conduction region. The contribution provided by s and p state electrons is negligible. The DOS cuts the Fermi level (E_F) showing the metallic behaviour of the system. Similarly, The DOS plot of Nb as shown in Figure 2. has a broad peak at E_F. High DOS at E_F indicates good conductivity of Nb. The increase in the DOS at E_F as the valence electrons is increased is a rigid-band-like effect resulting from the positive slope of the DOS as a function of energy in this energy range. This increase reflects the superconducting transition temperature of Nb. Sharp peaks occur at - 1.7 eV, - 0. 15 eV and 3.2 eV which is mostly contributed by d states of Nb to the total DOS. Like W, d states of Nb decomposes into d-eg and d-t_{2g} state electrons. d-t_{2g} states contributes mainly in the valence region and d-eg states to the conduction region. The hybridization effects in Nb is large as compared to W.

Band structures

The band structures plot of W and Nb is shown in Fig. 3 and Fig. 4 for its ground state b.c.c structure in the first Brillouin zone. It has four high symmetry points indicated by Γ, H, N and P. These points are connected by lines, labeled Δ, G, Σ and Λ. These four lines define a path through the Brillouin zone for both W and Nb.[9] The DOS plot shown in Fig. 1 and 2 supplements the band structures of the systems.

The lowest lying bands are due to s states of W and Nb atoms. The second bands which lie at -6.2 eV and -2.4 eV are the energy bands of W due to its s and p state electrons. Peaks are observed at -1.7 eV at Γ point and 3.9 eV at the H point. Both are due to the d state electrons. Similar band structure behaviour is observed in case of Nb as shown in Fig. 4. The difference being the peaks are at different energy ranges. For Nb, peaks are observed at energy range of - 1.7 eV at P point, - 0. 15 eV at H → N direction and 3.2 eV at Γ point. From the plots of band structures it can be found that both has a metallic behaviour.

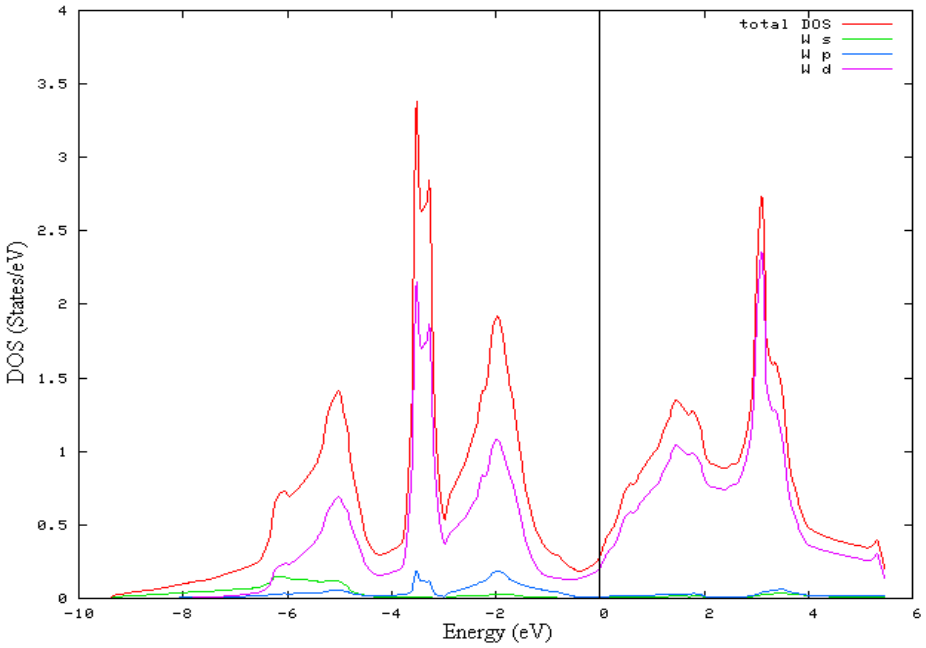

Figure1. DOS plot of W with partial DOS of s, p and d states.

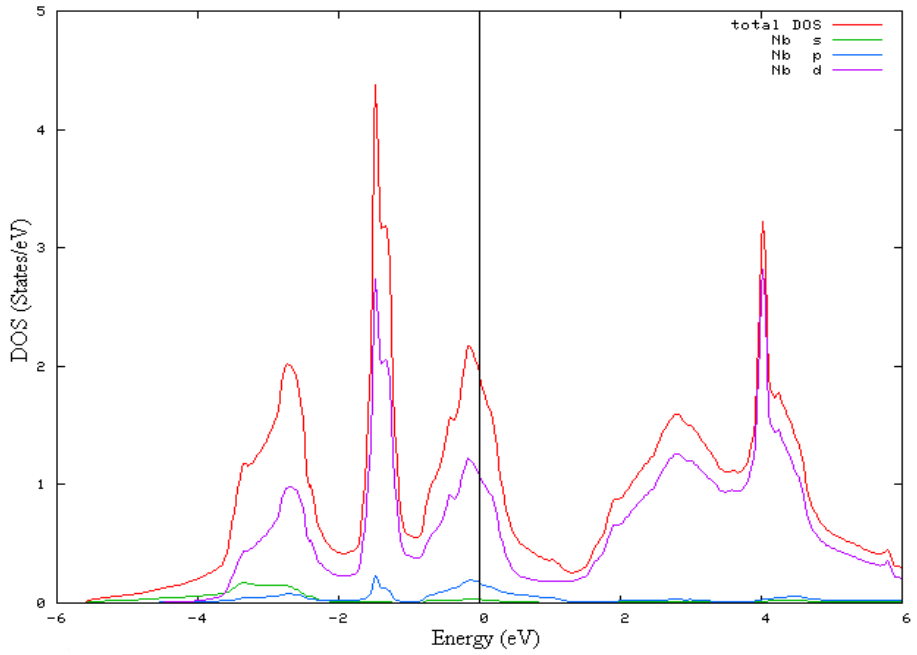

Figure 2. DOS plot of Nb with partial DOS of s, p and d states.

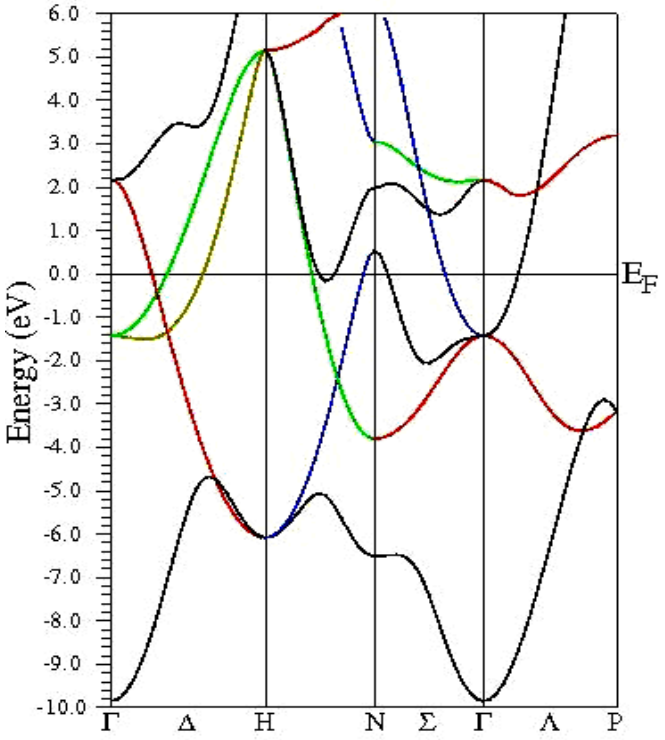

Figure 3. Band structures plot for bcc W.

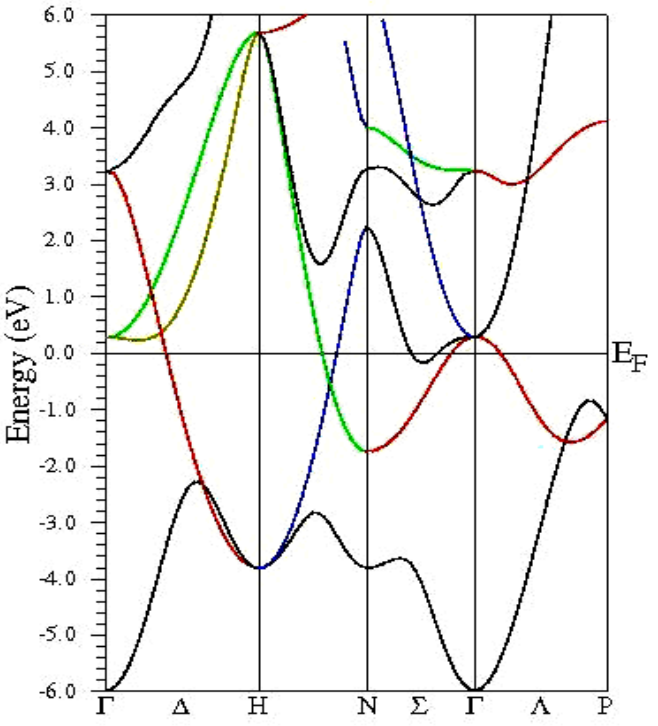

Figure 4. Band structures plot for bcc Nb.

CONCLUSIONS

We have reported the FP-LAPW calculations of the energy band structures and DOS of W and Nb. It is observed that both W and Nb shows metallic character with high DOS at Fermi level for Nb. The contribution to DOS and band structures is due to d states of W and Nb. High DOS at E_F are indicative of superconductivity.

ACKNOWLEDGEMENT

RKT acknowledges a research grant and SD a research fellowship (JRF) from DAE (BRNS), Mumbai, India.

REFERENCES

1. Vorburger TV, Penn D & Plummer EW (1975). Field emission work functions. *Surf Sci*, **48,** 417-431.
2. Mrovec M, Vitek V, Nguyen-Manh D, Pettifor DG, Wang LG & Sob M (1999). Study of the mechanical behavior of BCC transition metals using bond-order potentials. *Mat Res Soc*, **651,** 199-204.
3. Mrovec M, Manh DN, Pettifor DG & Vitek V (2001). Bond-order potentials with analytic environment-dependent tight-binding integrals:application to BCC molybdenum. *Mat Res Soc Symp Proc*, **653**, Z6.3.1-Z6.3.6.
4. Kohn W & Sham L J (1965). Self-consistent equations including exchange and correlation effects. *Phys Rev A*, **140**, 1133-1138.
5. Blaha P, Schwarz K, Madsen G, Kvasnicka D & Luitz J (2001). An augmented plane wave plus local orbitals program for calculating crystal properties. Tech. Universitat, Wien, Austria.
6. Perdew J P, Burke S & Ernzerhof M (1996). Generalized gradient approximation made simple. *Phys Rev Lett*, **77**, 3865-3868.
7. Posternak M, Krakauer H, Freeman AJ & Koelling DD (1980). Self-consistent electronic structure of surfaces: Surface states and surface resonances on W (001). *Phys Rev B*, **21**, 5601-5612.
8. Wei SH, Krakauer H & Weinert M (1985). Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. *Phys Rev B*, **32**, 7792-7797.
9. Ghimire MP & Thapa RK (2010). Band structures calculation of NbN and Nb. *Mynetresearch.com* (27 February 2010).

