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FP-LAPW calculations of electronic band structure of NbC and NbN

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ABSTRACT

We have studied the equilibrium lattice constants and energy band structures of NbC and NbN using the full-potential linearized augmented-plane-wave (FP-LAPW) method within the framework of the density functional theory (DFT). The calculation has been performed by using the generalized gradient approximation (GGA) for the exchange and correlation potential. Computations have been performed using the WIEN2k codes. The result obtained is reasonable and compares well with the experimental data and other calculations.

Key words: Linearized augmented plane wave; lattice constant; density functional theory.

INTRODUCTION

In recent years, the advent and application of highly sophisticated experimental methods for determining the properties of solids has resulted in a growing demand for detailed theoretical knowledge for critically analyzing and interpreting the experimental results. As such, considerable attention has been paid to the formulation of quantum mechanical theories which describe the dynamics of many interacting electrons in an external potential. In this quest, an important breakthrough was achieved with the development of density-functional theory (DFT)[1] according to which under certain conditions, the charge density of the electrons completely determines all the ground state properties of an interacting electron gas. In principle, the density-functional theory enables an accurate evaluation of the electronic part of the total energy and with the inclusion of Coulomb interaction between the nuclei enables the evaluation of all structural properties of solids.

The most precise way to evaluate the electronic structure is to solve the Kohn-Sham equations[2] which is a tedious job. However, recent advances in computational and theoretical approaches have enabled one to solve these equations exactly.

The transitional metal carbides and nitrides (TMCNs) possess many interesting properties. In the microscopic level they exhibit three different types of bonding: metallic, ionic and covalent.[3-8] These unusual combinations of bonding mechanisms are manifested in their macroscopic properties. They exhibit ultra hardness[4,6] as a result carbides

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are extensively used as cutting tools and wear -resistant surfaces. These compounds also possess very high melting point and metallic conductivity.[9] However, the most striking property of these compounds is their defect structure due to which they often crystallize in sodium chloride structure.[10]

In this paper, we report the equilibrium lattice constant and energy band structure calculations of niobium carbide (NbC) and niobium nitride (NbN). NbC is one of the most widely used materials for hardness and corrosion resistant coating. It is used to provide solutions to the most demanding high temperature materials problems. NbN on the other hand is being investigated as an electrically conducting barrier, since it has a high superconducting critical temperature (T_c~20K). The above mentioned facts have led physicists to investigate NbC and NbN for their use in industry.

METHOD

The calculations were performed using the full-potential linearized augmented-plane-wave (FP-LAPW) method[11-16] within the framework of the density functional theory. In the calculation, the generalized gradient approximation (GGA)[16] was used for the exchange and correlation potential. For computational purpose, we used the WIEN2K codes.[18,19] The input parameters used for the calculation of band structure is shown in the table below:

System	Experimental Lattice Constant (*Å*)	Crystal Type
NbC [10]	4.47	F.C.C.
NbN [10]	4.39	F.C.C.

RESULTS AND DISCUSSIONS

Niobium carbide (NbC)

Figure 1 shows the volume optimization plot of NbC obtained by GGA calculations. From the volume optimization curve, the calculated value of the lattice constant comes out to be 4.496 *Å*, which is in good agreement with the experimental value[10] of the lattice constant. Figure 2 shows the band structure plot of NbC. It is characterized by an energetically low-lying band due to the 2s states of the carbon atoms. This band displays a maximum dispersion between *Γ* and *L* of ~ 3.6 eV. The next lowest band originates from 2p-C in some part of the Brillouin zone and 4d-Nb in another part of the zone as evidenced by an overlap and a mixing between these bands as

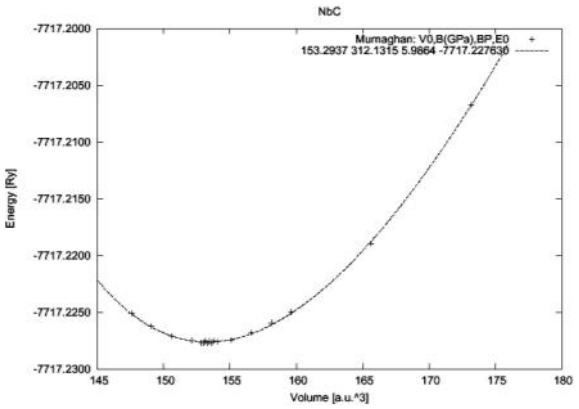

Figure1. Plot of total energy as a function of volume for NbC.

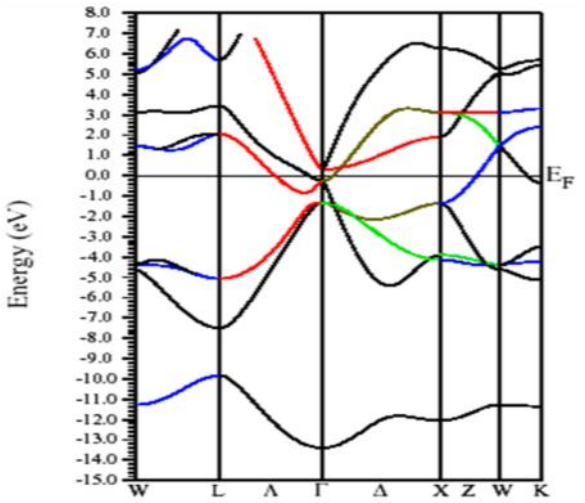

Figure 2. Electronic energy band structure of NbC.

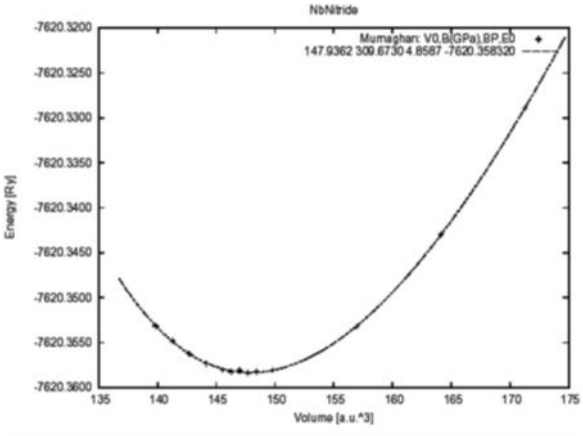

Figure 3. Plot of total energy as a function of volume for NbN.

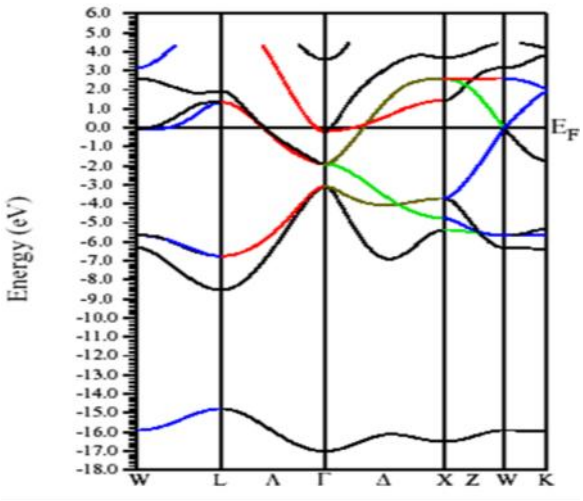

Figure 4. Electronic energy band structure of NbN.

one goes from *Γ* to *X*(Δ). The highest bands in the plot are due to 5s-Nb since the repulsive interaction with 2s-C band shifts this band to higher energies above the Fermi level. From the plot we found the Fermi energy E_F = 13.189 eV and the band gap E_g ~ 1.85 eV. Both these values agree well with the results of Amriou *et al.*,[20] who obtained E_F = 14.755 (14.355) eV and E_g = 1.879 (2.356) eV by LDA (GGA) calculations.

Niobium nitride (NbN)

Figure 3 shows the Total energy as a function of volume for NbN obtained by GGA calculations. From the plot, the calculated value of the lattice constant is found to be 4.443 A^0, which is in good agreement with the experimental value[10] of the lattice constant. The band structure of NbN is shown in Figure 4. The band structures and band ordering for NbN shows features similar to that of NbC in the region below the Fermi energy. Similar to the case of NbC, the band structure of NbN is characterized by an energetically low-lying band due to the 2s states of the nitrogen atoms. This band displays a maximum dispersion between *Γ* and *L* of ~ 2.5 eV. The next lowest band originates from 2p-N in some part of the Brillouin zone and 4d-*Nb* in another part of the zone as evidenced by an overlap and a mixing between these bands as one goes from *Γ* to *X*(Δ). The highest bands in the band structure plot are due to 5s-Nb since the repulsive interaction with 2s-N band shifts this band to higher energies above the Fermi level. From the plot, the calculated value of the Fermi energy and the band gap are found to be E_F = 15.965 eV and E_g ~ 6.12 eV respectively. These values of E_F and E_g compares well with those of Amriou *et al.*[20] who obtained E_F = 15.72 (15.59) eV and E_g =5.542 eV by LDA (GGA) calculations.

The essential features of the band structure found in our calculation are in good agreement with the results of Amriou *et al.*[20] using LDA calculations, Klein *et al.*[7] using linear combination of atomic orbitals (LCAO) method, Gupta and Freeman[8] using APW method and many other calculations.[21-25] A comparison of the electronic band structure of NbC and NbN (Figs. 2 and 4) show that the Fermi level of NbN is slightly higher than that of NbC, this can be attributed to the increase in the number of valence electrons from eight in NbC to nine in NbN. Therefore, the increase in E_F is caused by the additional valence electron. A comparison of the band

structure plots as obtained by us with those of Amriou *et al*.[20], show that the essential features of the electronic band structure are almost identical and the plots match very well apart from differences in values of E_F and E_g.

CONCLUSION

In this paper, volume optimization and band structure of NbC and NbN is presented. The result obtained has been compared with experimental data and other results obtained by different methods. The FP-LAPW results reported here are found to be in good agreement with the experimental data and other calculations.[21-25]

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