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FP-LAPW Calculations of Electronic Band structure of W and GaAs

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ABSTRACT

We have presented here the equilibrium lattice constants and energy band structures of W and GaAs 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.

1 INTRODUCTION

The advent and application of highly sophisticated experimental methods for determining the properties of solids in recent years has resulted in a growing demand for a detailed theoretical knowledge for critically analyzing and interpreting the experimental results. Therefore 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.

In this paper, we report the equilibrium lattice constant and energy band structure calculations of tungsten and gallium arsenide (GaAs).

2 Calculations

The calculations have been performed using the full-potential linearized augmented-plane-wave (FP-LAPW) method [3],[4],[5],[6],[7] within the framework of the density functional theory. In the calculation, the generalized gradient approximation (GGA) [8] has been used for the exchange and correlation potential. For computational purpose, we have

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made use of the WIEN2K codes [9],[10]. The input parameters used for band structure calculations are shown in the table below:

System	Experimental Lattice Constant	Crystal Type
W[11]	3.16 A^o	B.C.C.
GaAs[11]	5.65 A^o	F.C.C.

3. Results and discussions

(a) Tungsten (W) :

Fig 1 shows the volume optimization plot of *W* obtained by using GGA calculations. From the plot, the theoretical value of the lattice constant is calculated which in this case comes out to be 3.181 A^o which is in close agreement to the experimental value[11] of the lattice constant. The electronic energy band structure plot of *W* using the full potential augmented plane wave (FP-LAPW) within the frame work of density functional theory is shown in Fig 2. The band structure plot reflects the typical structures found in bcc materials. It is seen that the Fermi level E_F is close to the centre of the *d* bands as would be expected since the *d* states of *W*, whose valence shell electronic configuration is $5d^4 6s^2$, is approximately half-filled. From the band structure plot, the calculated value of the Fermi energy of *W* comes out to be 12.55 eV, which is set as zero in the band structure plot. The band structure plot compares well with the self-consistent full potential linearized augmented-plane-wave (LAPW) calculation of Wei *et al* [12] and of Jansen and Freeman [13]. The band structure

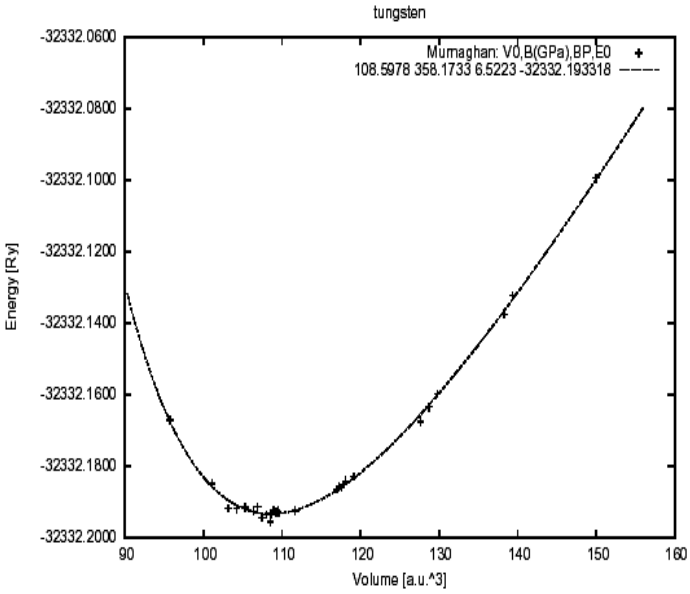

Fig 1: Volume optimization plot of W obtained by GGA calculations.

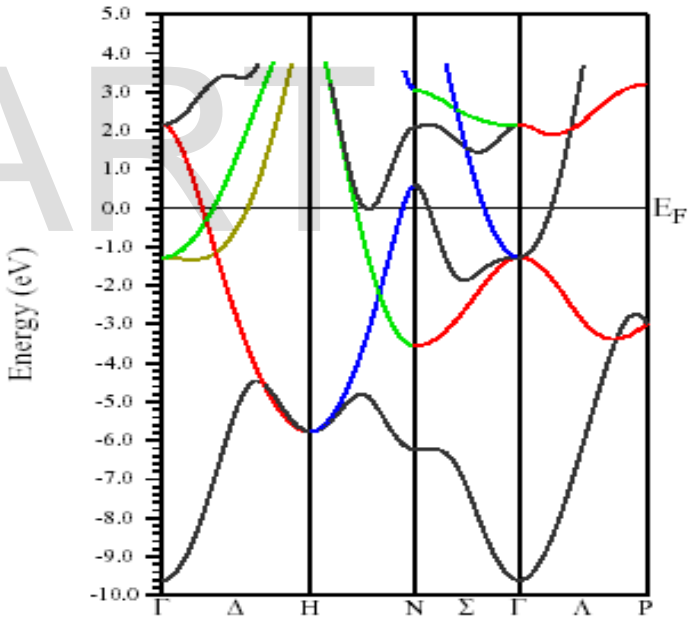

Fig 2 : Electronic energy band structure of *W*.

also shows similarity with the results of Christensen and Feuerbacher [14] using the relativistic-augmented-plane-wave method. Fig 3 shows the band structure plot of Jansen and Freeman [13] for bcc tungsten using the all-electron full-potential linearized augmented-plane-wave (FLAPW) method.

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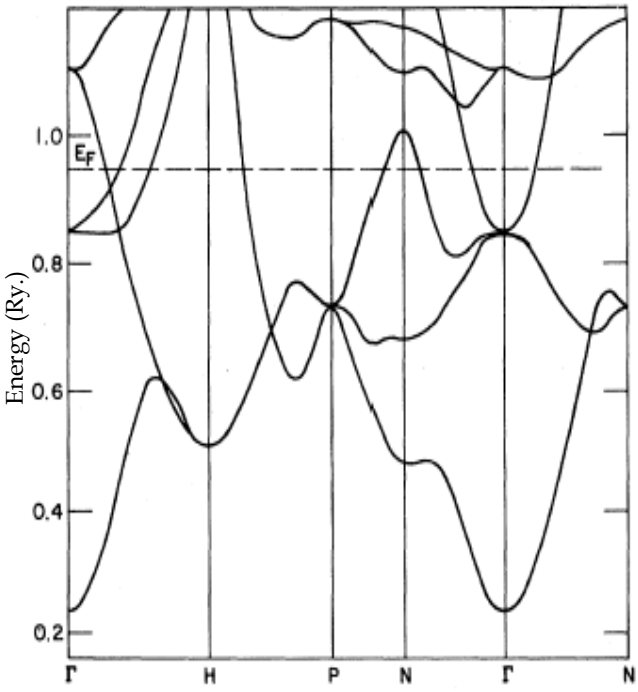

Fig 3: Band structure of bcc tungsten [13] for $a = 5.95\,a.u.$

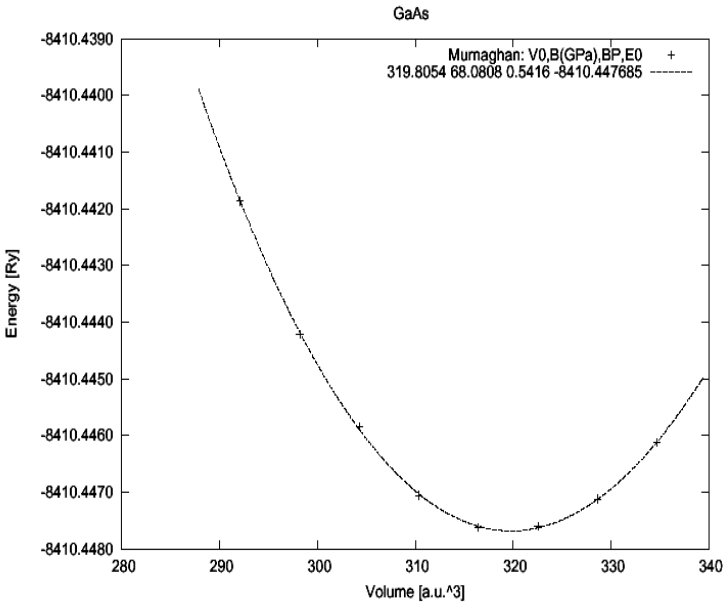

Fig 4: Volume optimization plot of *GaAs*.

Figs 2 and 3 clearly show that the essential features of the electronic band structure in the two cases match very well.

(b) Gallium Arsenide (GaAs) :

The plot of total energy as a function of volume for the case of *GaAs* obtained by GGA calculation is shown in Fig 4. From the plot, the value of the lattice constant is determined to be 5.745 A^o, which is in good agreement with the experimental value[11]. The band structure of *GaAs* is shown in Fig 5. From the plot, the value of the Fermi energy and the band gap are found to be $E_F = 5.02$ eV and $E_g \sim 0.75$ eV respectively. The plot of electronic band structure shows features that agree well with those of Chelikowsky and Cohen [15]. However, the band gap in the calculation of Chelikowsky and Cohen [15] is about 1.4 eV, which is almost double of our calculated value.

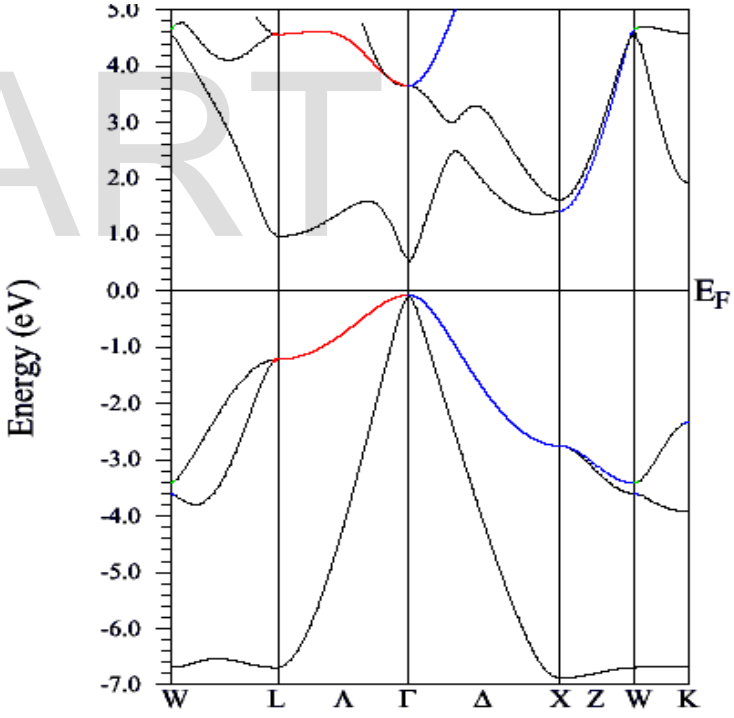

Fig 5: Electronic energy band structure of *GaAs*.

4. Conclusion

In this paper, volume optimization and band structure of W and GaAs is presented. The result obtained has been compared with experimental data and other results obtained

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by different methods. The FP-LAPW results reported here are found to be in good agreement with the experimental data and other calculations. We wish to extend the work to include other semiconductors and transition metals.

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