Band Structure and Superconducting Properties of Te under High Pressure

D. Singh

Department of Physics, MM University, Ambala, India

ABSTRACT

In the present work, the self-consistent ab initio calculations are performed for the electronic band structure properties of Te under high pressure using density functional theory (DFT) based tight-binding linear muffin-tin orbital (TB-LMTO) method. In this approach the local density approximation (LDA) was used for the exchange-correlation potential. The calculated band structure parameter parameters like electronic density of state (DOS) and Fermi energy etc., show that high pressure BCC phase is metallic as compared to ambient phase which is reported as semiconducting phase. The calculated band structure parameter parameter. are further used to study the superconductivity properties of Te at high pressure using Mc. Millan formula. *These theoretically calculated results are found in agreement with earlier reported experimental work.*

Keywords: Density functional theory (DFT), linear muffin tin orbital method (LMTO), band structure, density of state, Fermi Energy.

I. INTRODUCTION

The chalcogens (i.e. Te, Se and S)I A) have been investigated experimentally and theoretically in the last decades because of their renewed interest in view of the fact that these elements undergo similar sequence of structural phase transitions with pressure. These results also show that under ambient pressure these materials are found to be semiconductors and transforms to metallic phase under pressure high pressure [1-4]. These materials also exhibit superconductivity in their high-pressure phases [5,6]. Out of these, Te got much attention because of it's interesting electronic and optical properties. Under ambient conditions Te exhibits hexagonal structure and is semiconductor in nature. Earlier reported high Pressure XRD measurements clearly reported the sequence of pressure induced structural phase transitions with increase pressure is from Hexagonal Te (I) to Monoclinic Te (II) to Orthorhombic Te (III) to β-po type Te(IV) to BccTe(V) a**t** 4, 6.2, 11 and 27 GPa [1] respectively. Since recently, we have also carried out theoretical calculations on this series of the chalcogens materials under ambient and high pressure; it is tempting to take up the whole series from theoretical point of view. And so continuing work on this series, present paper reports ab-initio electronic band structures calculations and superconducting properties for Te at high pressure which has been carried out using density functional theory based linear muffin tin orbital method with in atomic sphere approximation. The organization of the paper is as follows. Section II gives the method of calculations. In section III the results have been discussed on electronic and superconducting properties of Te at 37GPa. Finally in section IV results have been summarized.

II. METHOD OF COMPUTATION

As mentioned, the band structure calculations at ambient & high pressure have been carried out density functional theory based TB-LMTO method with in atomic sphere approximation (ASA). This is the exact transformation of Anderson LMTO method [7] and it combines the desirable features of fixed basis method as well as partial wave method. All the relativistic contributions except spin-orbit couplings are included. The exchange-correlation potential with in local density approximation (LDA) is calculated using formalism of Von-Barth and Hedin[8]. The basic set is corrected for overlapping sphere geometry by including combined correction terms which account for non-spherical shape of atomic cells and the truncation of higher partial waves inside the sphere so that the error in the LMTO method is minimized. All angular momentum components upto L = 2 have been retained. LMTO program is used to generate the potential parameters. The total and projected partial DOS are calculated using tetrahedron method. The band structure is calculated on a mesh of 512 k points in the irreducible part of the BZ. Energy as well as k convergence is checked by increasing the number of k-points. The eigen values are converged upto 10^{-5} Ryd. McMillan Formula [9] is used to calculate superconducting transition temperature which is a function of the electron-phonon and electron-electron coupling constants within the framework of strong-coupling theory. The essential parameters required for calculating T_c values have been obtained from the self-consistent tight binding linear muffin-tin orbital method (TB-LMTO) and then with the help of these electronic parameters one can easily calculate superconducting temperature theoretically [9].

III. RESULTS AND DISCUSSIONS

To find the equilibrium lattice parameters, the total energies were computed by changing the cell volume and then these energies are fitted with Birch equation of state to obtain P-V relation. In order to calculate the band structure, crystal structural parameters like lattice parameters at different pressure, symmetry etc. is derived from our earlier work [1]. The 5*s*, 5*p*, 5*d* valence configuration was chosen to represent the basis set. The self-consistent band structure calculations are carried out for 512- K points in the entire Brillouin zone. Using equilibrium lattice parameters we have calculated band structure and DOS for high pressure bcc phase of Te from 28 GPa upto 37 GPa. In Te, electrons up to 4*d* constitute the atomic core while 5*s* and 5*p* electrons are the valence electrons, which are responsible for different solid state properties like band structure, DOS etc. It is found from the band structure that the lowest lying bands are due to 5*s* electrons whereas next-higher energy bands in the valence region just below E_F are predominately due to the 5*p* electrons. The bands crossing the Fermi-level are found to be coming mainly from 5*p* electrons which are responsible for metallic character of this phase. The conduction band above E_F is mainly due to the 5*d* electrons of Te. Thus the lower bands are mainly due to 5*s* electrons while 5*p* electrons mainly contribute the upper bands. Similarly, the contribution in total DOS due to 5*s* electrons is found in lower energy region of valence band whereas 5*p* and 5*d* are found to contribute mainly in the conduction band. The major contribution to the density of states at Fermi level [$N(E_F)$] is, therefore, coming from 5*p* electrons. Fermi-energy is observed to be shifting gradually to higher energy with increase in pressure as shown in Fig. 1.

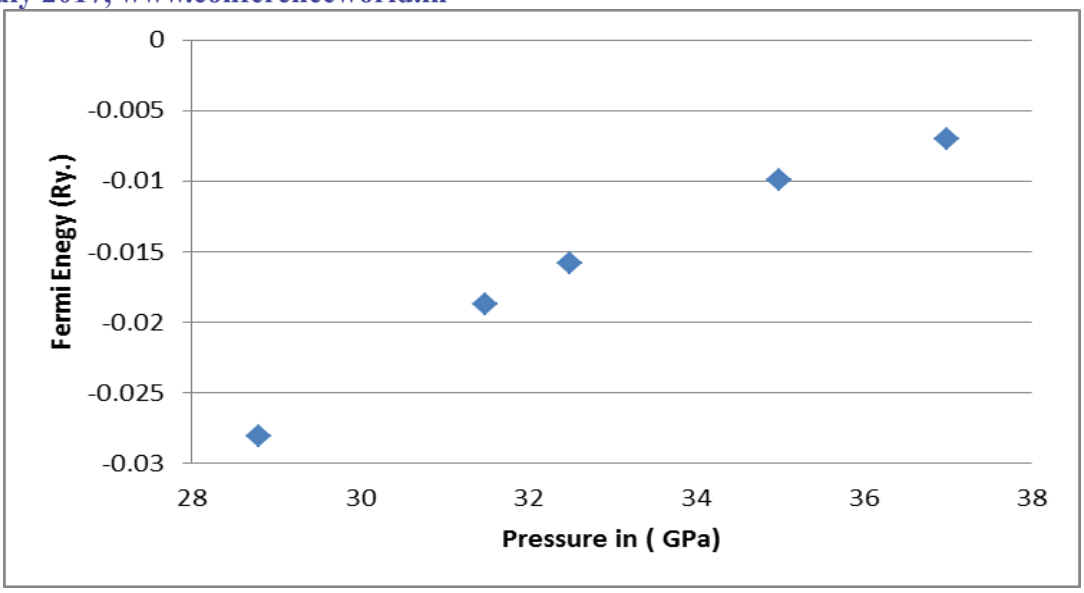

Fig. 1: The variation of the Fermi energy with pressure in Te high pressure BCC phase

The absence of band gap and non-zero DOS at E_F shows that this high pressure BCC phase of Te is metallic in nature. However, ambient pressure phase (Hexagonal) is semi-conducting phase because there is a band gap of 0.42 eV [1]. The conduction band width, which is difference in energy between Fermi level and lowest energy eigen value corresponding to the Γ-point is calculated for different pressures and is found to become broader with increase in pressure as shown in Fig. 2.

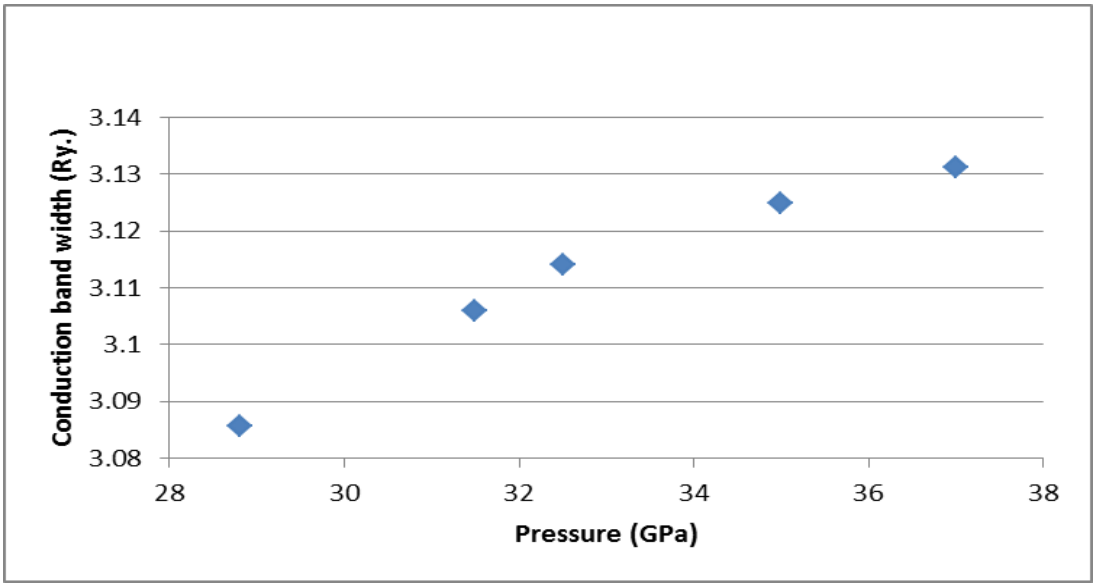

Fig. 2: The variation of the conduction band width with pressure in Te high pressure BCC phase

Further, as mentioned earlier, McMillan's formula [9] is used to calculate superconducting transition temperature (T_c) which is given as:

$$T_c = \frac{\Theta_D}{1.45} \exp \frac{\{1.04\,(1+\lambda)\}}{\{\lambda - \mu^*(1+0.62\lambda)\}} \qquad (1)$$

Where μ^* is the electron – electron interaction constant, θ_D is the Debye's temperature and λ is the electron-phonon coupling constant.

The electron – electron interaction constant μ^* is estimated from empirical expression given by Bennemann and Garland:

$$\mu^* = 0.26 \frac{N(E_F)}{1 + N(E_F)} \qquad (2)$$

The electron-phonon coupling constant λ can be written as:

$$\lambda = \frac{N(E_F)\langle I^2 \rangle}{M\langle \omega^2 \rangle} \qquad (3)$$

Where M is the atomic mass, $\langle \omega^2 \rangle$ is the average of square of the phonon frequency and $\langle I^2 \rangle$ is the square of the electron phonon matrix element averaged over the Fermi surface. In the atomic-sphere approximation $\langle I^2 \rangle$ can be written as:

$$\langle I^2 \rangle = 2 \sum_l \frac{(l+1)}{(2l+1)(2l+3)} [M^2_{l,l+1}] \frac{N_l(E_F)\, N_{l+1}(E_F)}{N(E_F)\, N(E_F)} \qquad (4)$$

Where $M_{l,l+1}$ is the electron-phonon matrix elements, which is given by the expression :

$$M_{l,l+1} = -\phi_l \phi_{l+1}[(D_l(E_F) - l)(D_{l+1}(E_f) + l + 2) + (E_F - v(s))s^2 \qquad (5)$$

Where Φ_l is the sphere boundary amplitude of the partial wave evaluated at E_F, $D_l(E_F)$ is the logarithmic derivative evaluated at the sphere boundary, $V(s)$ is the potential at the sphere boundary, E_F is the Fermi energy and s is the sphere radius. The matrix elements $\langle I^2_{sp} \rangle$ and $\langle I^2_{pd} \rangle$ are calculated in a manner similar to the earlier work on P by Rajagopalan et.al [10] and on Zr by Palanivel et.al.[11], $\langle \omega^2 \rangle$ which appears in eq.(2) is taken to be $0.5\theta^2_D$ [11]. The Hopfield parameter (η) [12] is the basic quantity which may be obtained from the results of band structure calculations and given by the relation:

$$\eta = N(E_f) < I^2 > \qquad (6)$$

It increases with increase in pressure with a slow rate. This indicates that the contribution from the electronic part is very small. To study the pressure dependence of the Debye's temperature, one has to look for the specific heat data which are not available for most of the materials in the high-pressure region and one should also consider the pressure effect of phononic contributions to which is reflected in the Debye's temperature θ_D. Due to the non-availability of the data above 30 GPa, we have adopted a simple but straight forward method to compute the pressure dependence of θ_D as suggested by Palanivel et.al.[11]. The variation of θ_D with pressure in the BCC phase can be computed by using expression.

$$\theta_D(p) = \frac{\sqrt{E_F}}{\sqrt{E_{F_o}}} \frac{a_o}{a} \theta_{D_o} \qquad (7)$$

Where a is the lattice constant, E_F is the Fermi energy and the variable with subscripts are the corresponding quantities under normal conditions The θ_D value for the BCC phase of Te is taken from the work of Bundy and Dunn [6] which is 183.3 K for normal conditions. The superconducting transitions temperature (T_c) values are

calculated taking into account the variation of the θ_D with pressure. The calculated values of superconducting transitions temperature (T_c) of Te in high pressure BCC phase are ploted in Fig. 3.

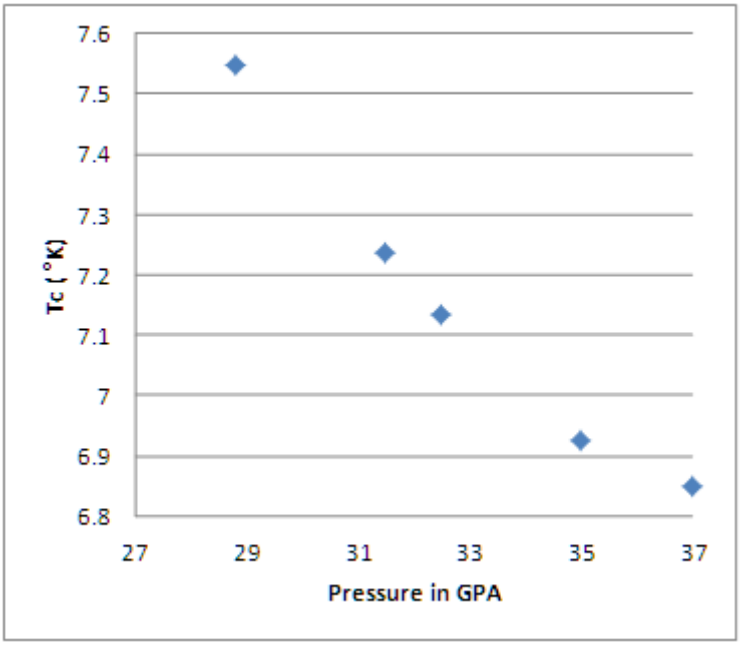

Fig. 2: The variation of the superconducting transitions temp. (T_c) with pressure in Te high pressure BCC phase

The value of T_c of high pressure BCC phase of Te at 37 GPa is 6.8 °K which is slightly higher than the experimental value of Eugene et.al [14]. It may be seen from the fig.3 that the T_c values of Te BCC phase decrease with increase in pressure which is in agreement with Akahama's et.al experimental observation [13] who measured the T_c values as a function of pressure up to 42 GPa. It is also in agreement with the experimental observations of Eugene's work [14].

IV. CONCLUSIONS

We have calculated and discussed the electronic band structure & DOS of Te in the BCC phase as a function of pressure. Further, the conduction bandwidth is found to be increase while $N(E_F)$ decreases with increase in pressure. The superconducting transition temperatures of Te BCC phase as a function of pressure is calculated using Mc.Millan Formula. The value of T_c of Te BCC phase at 37 GPa is 6.8 K which is in agreement with experimental work of Eugene et.al. . It is observed that the T_c values of Te BCC phase decrease with increase in pressure which is in agreement with Akahama's et.al experimental work.

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