



Structural and Electronic Properties of Terbium Telluride

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ABSTRACT: In the present study, the structural and electronic properties of terbium telluride in rock-salt (NaCl, B1) structure are investigated. To study these properties, the Realistic Interaction Potential Approach (RIPA) model and first principle calculation density functional theory (DFT) have been used. Present compound shows NaCl to CsCl structural phase transition. The structural properties, including phase transition pressure, volume collapse and other ground state properties are obtained and compared with existing literature. The calculated equilibrium structural parameters are in good agreement with the available results.

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Key words: Rare earth, Structural properties, High pressure, Phase transition.

I. INTRODUCTION

The rare earth (RE) chalcogenides undergo a combination of structural and valence transitions under pressure due to their equilibrium electronic structure. Many of them exhibit no integer valence at high pressure. This valence fluctuation arising from instability of f-electrons of these rare earth atoms. The hybridization of the 5f-electrons with conduction electrons is also an interesting phenomena of these compounds. These RE compounds show some complex properties like Kondo effect, magnetic anisotropy, heavy fermion or intermediate valence behaviour [1,2]. In this group of RE chalcogenides rare earth tellurides have paid more attention. Most of the mono rare earth tellurides are paramagnetic and many of them are antiferromagnetically ordered at very low temperatures. Using first-principles calculations within the self-interaction corrected local spin-density approximation the valence and structural transitions of the rare earth monote telluride TbTe are studied under pressure by Petit et. al. [3]. The crystallographic distortion of lattice distortion in terbium telluride (TbTe) with the variation of temperature is reported experimentally by Hulliger et al. [4].

According to the above literature TbTe monote telluride is very less explored material. We have applied the

Realistic Interaction Potential Approach (RIPA) model for studying structural phase transition and volume collapse of TbTe. For calculating electronic properties, the first principle calculation density functional theory (DFT) has been used. We have also reported the electronic band structure (BS) and density of states (DOS) for TbTe. The presentation of this paper is as follows: In Section 2 the method of computation is described. In Section 3, the results with some predictions are discussed. Lastly, in Section 4, we have concluded the results.

II. METHOD OF CALCULATION

The effect of pressure directly results in compression leading to the increased charge transfer (or three body interaction effect [5,6]). These effects have been incorporated in the Gibbs free energy ($G = U + PV - TS$) as a function of pressure and three body interactions (TBI). Here, U is the internal energy of the system equivalent to the lattice energy at temperature near zero and S is the entropy. The Gibbs free energies for rock-salt (B1-type) and cesium-chloride (B2-type) structures at room temperature $T=300K$ are given by:

At temperature $T=0K$ and pressure (P) the Gibbs free energies for BX (X=1,2) phase is:

$$G_{BX}(r) = \frac{-\alpha_M^X Z^2 e^2}{r^X} - \frac{12\alpha_M^X Z e^2 f_m(r)}{r^X} - \left[\frac{C^X}{r^{X6}} + \frac{D^X}{r^{X8}} \right] \dots(1)$$

$$+ 6b\beta_{ij} \exp[(r_i + r_j - r^X) / \rho] + 6b\beta_{ii} \exp[(2r_i - Y_X r^X) / \rho]$$

$$+ 6b\beta_{jj} \exp[(2r_j - Y_X r^X) / \rho] + PV_{BX}(r^X) - TS^X$$

Where $X=1$ (Phase 1=B1), 2 (Phase 2=B2), and $Y_x=1.414, 1.154$, for NaCl (B1) and CsCl (B2) structures respectively.

With M as the Madelung constant. C and D are the overall van der Waal coefficients for NaCl and CsCl structure respectively, A_{ij} ($i,j=1,2$) are the Pauling coefficients defined as $A_{ij}=1+(Z_i/n_i)+(Z_j/n_j)$ with Z_i (Z_j) and n_i (n_j) as the valence and the number of electrons of the i (j)th ion. Z_e is the ionic charge and b () are the hardness (range) parameters, r is the nearest neighbour separations $f_m(r)$ is the modified three body force parameter which includes the covalency effect with three body interaction, r_i (r_j) are the ionic radii of ions i (j).

These lattice energies consist of long range Coulomb energy (first term), three body interactions corresponding to the nearest neighbour separation r (second term), vdW (van der Waal) interaction (third term), energy due to the overlap repulsion represented by Hafemeister and Flygare (HF) type potential and extended up to the second neighbour ions (fourth, fifth and sixth terms).

Covalency effects have been included in three-body interactions in the second terms of lattice energies given by eqn. (1). Now modified three body parameter $f_m(r)$ becomes

$$f_m(r) = f_{TBI}(r) + f_{cov}(r) \quad (2)$$

The relevant expressions of $f_{TBI}(r)$ and $f_{cov}(r)$ are given in our earlier work [5-7]. Now the entropy differences in the last term of Eqs. (1) can be calculated from the relation used by our earlier work [8].

For quantum espresso irreducible k-points are generated according to the Monkhorst-Pack scheme [9]. The Kohn-Sham single-particle functions were expanded on a basis of plane-wave set with a kinetic energy cut-off of 32 Ry. Brillouin-zone was sampled with $8 \times 8 \times 8$ k-point mesh, in order to get well converged ground state energy. The exchange and correlation effects have been treated within the generalized gradient approximation (GGA).

III. RESULTS AND DISCUSSION

The structural properties like phase transition pressure and volume collapse of TbTe are illustrated by calculating the lattice energies of B1 and B2 structure from present model. The structural phase transition pressure is calculated by minimizing the Gibbs free energies for the equilibrium lattice parameter for the B1-structure and B2-structures. The lattice energies U_{B1} and U_{B2} are obtained to calculate Gibbs free energy difference $G=(G_{B1}-G_{B2})$ at different pressures. This Gibbs free energy contains $[b, f_m(r)]$, the three model parameters. Using lattice parameter, the first space derivatives of the lattice energy (U) and equilibrium condition, these model parameters have been calculated [5-8]. The input parameters have been taken from [6]. Gibbs free energy difference G have been plotted with the variation of pressure in Fig. 1 for describing the phase transition pressure of TbTe. At the phase transition pressure a sudden collapse in volume takes place at the transition pressure. This discontinuity in volume of TbTe is presented in Fig. 2.

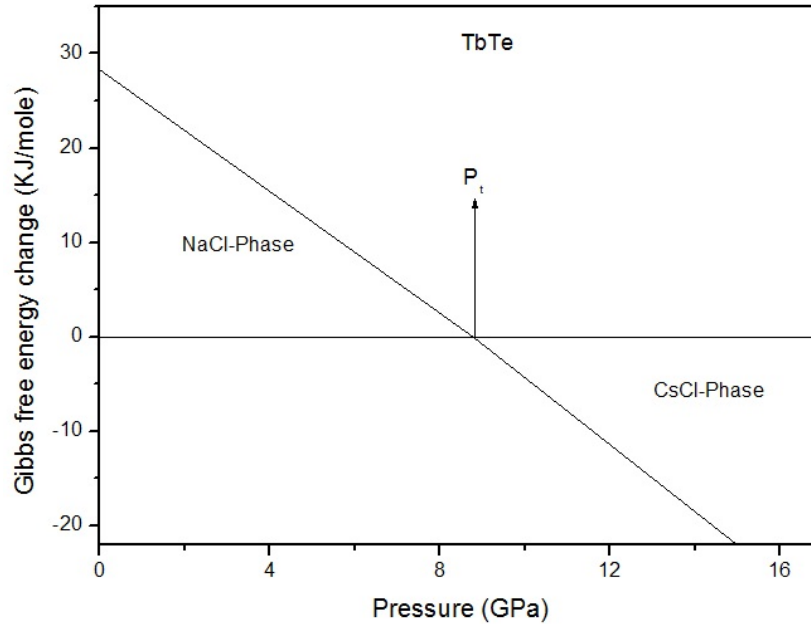


Fig. 1. Gibbs free energy change with pressure for TbTe.

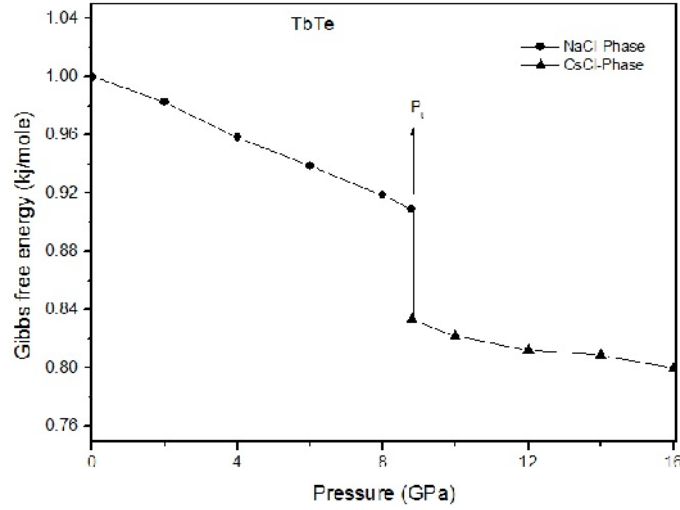


Fig. 2. Volume change with the variation of pressure for TbTe.

Basic self consistent field (SCF) methods are used for total energy calculations of large systems where the wave functions are used to evaluate second order and high order molecular properties. We have used, the first principles pseudopotential (PWSCF) method the calculation of phase transition pressure is carried out by estimating enthalpy in both the structures. These values of phase transition pressures and volume collapses from model (8.8 GPa and 8.9%) and first principle calculations (10.0 GPa and 9.5%) are tabulated in Table 1. These values are compared with other theoretical results of TbTe and are in good agreement with them [3].

Table 1: Phase transition and volume collapse of TbTe.

Crystal	Phase transition pressure (GPa)		Volume collapse (%)	
	Present	Others	Present	Others
TbTe	8.8 10.0	9.5 ^a	8.9 9.5	11.0 ^a

a-ref [3]

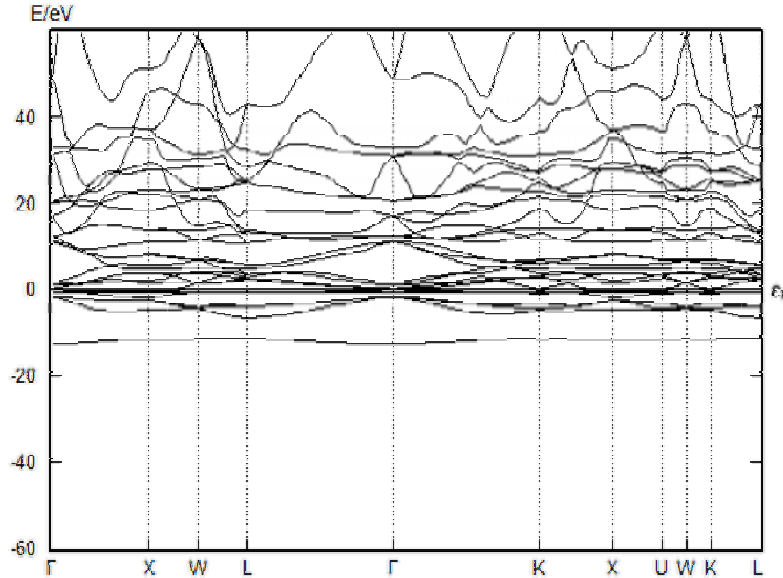


Fig. 3. Electronic Band structure (BS) of TbTe in NaCl phase.

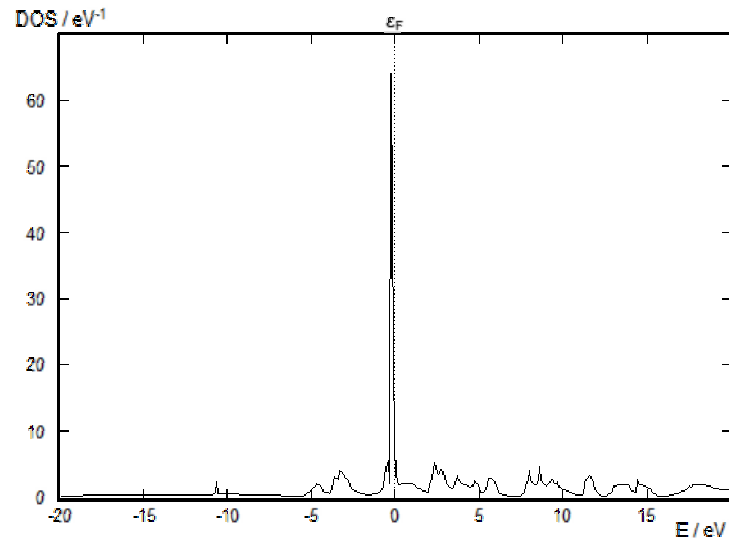


Fig. 4. Total density of States of TbTe in NaCl phase.

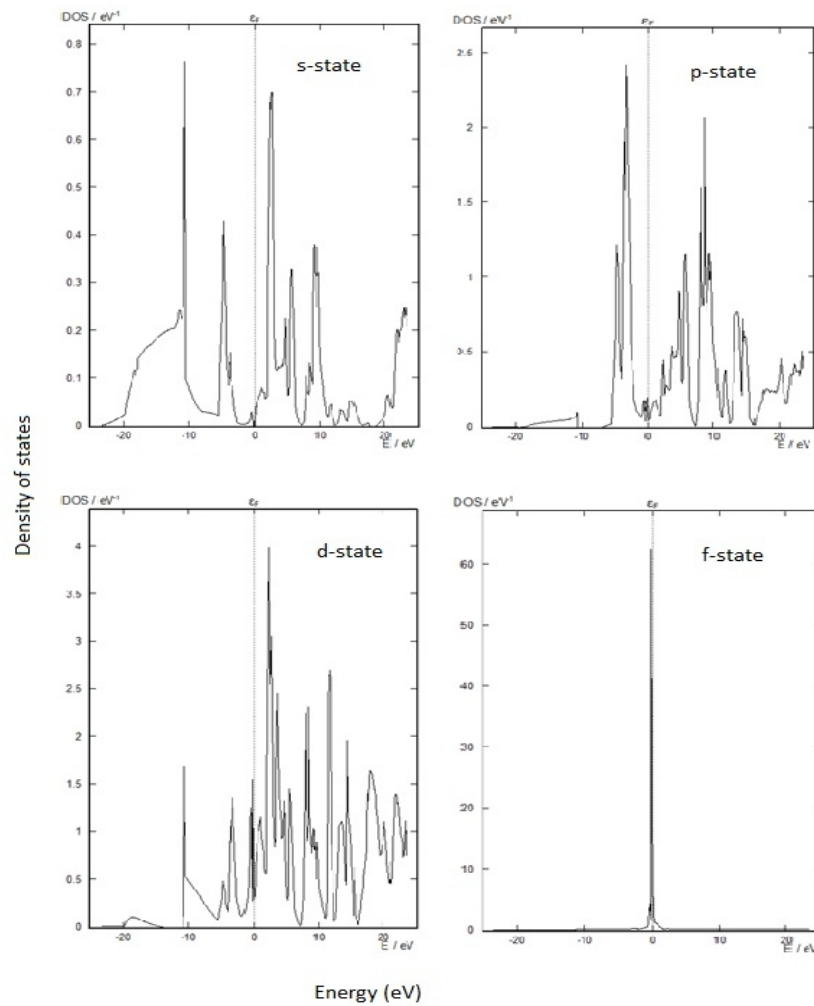


Fig. 5. Partial Density of state (PDOS) in the NaCl phase of TbTe in s, p, d and f states respectively.

To explore the electronic properties, we have studied the band structure (BS), density of states (DOS) and partial density of state (PDOS) of TbTe in NaCl-type structure. TbTe fit in to the large close of NaCl structured rare earth monochalcogenides. For TbTe, the electronic band structure (BS) and density of states (DOS) is presented in Fig. 3 and 4, respectively in the rock-salt phase under normal conditions. It is clearly seen that the bands are overlapped at the Fermi level. This behavior indicates the metallic nature of TbTe rare earth monochalcogenide in NaCl structure. For further studying the contribution of all the atoms in the electronic structure the partial density of states (PDOS) has been plotted.

These PDOS are presented in Fig. 5 for s, p, d and f states respectively. From PDOS it is clearly seen that the peaks are lie at -10eV and 2.5eV in s-state, -2.0eV and 9.0eV in p-state and -2.0eV in d-state respectively, while in f-state the peaks lie at Fermi level. The metallic behaviour of TbTe in NaCl phase is obviously seen due to f-state.

IV. CONCLUSION

For structural properties of the terbium telluride, the Realistic Interaction Potential Approach (RIPA) model has been applied. According this study, the present rare earth compound crystallizes in six fold coordinated NaCl-type structure at ambient conditions and under pressure, they transform to the eightfold-coordinated CsCl-type structure. At the NaCl to CsCl phase transition, the volume collapse discontinuity in pressure volume phase diagram recognizes the occurrence of first order phase transition. This study shows that the structural phase transition and volume collapses from

present model and first principle calculation are in good agreement with available data. In order to examine the electronic study, electronic band structure, density of state and partial density of states have been studied. On the basis of this it can be concluded that present compound shows the metallic nature in the stable NaCl-phase.

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