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Elastic Constants And Fermi Surface Topology change in Calaverite $AuTe_2$: A Density Functional Study

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Abstract. Structural, elastic, electronic and Fermi surface studies of $AuTe_2$ have been carried out by means of first principles calculations based on density functional theory. The calculated ground state properties agree well with the experiment. Fermi surface and elastic constants are predicted for the first time and from the calculated elastic constants we find the compound to be mechanically stable satisfying the stability criteria of monoclinic structure. In addition, we also find the c-axis to be more compressible than the other two which is also speculated from the present work. The metallic behaviour of this compound is confirmed from the electronic band structure calculation as we find the bands to cross the Fermi level (E_F). In addition, we also observe a FS topology change under pressure which is also explained in the present work.

Keywords: Electronic structure, Elastic constant, Fermi Surface
PACS: 31.15.-p; 62.20.D-; 71.18.+y.

INTRODUCTION

Gold telluride (or) Calaverite is a natural common gold bearing mineral besides native gold. The X-ray refinement study of the $AuTe_2$ confirms the average monoclinic distorted CdI_2-type structure with space group of C2/m symmetry[1]. Triest et al.[2] reported the electronic structure and photo electronic spectra of Calaverite. Apart from the numerous experimental reports there are other theoretical studies are available where authors explained the structural, electronic, and dynamical properties of $AuTe_2$ structure at ambient and high pressures.[3,4] In the present study we have calculated the Fermi surface and mechanical properties of $AuTe_2$ which are very vital in understanding minerals from different prospective.

METHODOLOGY

All the ground state properties and elastic constants calculations were performed using CASTEP[5] package which is based on plane wave pseudo potential method. The total energies are obtained based on Generalized Gradient Approximation of Perdew-Burke-Ernzerhof (GGA-PBE). A plane wave kinetic energy cut off of 620 eV is used. The first Brillouin zone of the unit cell is sampled according to the Monkhorst-Pack scheme with 10x10x9 k-mesh. The structural optimization was performed by relaxing all the atoms, volume of the unit cell with respect to the total energies, forces and stresses at ambient condition.

We have studied the electronic properties using full-potential linear augmented plane wave (FP-LAPW) method based on first-principles density functional calculations as implemented in the WIEN2k[6]. In this present study we have calculated the electronic band structure, density of states and Fermi surface with the inclusion of spin-orbit coupling. All our calculations are performed using the optimized parameters from the CASTEP calculation.

RESULTS AND DISCUSSION

The understanding of the structural stability and mechanical properties of any mineral is important and mandatory as they provide useful information required in the field of Earth sciences. For this reason we have calculated the band structure and mechanical properties of the $AuTe_2$. The calculated ground state properties agree well with the available experimental results.

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TABLE 1. Ground state lattice parameters of $AuTe_2$

Parameters	Present work	Exp.[7]
a (Å)	7.4536	7.182
b (Å)	4.2994	4.402
c (Å)	5.1550	5.056
β(Degree)	89.90	89.99
V ($Å^3$)	165.20	159.85
Te(u)	0.6652	0.6890
Te(w)	0.2867	0.2888

Electronic Structure And Fermi Surface

The calculated band structure along the high symmetry directions of the Brillouin zone and the density of states of $AuTe_2$ is illustrated with spin orbit coupling at zero pressure and are shown in Figure 1(a, b). The metallic nature of this studied compound is confirmed from the band structure plot as we find the two bands to cross the Fermi level and are shown in different color in the Figure 1(a). At zero pressure there are two Fermi surface corresponding to the two bands crossing the Fermi level as shown in Figure 2 (a, b) (green and blue color). The 1st surface is the hole sheet along Γ-Z direction (Figure 2(a)) and the second surface consists again hole pocket along Z-A and Z- Γ direction. More interestingly the pressure effect shows the FS topology change within the corresponding surface and are shown in Figure 2 (c, d). Under 1 GPa pressure we observe a new electron pocket to appear at Γ point in the first surface (see the blue color band) due the downward movement of the band and the corresponding FS is shown in Figure 2(c) and simultaneously we find the hole pocket to vanish in the second surface along the Z-A direction due to the upward movement of the band and is evident from the Figure 2 (d) (green color band). Again at 3 GPa pressure we have seen the hole surface to get connected in the 1st FS as shown in Figure 2 (e), and the second surface remain unaltered, which may further induce the structural transition in $AuTe_2$ as reported experimentally, where the authors have found the same at 2.5 GPa[9] and the pressure range agree well with our calculated pressure where we have seen the FS topology change. Overall we find the simultaneously upward and downward movement of the band for this compound resulting the FS topology change to occur.

The total density of states (DOS) along with the *l*-projected DOS is given in Figure 1(b). It can be clearly seen from Figure 1(b), that the total DOS contribution comes from both the atoms. From *l*-projected DOS it is evident that the maximum contribution arise mainly from the Au *5d* and Te *5p* states which imply the moderate hybridization existing between these two states there by indicating a possible covalence between them.

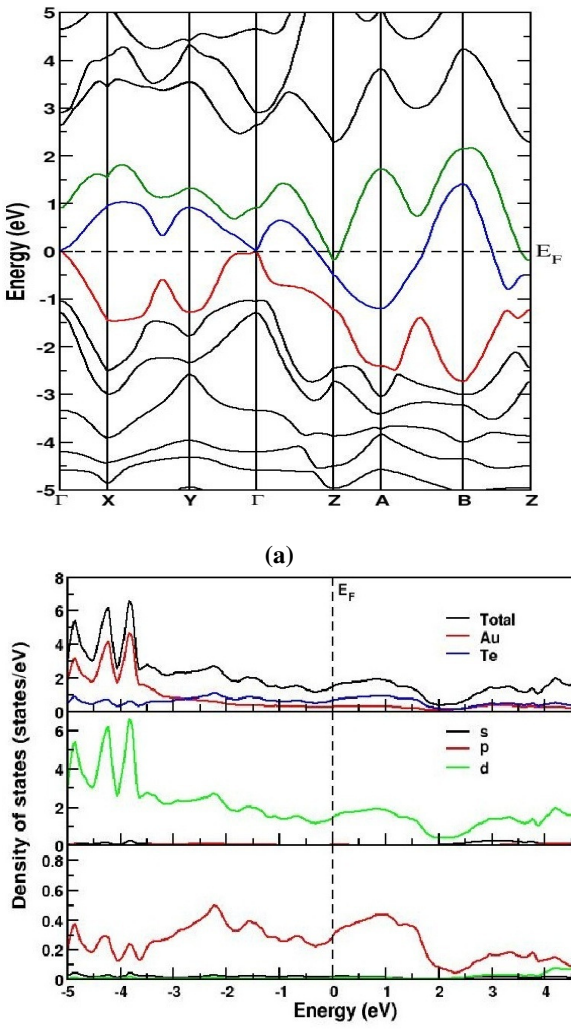

FIGURE 1. The (a) Band structure and (b) Density of states of $AuTe_2$.

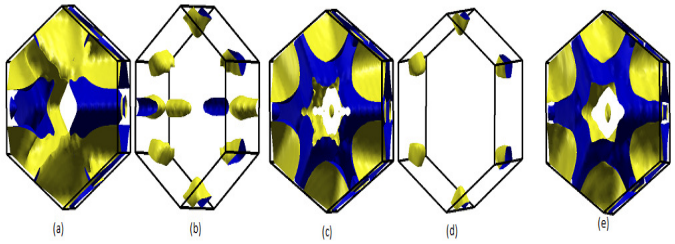

FIGURE 2. Fermi surface of $AuTe_2$ (a, b) 0 GPa (c, d) 1 GPa and (e) 3 GPa.

Elastic Constants

Elastic properties are fundamental for any crystalline material to describe its stiffness against applied strain. The investigated compound crystallizes in monoclinic space group, and it has 13 independent elastic constants. The calculated single crystal elastic constants (EC) at the theoretical equilibrium volume are tabulated in Table 2. The computed elastic constants satisfy the Born-Huang's mechanical stability criteria of monoclinic structure[7], implying $AuTe_2$ to be mechanically stable. From Table 2, it is quite evident that $C_{22}>C_{11}>C_{33}$, which shows that C_{22} is high in comparison with the other EC which indicate that particular axis to be more stiffer than the other axes. The calculated single crystal bulk modulus from elastic constants is found to be 47.20 GPa.

Conclusions

We have calculated the electronic, elastic and FS of $AuTe_2$. We find a change in the FS at 1 and 3 GPa. DOS reveal a strong covalent bond between the Au *5d* and Te *5p* states. EC confirm that c-axis is more compressible than other two axes.

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TABLE 2. Elastic constants of $AuTe_2$ in GPa.

C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}
100.1	101.1	52.5	18.0	20.0	24.8	47.4	40.0	-3.8	44.4	12.2	9.7	-7.1

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