THEORETICAL STUDY OF ELECTRONIC PROPERTIES OF Ag_2Te

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The electronic band structure and density of state calculations were performed for the low-temperature modification of a silver chalcogenide - β-Ag_2Te through Atomistic Simulation Software Quantum ATK. The structures are characterized by three, four and five coordinations of silver by the chalcogen. According to the band structure calculations, β-Ag_2Te is semiconductor with an about 0.1–0.2 eV forbidden zone. The calculations have shown that β-Ag_2Te has a very low DOS in the energy range from about –0.1 to +0.5 eV.

Keywords: electronic band structure, chalcogenide, density of state, silver, semiconductor.
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INTRODUCTION

Ag_2Te, one of silver chalcogenides, is known as Hessite mineral in nature. It was used as ionic conductor at high temperature phase. The zone structure of Ag_2Te was studied through local spherical wave (LSW) mathod. In accordance with the LSW calculation of the zone structure, this compound is semi-metallic having approximately $0,1 \div 0,2eV$ energy cover (forbidden zone). It undergoes a phase transition below 417K into the phase, a narrow gap semiconductor, where the ion migration is frozen and the compound is nonmagnetic. Ag_2Te changes from a regular structure to a chaotic structure at low temperatures. The transition temperature of Ag_2Te is 1450°C. The gap of β-Ag_2Te is in the range of several tens meV, the mobility of carriers is high and the effective mass is of the order of 102 m_0 (m_0 is the free electron mass) [1, 2].

It is known that the low-temperature (β) phases for Ag_2Te has large and positive magneto-resistance. This compound is non-magnetic. In order to understand the origin of magneto-resistance, it is important to have profound knowledge about its electronic structure.

The Ag chalcogenides are of great importance first of all due to the high ionic conductivity (of Ag+) of the high temperature (α) structure and electronic conductivity. The high ionic conductivity in the α phase of the Ag_2Te is due to the static distribution of silver atoms in the lattice. These compounds show a transition at rather low temperatures from the β structure to α structure. The transition temperature is 139°C for Ag_2Se and 145°C for Ag_2Te [3].

The electrical transport properties of Ag_2Te have been extensively studied and reported [4-7]. In these studies, a very small temperature range is studied and the phase transition environment is studied. According to the results of the band structure calculations it is small gap (20-50 meV) semiconductor. The deviation from stoichiometry determines both the electronic conductivity and activation energy. The mobility of electrons and holes is high with small effective mass. Concentration of electron - carriers is about $3 \times 10^{18} cm^{-3}$. Earlier, the lattice parameters of β-Ag_2Te were calculated by Van der Lee, A. and J.L. de Boer. Lattice parameters and coordinates of β-Ag_2Te are from an accurate single crystal refinement by the mentioned researchers [7].

RESULTS

In this article the electronic band structure and density of state were calculated for β-Ag_2Te using the Atomistic Simulation Software Quantum ATK method [8].

Figure 1 shows the atomic structure of β-Ag_2Te. As it can be seen from the figure, the extraordinary superconducting properties of β-Ag_2Te is associated with these linear chains of Ag atoms.

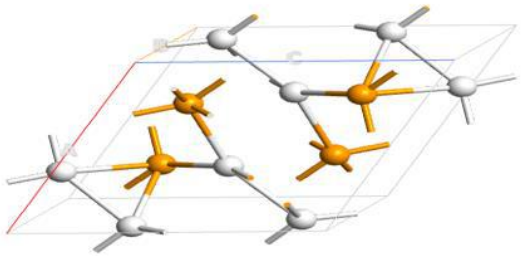

Fig. 1. Atomic structure of β -Ag_2Te.

Besides the metal–chalcogen distances corresponding to bonding, there are also metal-metal-distances as in pure metals. Table 1 presents the interatomic distances for β-Ag_2Te. β -Ag_2Te has two types of silver atoms in its structure. Both types of Ag atoms have a four-fold coordination by Te atoms. The Ag-Ag distances range from 2.84 to 3.13 Å. The chalcogen packing is distorted face-cantered cubic.

The band structure of β-Ag_2Te plotted for high symmetry points Γ-X- M-Γ-R-X at T=300K is given in figure 2. The band structure calculated based on density functional theory within spin-polarized PBE-GGA approximation.

Figure 3 presents some calculated results of the density of state (DOS) constructed for *s*-, *p*- and *d*-electrons of β-Ag_2Te.

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Table 1.

Interatomic distances between atoms in β-Ag_2Te crystal ($\AA$)

Ag(1)-Te	2.877	2.895	2.965	3.016
Ag(2)-Te	2.842	2.905	3.011	3.034
Ag(1)- Ag(1)	2.841	3.010	-	-
Ag(2)- Ag(2)	3.053	-	-	-
Ag(1)- Ag(2)	3.061	3.133	2.909	

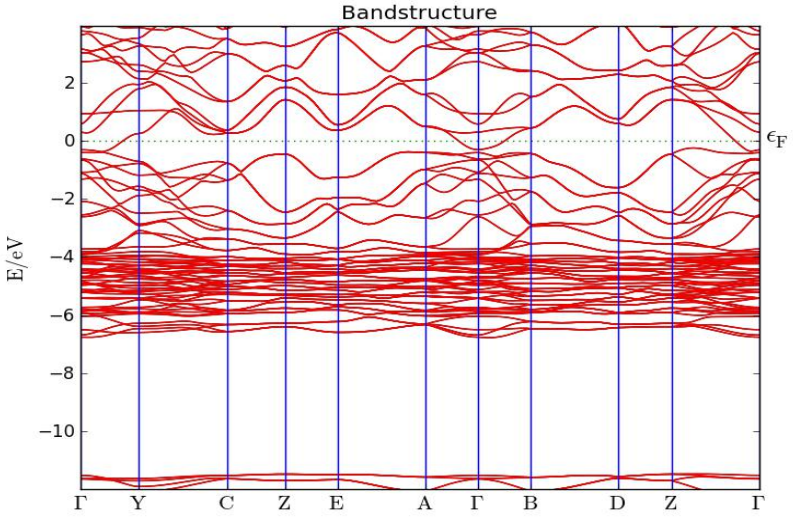
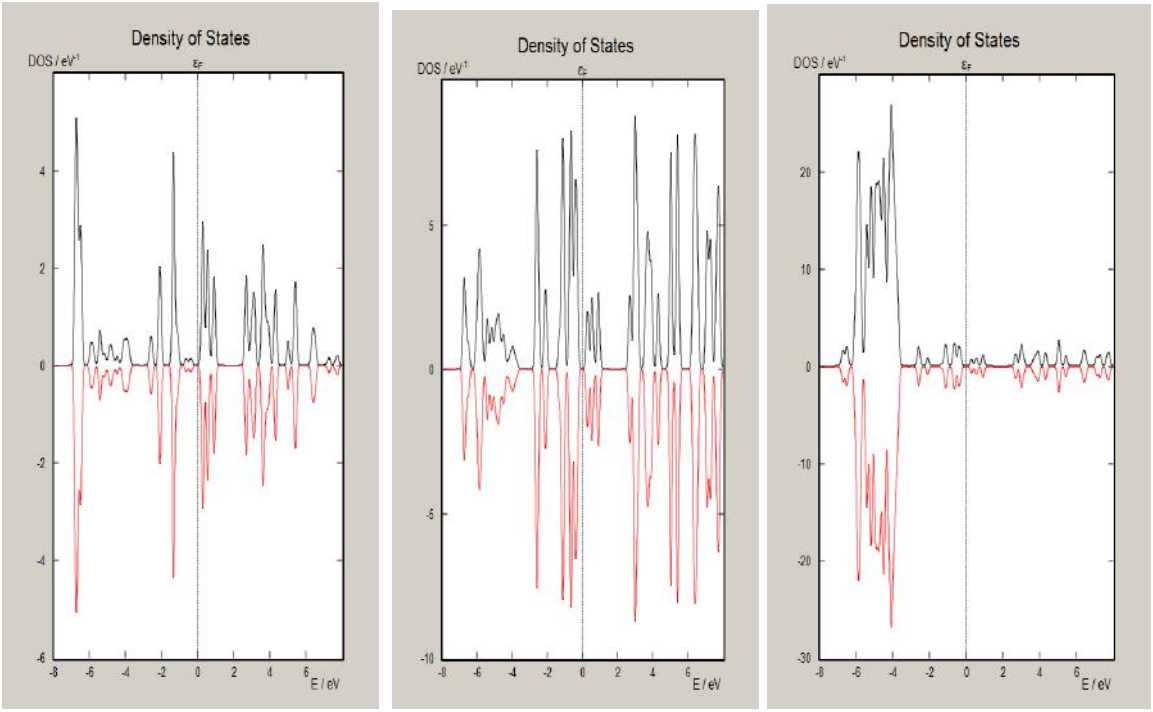


Fig. 2. Electronic band structure of β-Ag_2Te.



a b c

Fig. 3. DOS for *s- (a); p-(b)* and d-(c) electrons of β-Ag_2Te.

CONCLUSION

The electronic band structure and density of state were calculated for low temperature β-Ag_2Te using the Atomistic Simulation Software Quantum *ATK* method It was found that the extraordinary superconducting properties of β-Ag_2Te is associated with the linear chains of Ag atoms. There is a small overlap between the conduction and valence band of β-Ag_2Te. In addition, DOS was calculated for *s- (a); p-(b)* and d-(c) electrons of β-Ag_2Te.

Based on the calculations, we can say that β-Ag_2Te have a very low *DOS* in the energy range from about –0.1 to +0.5*eV*.

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