JOURNAL OF BAKU ENGINEERING UNIVERSITY - PHYSICS
2025. Volume 9, Number 1 *Pages 17-21*

UDC 621.315.592.541.65
DOI: https://doi.org/10.30546/09081.2025.001.8008

BAND STRUCTURE OF $TlInSe_2$ AND $InGaTe_2$ TRIPLE COMPOUNDS

U.S. ABDURAHMANOVA

Baku Engineering University,

Bakı, Azerbaijan

E-mail: uabdurahmanova@beu.edu.az

ARTICLE INFO

Article history
Received:2025-09-18
Received in revised form:2025-07-04
Accepted:2025-07-14
Available online

Keywords:
triple compounds, tetragonal syngony, band structure, semiconductors.

ABSTRACT

In this research work we present the results of calculations of energy spectra and band structure of $TlInSe_2$ and $InGaTe_2$ triple compounds crystallized in the tetragonal syngony. For calculations we used pseudopotential method and functional density theory in the approximation of the combined gradient using LAPW method and WIEN 2K program code. Some properties of these compounds are determined based on their band structure. It is known that search for new semiconductor materials is usually carried out in the direction of expansion of the group of crystal structure of already known materials. In particular, study of crystal structure of TlSe showed that this phase is distinguished by extreme specific features. TlSe lattice turns out to be composed of two independent structural units - from octahedron with ionic bond Tl^{+}- Se and tetrahedron with covalent bond between Tl^{3+}-Se and therefore chemical formula of TlSe should be written as $Tl^{+}Tl^{+3}Se_2$. Thus, by replacing the trivalent thallium atom with corresponding trivalent atoms, in particular, gallium and indium, in the TlSe lattice, a new class of semiconductor compounds of the $A^{III}B^{III}C_2^{VI}$ type was obtained.

1. Introduction

The great interest in type $A^{III}B^{III}C_2^{VI}$ compounds is that they do not have pairs of valence electrons, the chemical bond is strongly asymmetric, the crystal structure has special features, and the chemical composition is managed within a certain crystal structure.

The crystal structures, electrophysical, thermal-physical, optical and photoelectric properties of the mentioned type crystals have been studied and the research in this direction is systematically continued [1- 3].

By studying the possibilities of applying these compounds, it was determined that compound $TlInSe_2$, which is a typical representative of the mentioned compounds, has high sensitivity in the visible and near- infrared parts of the spectrum, memory switching properties, and tenso sensitivity. It was determined that $TlInTe_2$ and $TlGaTe_2$ compounds which are structural analogues of this group, have high tenso-sensitivity and memory switching properties.

Triple semiconductor compounds are characterized by their specific characteristics. $TlSe$ -type crystals also have the possibility of wide application in semiconductor tensometry. Compound $TlInSe_2$ is particularly promising in this regard. It has very high strain sensitivity, which can be increased and controlled depending on temperature, deformation, and the effect of electromagnetic waves.

X-ray structural studies have shown that some of the triple semiconductor compounds of $A^{III}B^{III}C_2^{VI}$ type have a chain structure, while the others have a layered structure [4]. The results of X-ray phase analysis showed that solid solutions based on compounds $TlInSe_2$ and $InGaTe_2$ crystallize in the tetragonal syngony [5]. The change of lattice constants of $TlInSe_2$ in the solubility regions depending on the composition mainly obeys Vegard's law.

The calculation of the energy spectrum using modern methods and programs, system analysis, identification of the results of compounds of the $A^{III}B^{III}C_2^{VI}$ type having a chain crystal structure have not been carried out before. Some properties, obtaining methods, growing technologies of the monocrystals of these type compounds have been determined [7-10].

In this work the results of calculation of energy spectra of $TlInSe_2$ and $InGaTe_2$ compounds are presented.

Results of the studies of $TlInSe_2$ compound show that, the upper level of the valence band of this compound is at the T_1 point and the lower level of the conduction band is located at the border of the Brullien zone of the volume-centered tetragonal lattice. However, indirect transitions are possible in this compound. Direct transition is not possible according to the selection rule. From these calculations, the following values were obtained for direct and indirect transitions in $TlInSe_2$: $\Delta E(indirect) = 1{,}21eV$ and $\Delta E(direct) = 1{,}3eV$ (figure 1).

The valence band can be divided into three groups depending on their composition and nature [12-14].

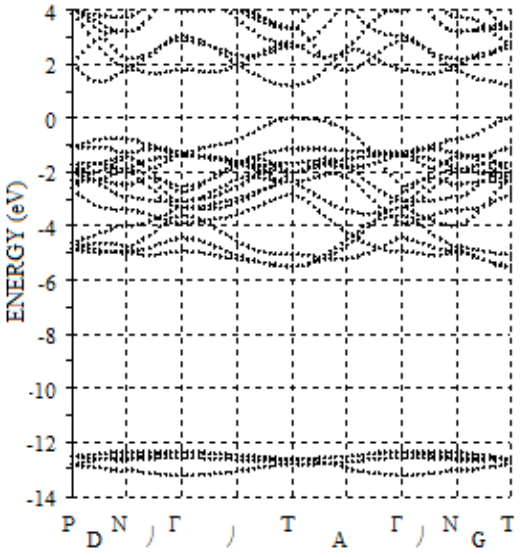

Figure1. Band structure of $TlInSe_2$

The energy spectrum of $TlInSe_2$ was calculated using the pseudopotential method. It was found that the top of the valence band is located at the highly symmetric point T on the surface of the Brillouin zone and the irreducible image corresponds to T3, and the bottom of the conduction band is located on the line D in the middle between the points P (π/α, π/α, π/c) and N (π/α, π/α,0), corresponding to the irreducible representation D1.

The transition with the lowest energy occurs between the states T3 and T4 and is forbidden in the dipole approximation. The width of the forbidden band obtained from calculations is about 1 eV. The valence band can be conditionally divided into three groups:

- The lowest group with four bands near -12.6 eV owes its origin to the 4s-states of Se.
- Another group of four bands in the region of –(4÷5.5) eV is associated mainly with the 6s-state of Tl atoms and the 5s-state of In.
- The upper group of ten bands in the region of (0÷3.5) eV is formed mainly by the 4p-state of Se atoms, the 6p-state of Tl atoms and the 5p-state of In atoms.

The data on the origin of the bands agree with the results of work, in which the photoemission spectra were studied and the band structure of $TlInSe_2$ was calculated using the plane wave addition method.

The theoretical conclusion of the work, which showed the presence of an isolated group consisting of two zones of the upper part of the valence band of the semiconductor compound $TlInSe_2$, was not confirmed in this work and in the work. Probably, this is due to the incorrect consideration of the screening of pseudopotentials inherent in the empirical method.

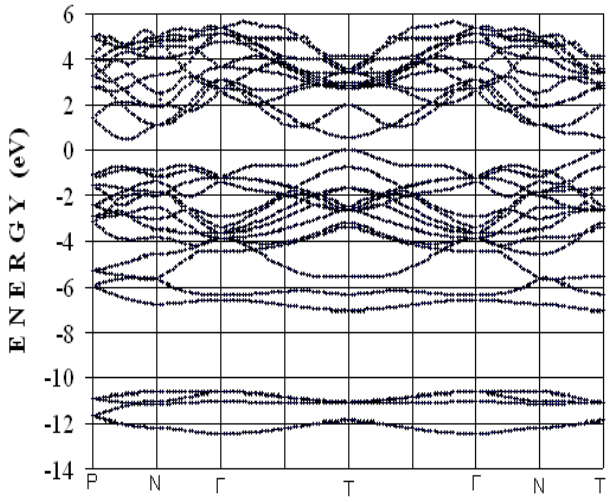

Figure 2. Band structure of $InGaTe_2$

The calculation of the electron spectrum of $InGaTe_2$ was carried out at the symmetric points G, T, N, P and along the lines connecting these points. The results of the calculation of the band structure are presented in figure 2. The valence band of $InGaTe_2$ consists of three subbands.

The lower group, consists of four bands, is separated from the others by a wide energy gap of ~6 eV. The group-theoretical analysis shows that these lower valence bands, located near -10÷11eV, owe their origin to the 5s- state of Te.

The next group of tetravalent bands, located at the energy level of about -5 eV, arises mainly from the *s*-states of In and Ga atoms.

The third large group of ten bands with a width of 5 eV is due to the *p*-states of In, Ga and Te atoms.

According to conducted calculations, the band gap is determined as 0.56 eV.

2. Methodology

The pseudopotential method is one of the main methods for calculating the energy spectrum of charge carriers in semiconductors [6,15]. The energy spectrum of $TlInSe_2$ one of the base samples

of $A^{III}B^{III}C_2^{VI}$ types of compounds, was calculated using the pseudopotential method. At this time, the analytical expression proposed by Konstantinov and others was used for atomic pseudopotentials. The form factors of ion potentials proposed by them consisted of 4 parameters

The idea of the pseudopotential method is first encountered in the work of Philips. In their work, Phillips and Kleinman developed the pseudopotential method and gave it a more rigorous formulation. In all cases, the pseudopotential theory is based on three fundamental physical approximations.

1. The first approximation is the self-consistent field approximation. In this approximation, the interaction between electrons is described by some average potential, which itself depends on the states of the electrons, and the electron states are in turn determined by the average potential.

2. In the second approximation, all electron states are divided into inner shells and conduction band states, and it is assumed that the wave functions of the inner shells are strongly localized.

3. The third fundamental approximation is the use of perturbation theory for electrons in the conduction band.

The electronic band structure of the $InGaTe_2$ crystal was determined at the symmetric points and lines of the Brillouin zone of the $InGaTe_2$ crystal using the LAPW method in the Density Functional Theory approximation and the WIEN2k software package and the results were analyzed. The Generalized Gradient Approximation (GGA) was used as the exchange-correlation potential.

For this purpose, the lattice parameters and atomic coordinates were first determined from first principles (ab-initio) by minimizing the energy and Hellman–Feynman forces.

To calculate the band structure of $InGaTe_2$, the optimized values of the lattice parameters a=8.3945 Å; c=6.8352 Å and the chalcogen parameter x=0.1730 were taken.

3. Conclusion

The band structure of $TlInSe_2$ compound was studied using the pseudopotential method, and the band structure of $InGaTe_2$ compound was studied using density functional theory. As a result of the studies, it was determined that, the valence band can be divided into three subgroups.

The valence band can be conditionally divided into three groups:

The lowest group with four bands near -12.6 eV is formed from the *4s*-states of Se, the next group of four bands (4÷5.5 eV) is releated to the *6s*-state of Tl and the *5s*-state of In atoms. The upper group of ten bands in the region of 0÷3.5 eV is formed by the *4p*-state of Se atoms, the *6p*-state of Tl atoms and the *5p*-state of In atoms.

Studies of the band structure of the $InGaTe_2$ compound represent that it was calculated using density functional theory and the valence band of the $InGaTe_2$ compound consists of three groups. The lowest group consists of 4 bands located at a distance of ~ 6 eV from the others. Theoretical-group analysis shows that these bands, located around –11 eV÷–10 eV, arise from the 5s states of tellurium atoms, the next group of 4 bands is located at the –5 eV level and arises from the *s*– states of indium and gallium atoms. The group of 10 bands with a width of 5 eV arises from the *p*– states of In, Ga and Te atoms.

REFERENCES

1. Müller D., Eulenberger G., Hahn H. (1997) Uber Tirnare Thallium-Chalkogenide Mitthalliumselenide Structures // Z. anorg. allg. Chemie, V. 398, №2, p. 207-220.
2. Mobarak M., Berger H., Lorusso G.F. et al. (1998). The Growth and Properties of Single Crystals of $GaInTe_2$, a Ternary Chalkogenide Semiconductor // J.Physics D: Appl. Physics, V. 31, №12, p. 1433-1437.
3. Gashimzade F.M., Orujov G.S. (1980). Calculation of the energy spectrum of electrons of ternary semiconductor compounds with the structure of thallium selenide // Azerb. USSR, v. 36, №12, p. 18-23.
4. Guseinov G.D., Mooser E., Kerimova E.M. et al. (1969). On some properties of $TlInS_2$(Se_2, Te_2) syngle crystals // Phys. Stat. Sol., v.34, p.33-44
5. Gojaev E.M., Jafarova S.R., Gulmammadov K.D., Mammadov E.M., Osmanova S.S., (2009). Synthesis and growth of TlInSe2 and TlGaSe2 single crystals // Inorganic materials, v. 45, №7, p.790-792.
6. Xeyne V., Koen M.L., Ueyr D., (1973). Pseudopotential theory, Moscow, «Mir», 557 pp.
7. Gojaev E.M, Orujov G.S., Kerimova R.A., and etc. (2006). Band structure and optical properties of the chain compound $TlInTe_2$ // Solid State Physics, v.48, № 1, p.40-43.
8. Abdurahmanova U.S., (2022). Synthesis and photoconductivity of crystal $InGaTe_2$ Journal of Physics, Baku Engineering University, Baku, Azerbaijan, ISSN 2521-6368, vol 6, No2, p. 72-77.
9. Orudzhev G., Mamedov N., Uchici H. et al. (2003) Band Structure and Optical Function of TernaryChain $TlInSe_2$ // J. Phys. Chem. Solids. V. 64. P. 1703.
10. Gonze X., Beuken J.M., Caracas R. et al. (2002) First_Principles Computation of Material Properties: the ABINIT Software Project // Allan. Comput. Mater. Sci. V. 25. P. 478–492.
11. Gojaev E.M, Jafarova Q.S., Safarova S.I., (2013), Band structure of TlInTe2 and thermal efficiency of solid solutions based on it // Thermoelectricity. № 1. p. 28–33.
12. Lencer D., Salinga M., Wuttig M. (2011) Design Rules for Phase change Materials in Data Storage Application // Adv. Mater. T. 23. № 18. C. 2030–2058.
13. Vinoqradov E.A., hasanli H.M., Javadov B.M., Tahirov V.I., (1979) Infrared reflection spectra of layered single crystals TlGaTe2, TlInTe2 and TlInSe2//SSP. v. 21. № 9. p. 2793–2796.
14. Navikova S.I., (1972), "Solid State Physics and Thermodynamics", Novosibirsk, p.56
15. Bachelet, G.B., Haman D.R., Shlüter V., (1982), Psevdopotensials that work: from H to Pu//Physical Review B, 26, N 8, 4199-4228