

Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

Procedia Engineering 8 (2011) 2–7

---



---

Engineering  
**Procedia**


---



---

2<sup>nd</sup> International Science, Social-Science, Engineering and Energy Conference 2010:  
 Engineering Science and Management

## Study on Electronic Structure of $\beta$ - $\text{In}_2\text{Te}_3$ Thermoelectric Material for Alternative Energy

Athorn Vora-ud<sup>a,\*</sup>, Chanchana Thanachayanont<sup>b</sup>, Suwit Jugsujinda<sup>a</sup>,  
 Vittaya Amornkitbamrung<sup>c</sup> and Tosawat Seetawan<sup>a</sup>

<sup>a</sup> Thermoelectrics Research Center and Program of Physics, Faculty of Science and Technology, Sakon Nakhon Rajabhat University, 680 Nittayo Rd., Muang District, Sakon Nakhon, 47000, Thailand

<sup>b</sup> National Metal and Materials Technology Center, National Science and Technology Development Agency, 114 Thailand Science Park, Phahonyothin Rd., Klong 1, Klong Luang, Pathumthani, 12120, Thailand

<sup>c</sup> Integrated Nanotechnology Research Center and Department of Physics, 123 Mitrapab Rd., Faculty of Science, Khon Kaen University, Khon Kaen, 40002, Thailand

**Elsevier use only:** Received 15 November 2010; revised 15 December 2010; accepted 20 December 2010

---

### Abstract

The objective of this research was simulated the electronic structure of  $\text{In}_2\text{Te}_3$  thermoelectric material by using discrete variational- $X\alpha$  (DV- $X\alpha$ ) cluster models method based on LCAO and HFS approximation for porbability of alternative energy. The Zineblende  $\text{In}_{32}\text{Te}_{14}$  cluster model was designed by using 216 space groups and atomic positions (x, y, z), Te (0, 0, 0) and In (0.25, 0.25, 0.25). The cluster model, energy level, density of state, bond overlap contour map were simulated and analyzed. The cluster model was obtained the values of energy gap of 1.52 eV, agree well with literature data and good thermoelectric material for alternative energy.

© 2011 Published by Elsevier Ltd. Open access under [CC BY-NC-ND license](http://creativecommons.org/licenses/by-nc-nd/3.0/).

**Keywords:** Electronic structure; Thermoelectric material;  $\text{In}_2\text{Te}_3$ ; DV- $X\alpha$  method; Alternative energy

---

### 1. Introduction

Indium telluride ( $\text{In}_2\text{Te}_3$ ) is semiconductor material for alternative energy such as nuclear materails [1] and thermoelectric materials [1]-[4] and other applications are composed digital electronic device [5], gas sensor [6] and strain gauge [7]. The two crystal phases of  $\text{In}_2\text{Te}_3$  are composed  $\beta$ - $\text{In}_2\text{Te}_3$  phase and  $\alpha$ - $\text{In}_2\text{Te}_3$  phase [3] form the X-ray studies have shown that it crystallizes in two polymorphic modifications [8]-[11]. The high temperature phase (above 523K) is a disordered  $\beta$ - $\text{In}_2\text{Te}_3$ , which has a defect Zinblende structure [12] and the low temperature  $\alpha$ - $\text{In}_2\text{Te}_3$  phase belong to the defect fluorite structure [13] with lattice parameter of  $a = b = c = 6.16 \text{ \AA}$  [2], [4] and  $a =$

---

\* Corresponding author. Tel.: +664-297-0295; fax: +664-297-0295  
 E-mail address: [tosawatseetawan@yahoo.com](mailto:tosawatseetawan@yahoo.com)

$b = c = 18.54 \text{ \AA}$  [3], [4], respectively.  $\text{In}_2\text{Te}_3$  is cubic symmetry [14] and the semiconducting properties have been widely studied during the last few decades [15] which it is interesting for photoconducting properties [16], [17] and also for its switching and memory effects [18], [19] is found to have two modifications labelled as  $\alpha$  and  $\beta$  corresponding to low and high temperature formation, respectively [20], [21]. The structural model is a network structure of distorted tetrahedral  $\text{InTe}_3$  units, which are composed an In atom and three Te atoms bound to the In atom, with neighbouring units sharing a Te atom [22]. In addition,  $\text{In}_2\text{Te}_3$  compounds with very interesting electrical and optical properties for eventual use in solar cell detectors [23]. Against this background, we focused attention study on electronic structure of  $\beta\text{-In}_2\text{Te}_3$  phase because and it has thermoelectric properties more than  $\alpha\text{-In}_2\text{Te}_3$  phase such as, the  $\alpha\text{-In}_2\text{Te}_3$  phase has Seebeck coefficient of 137, 148, and  $162 \mu\text{VK}^{-1}$  at 323, 343, and 363 K, respectively [3], part  $\beta\text{-In}_2\text{Te}_3$  phase has large Seebeck coefficient about  $400 \mu\text{VK}^{-1}$  at 600 K [2] and it has natural nanostructure and low thermal conductivity properties [2], [24], [25] for good thermoelectric generation and alternative energy. However, the electronic structures of  $\beta\text{-In}_2\text{Te}_3$  phase the semiconductors have a few reported and unclearly such as, energy level and density of state etc.

In this work, we are simulated the electronic structures of  $\text{In}_2\text{Te}_3$  by DV-X $\alpha$  method. The electronic structures are composed of spin energy level, density of state, bond overlap and contour maps and analyzing to determine energy gap and chemical bonds of cluster model.

## 2. Computational Details

The steps of computational detail of DV-X $\alpha$  method is showed more carefully by *T. Seetawan et al.* [26]. Firstly, the simulation electronic structures of  $\text{In}_2\text{Te}_3$  is designed the unit cell volume by using ordinary data of the crystal structure of  $\text{In}_2\text{Te}_3$  with lattice parameters of  $a = b = c = 6.16 \text{ \AA}$ , the space group of  $216(F-43m)$  [2], [4], [27] and position atoms [27]. The atoms is generated random for stuffing atoms to unit cell. The cluster model is designed by deleting atoms base on unit cell and checking symmetry of cluster model. The orbitals of cluster model are calculated from symmetry by using Symorb [28] for easy in simulation with DV-X $\alpha$  method which assuming the Hartree-Fock-Slater approximation [29-31]. The exchange-correlation between electrons,  $V_{XC}$ , is expressed using Slater's X $\alpha$  potential [32] is  $V_{XC} = -3\alpha [3\rho(r)/8\pi]^{1/3}$ , where  $\rho(r)$  is the electron density at position  $r$ , the parameter  $\alpha$  is fixed at 0.7, and the self-consistent charge approximation is used in calculation. The matrix elements of the Hamiltonian and the overlap integrals are constructed by a linear combination of numerically generated atomic orbitals (LCAO). The DV-X $\alpha$  calculations is carried out using a personal computer which consists of AMD sempron of 2.45 GHz, 850 chipset and 2.00 GB DDR2. The used atomic orbitals are 1s, 2s, 2p, 3s, 3p, 3d, 4s 4p, 4d, 5s and 5p for In and Te atoms.

## 3. Results and Discussion

The  $\text{In}_{32}\text{Te}_{14}$  cluster model was showed in Fig. 1. The  $\text{In}_{32}\text{Te}_{14}$  cluster model was showed (a) 100, (b) 111, (c) 210 and (d) 221 planes and polyhedron which these plane is principle plane as can be observing by XRD technique [8]-[11] and highest symetries of 26 (Td) which agree with cubic symmetry [14]. The total charge, Dipole and Quadropole of cluster model are  $(\text{In}_{32}\text{Te}_{14})^{68}$ ,  $0.17764\text{E-}14$  and  $0.28459\text{E+}04$  which interest for investigation to studying the behavior of the thermopower and magnetoresistance, which characterize the carrier concentration [1]. The cluster model and related parameters were further analyzed of the energy levels and density of states spin orbitals by Mulliken population analysis [29]-[32]. The partials spin energy level were composed of In 4d, In 5s, In 5p, Te 4d, Te 5s and Te 5p orbitals and total spin energy level of cluster model as shown in Fig. 2.

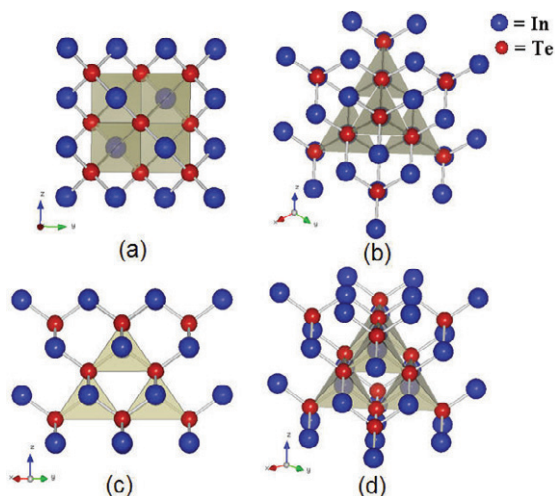


Fig. 1  $\text{In}_{32}\text{Te}_{14}$  cluster model show (a) 100, (b) 111, (c) 210 and (d) 221 planes

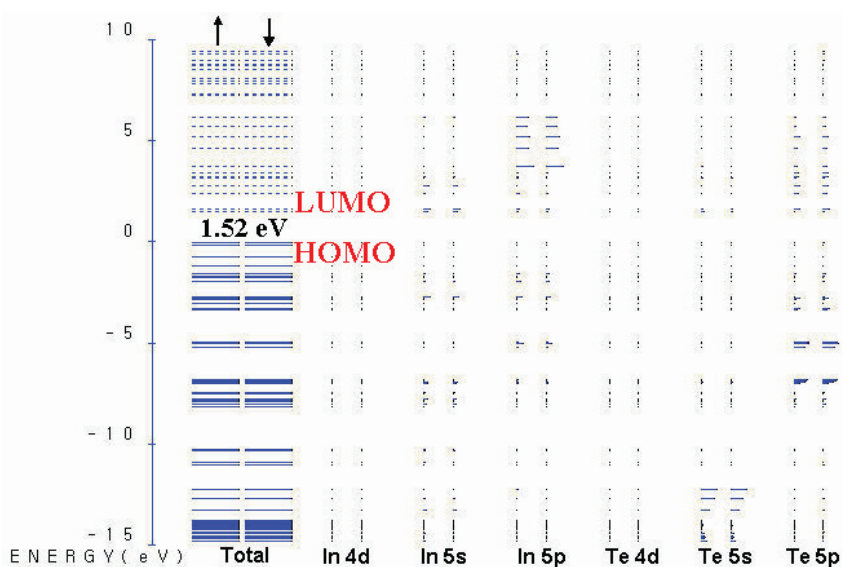


Fig. 2 The partial and total energy level spin orbitals of  $\text{In}_{32}\text{Te}_{14}$  cluster model

The cluster model has characteristic band gap energy which obtained between conduction band (dash line) or the highest occupied molecular orbital (HOMO) which energy level is zero and valence band (solid line) or lowest unoccupied molecular orbital (LUMO) of total energy level.

The energy gap was related to the conductivity of the cluster models found the difference between the lowest energy level of the conduction band and the highest energy level of the valence band. The energy gap of  $\text{In}_2\text{Te}_3$  is 1.52 eV agreed the literature data of 1.5 eV [33] and 1.58 eV [34] which it is direct gap [3] and the reported of optical gap 1.02, 1.07, 1.125 and 1.165 eV at 300, 473, 523 and 573 K [35], respectively were optical properties for eventual use in solar cell detectors [23]. The gap enhancement can be achieved with doping transition atom with energy-narrow d states form virtual bound states with the conducting electrons, resulting in sp-d hybridization [36]. The partial and total density of state spin orbitals were showed in Fig. 3. Figure 3 was composed density of state spin orbitals (a) partial In 5s orbitals, (b) partial In 5p orbitals, (c) partial Te 5s orbitals, (d) partial Te 5p orbitals and (e) all orbitals and total density of state spin orbitals. The bond overlap population between In and Te atoms was showed in Fig. 4. The bonding and anti-bonding orbital of In and Te atoms dependence on energy level which

bonding is valence band and anti-bonding is conduction. Bond order of 1 In-5Te, 1In-7Te and 1In-23Te are 0.249, 0.513 and 0.333, respectively, which indicate by summation of bonding and anti-bonding values.

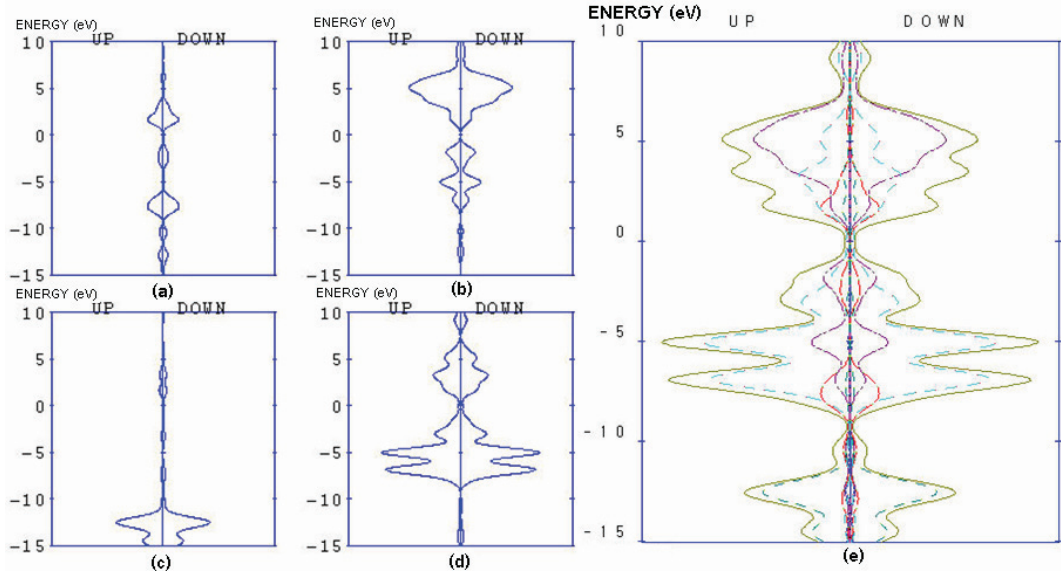


Fig. 3 the partial and total density of state spin orbitals of  $In_{32}Te_3$  cluster (a) In 5s, (b) In 5p, (c) Te 5s, (d) Te 5p and (e) all orbitals and total.

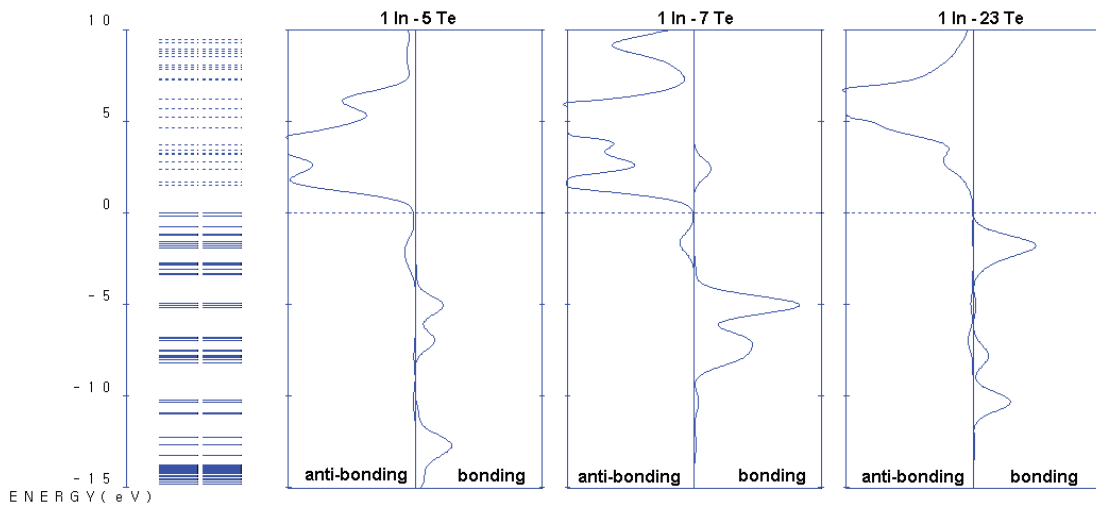


Fig. 4 bonding and anti-bonding orbital of In and Te atoms 1In-5Te, 1In-7Te and 1In-23Te

The contour map of total electron density and wave function number electron density are W86, W87 and W88 as shown in Fig 5. These wave function numbers were interacted atomic orbital which corresponding to  $In_{32}Te_{14}$  cluster model in 210 plane in figure 1 (c).

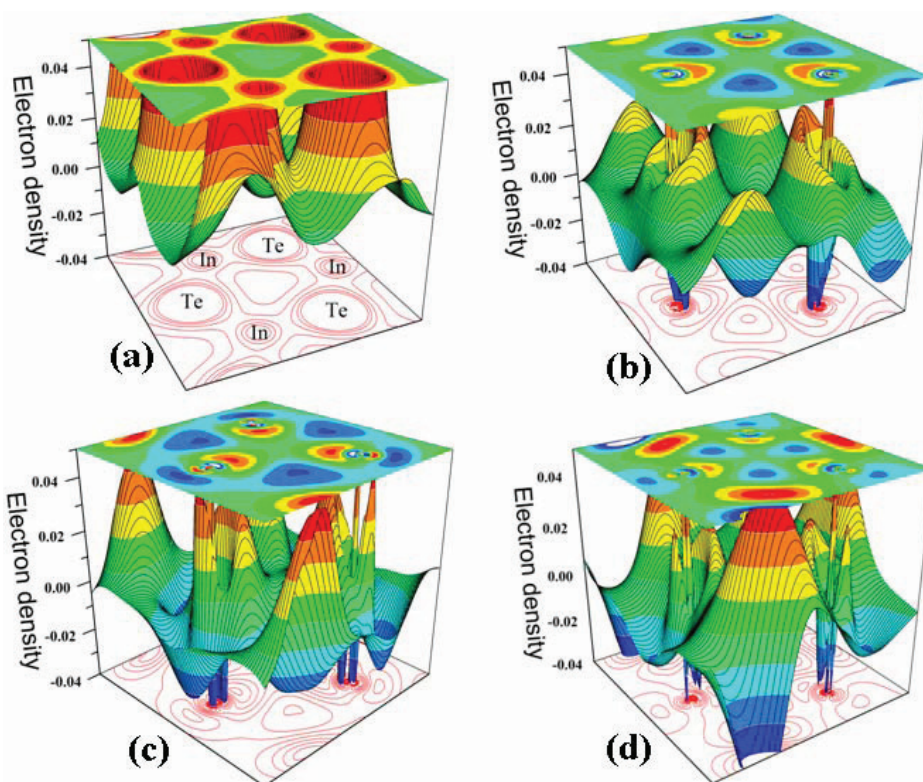


Fig. 5 Contour map electron density of In and Te atom (a) total, (b) W86, (c) W87 and (d) W88 wave function numbers

#### 4. Conclusion

The electronic structure of  $\text{In}_2\text{Te}_3$  was simulated by DV-X $\alpha$  method compose of the cluster model, energy level, density of state, bond overlap contour map. The energy gap of  $\text{In}_2\text{Te}_3$  is 1.52 eV agreeing the literature data. Bond order of 1 In-5Te, 1In-7Te and 1In-23Te are 0.249, 0.513 and 0.333, respectively. The contour maps of electron density were interacted atomic orbital which corresponding to  $\text{In}_{32}\text{Te}_{14}$  cluster model in 210 plane. The  $\text{In}_2\text{Te}_3$  was good thermoelectric material for alternative energy

#### Acknowledgement

The financial support from Thailand Graduate Institute of Science and Technology, NSTDA (TGIST: TG-33-99-52-037M) is gratefully acknowledged.

#### References

- [1] V.V. Shchennikov, K.V. Savchenko and S.V. Popova: Phys. Solid. State. vol. 42, no.6, pp. 1036-1040, 2000.
- [2] S. Yamanaka, M. Ishimaru, A. Charoenphakdee, H. Matsumoto and K. Kurosaki: J. Electron. Mater. vol. 38, no.7, (2009), pp. 1392-1396.
- [3] D. Lakshminarayana, P.B. Patel, R.R. Desai and C.j. Panchal: J. MRS. Mater. Electron., vol. 13, pp. 27-31,2002.
- [4] R.R. Desai, D. Lakshminarayana b, P.B. Patel, P.K. Patel and C.J. Panchal: Mate. Chem. Phys., vol. 94, ,pp. 308-314,2005.
- [5] H. Zhu, K Chen, Z. Ge, H. Xu, Y. Su. J. Yin, Y. Xia and Z. Liu: J. Mater. Sci. vol. 45, pp. 3569-3573,2010.
- [6] D. Lakshminarayana, P.B. Patel, R.R. Desai and C.J. Panchal: Sens. Actuators. B. vol. 107, pp. 523-526, 2005.
- [7] D. Lakshminarayana, P.B. Patel, R.R. Desai and C.J. Panchal: Sens. Actuators A. vol. 121, pp. 405-409, 2005.
- [8] A.I. Zaslavskii and V.M. Seregeeva: Sov. Phys. Solid. State. vol. 2, pp. 2556,1961.
- [9] G.L. Bleris, T. Karakostas, J. Stoemenos and N.A. Economou: Phys. Status. Solidi (a). vol. 34, , pp. 243,1976.
- [10] T. Karakostas and N.A. Economou: Ibid. vol. 31, pp. 89,1975
- [11] A.I. Zaslavakii, N.F. Karethko and Z.A. Karachentseva: Sov. Phys. Solid. State. vol. 13, pp. 2152,1972.
- [12] H. Hahn and W. Klinger: Z. Anorg. Chem. vol. 97,pp. 260,1979.



- [13] H. Inuzuka and S. Sugaike: Proc. Japan Acad. vol. 30, pp. 383, 1954.
- [14] R. Robles, A. Vega and A. Mokrani : Otic. Mater. vol. 17, pp. 497, 2001.
- [15] M. Emziane, J.C. Berne Ádea, J. Ouerfelli, H. Essaidi and A. Barreac: Mater. Chem. Phys. vol. 61, pp. 229, 1999.
- [16] D.B. Anan'ina, V.L. Bakumenko, G.G. Grushka and L.N. Kurbatov: Sov. Phys. Semicond., vol. 10, no.1, pp. 3-6, 1976.
- [17] D.N. Bose and S. De Purkayastha: Mat. Res. Bull. vol. 16, pp. 635, 1981.
- [18] S. Balevicius, A. Cesnys and A. Deksnys: Phys. Stat. Sol. (a) vol. 32, pp. K11, 1975.
- [19] S. Balevicius, A. Cesnys and A. Deksnys: Phys. Stat. Sol. (a) vol. 35, , pp. K41, 1976.
- [20] A.I. Zaslavskii, N.F. Kartenko and Z.A. Karachentseva: Sov. Phys. Solid. State., vol. 13, no.9, pp. 2152, 1972.
- [21] T. Karakostas and N.A. Economou: Phys. Stat. Sol. (a) vol. 31, pp. 89, 1975.
- [22] Y. Kawakita, R. Matsubara, H. Nakashima and S. Takeda: J. Non-Cryst. Solids vol. 232, pp. 483, 1998.
- [23] M.A.M. Seyam: Appli. Surf. Sci. vol.181, pp.128, 2001.
- [24] P. Pichanusakorn and P. Bandaru: Mater. Sci. Eng. R. vol. 67, pp. 19, 2010.
- [25] J.C. Zheng: Front. Phys. China. vol. 3, no.3, pp. 269, 2008.
- [26] T. Seetawan, A. Vora-Ud, P. Chainaronk, C. Thanachayanont, V. Amornkitbamrung: Comp. Mater. Sci., vol. 49, pp. S225, 2010.
- [27] P. Villas and L.D. Calvet, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases, Second Edition*, vol.4, pp. 5195, 1996.
- [28] H. Nakamatsu, H. Adachi and T. Mukoyama: Bull. Inst. Chem. Res. Kyoto Univ. ,vol. 69, no.4, pp. 342, 1991.
- [29] C. Satoko, M. Tsukada, H. Adachi: J. Phys. Soc. Jpn. vol. 45, pp. 1333, 1978.
- [30] M. Morinaga, N. Yakawa, H. Adachi: J. Phys. Soc. Jpn. vol. 53, pp. 653, 1984.
- [31] J. Guo, D.E. Ellis, D.J. Lam: Phys. Rev. B vol. 45, pp. 3204, 1992.
- [32] J.C. Slater: *Quantum Theory of Molecules and Solids, The Self-Consistent Field for Molecules an Solids*, (fourth ed., Springer, New York, 1974).
- [33] M.A. Santana-Aranda, J. Luyo-Alvarado, M. Meléndez-Lira, M. Zapata-Torres, A. Zapata-Navarro, S. Jiménez-Sandoval, R. Castro-Rodriguez, J.L. Peña: Superficies. Y. Vacio. vol. 8, pp. 69, 1999.
- [34] L. Yanwu, W. Dingsheng and R. Ailun: Chinese. Phys. Lett., vol. 7, no.2, , pp.75, 1990.
- [35] N.A. Hegab, A.E. Bekheet, M.A. Afifi, A.A. El-Shazly: Appl. Phys. A vol. 66, pp. 235, 1998.
- [36] V. Skyarchuk and Y. Plevachuk: J. Non-Cryst. Solids vol. 353, pp. 3216, 2007.