Original Article

Bulletin of Pure and Applied Sciences.
Vol.36 D (Physics), Issue (No.1) 2017: P.75-79
Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI 10.5958/2320-3218.2017.00010.0

Electronic Band Structure of Bulk Materials of Bismuth Antimony Nanowires

Ashok Kumar Singh, Ali Ahmad Ansari, Jagriti

Ashok Kumar Singh
Department of Physics, H.N.K. Inter College, Ara, Bihar, India

Ali Ahmad Ansari
Research Scholar
University Department of Physics, B.R.A.B.U. Muzaffarpur, Bihar, INDIA -842001

Jagriti
Research Scholar
University Department of Physics, B.R.A.B.U. Muzaffarpur, Bihar, INDIA -842001

Corresponding author:
Ali Ahmad Ansari
Research Scholar
University Department of Physics,
B.R.A.B.U. Muzaffarpur, Bihar, India-842001

E-mail: madanjeebrabu@gmail.com

Received on 30.04.2017,
Accepted on 29.06.2017

Abstract

We have developed a model for the miniband gap and the related nonparabolic dispersions at the limiting of bismuth antimony. We have used an interactive one dimensional two band model and developed an analytical approximation for this model. We have studied the band edges and electronic phases as a function of grow the orientation, wire diameter and stoichiometry, including the semimetal phases, the indirect semiconductor phases and the direct semiconductor phases. We have found that bulk materials of bismuth antimony and their alloys have the same symmetry with a rhombohedral lattice structure. There are two atoms per unit cell. The trigonal axis with a threefold symmetry, the binary axis with a twofold symmetry and the bisectrix axis form a natural cartesian coordinate frame. A mirror plane is formed by the trigonal axis and the bisectrix axis which is perpendicular to the binary axis. The band structure does not change notably with temperature.

INTRODUCTION

Lin etal [1] have synthesized and studied some elctronic properties of $Bi_{1-x}Sb_x$ nano wires of different diameters and different composition of antimony. Rabin etal [2] studied for the composition of range of different nanowire diameter below the temperature of 77K oriented in the trigonal direction with their wire axis. Nikolaeva etal [3] studied $Bi_{1-x}Sb_x$ wires of larger diameters on the order of microns for their strain effect in the wire direction of their electrical resistivity. Tang and Dresselhams [4] have given systematic presentation on the electronic band structure of $Bi_{1-x}Sb_x$ thin films as a function of growth orientation; film thickness E. Smith [5] observed a number of properties in bulk bismuth materials, such as non parabolic dispersions and abnormal magneto resistance. Hicks etal [6] studied that thermoelectric materials could have enhanced figure of merit of the materials were synthesized in the form of low dimensional systems and nanosystems. Rogacheva et al [7] showed the conditions of the sample and measurements using different experimental techniques may also result different values at certain phase transition points.

METHOD

The quantum continement effect of nanowires may change the symmetry properties of the carrier pockets, the positions in energy of the band edges and possibly the shape of the dispersion relations at the T point, the L points and the H points. A trivial quantum confinement does not change the inverse effective mass tenor or the shape of dispersion. A nontrivial quantum confinement changes the inverse effective mass tensor and the shape of the dispersion. For the T point and the H points, the dispersions of the band edges are parabolic and the quantum confinement effect is trivial. The valence band edge at the T points will decrease in energy. For the L points, the dispersions of the band edges are non parabolic and the quantum confinement effect is nontrivial; so that the traditional square well model is not accurate any more. There coexists an electron pocket and a whole packet at each L point. Thus conduction band edge and valence band edge for the L point are every close to each other in energy and are strongly coupled, which results in the nonparabolicity of the dispersion for the L point electrons and holes are possibly even linearly if the two bands are touching. The shape of the dispersion is also correlated with the magnitude of narrow band gap. The relation between the narrow band gap and the dispersion for bulk bismuth is described by a two band model

$$p.\alpha^{[L,Bulk,Bi]}.p = E(\kappa)\left[1+\frac{E(\kappa)}{Eg^{[L,Bulk,Bi]}}\right] \quad \text{..... (1)}$$

Where $\alpha^{[L,Bulk]}$ is the inverse effective mass tensor of the L point carrier pocket of bulk bismuth and it is assumed that $\alpha^{[L,Bulk]}$ for both the conduction band edge and the valence band edge are the same due to the strong interaction between these two bands

.

RESULTS AND DISCUSSION

Fig (1) shows the electronic phase diagrams band gap of $Bi_{1-x}Sb_x$ nanowires with diameter 100 nanometer as a function of growth orientation and stoichiometry. The semimetal phase regions, indirect semiconductor phase regions and the direct semiconductor phase regions are marked for each orientation. The antiomony composition x is denoted by the radius of circles as shown in fig (2) when wire width is 100 nm the electronic phase starts from a semimetal, where the top of valence band edge is located at the T point at $x = 0$. As the antimony composition increases, phase changes at $x = 0.15$ the top of the valence band

edge becomes located at an L point and the electronic phase becomes a direct gap semiconductor. For higher antimony concentration *x*, the top of the valence band edge shifted to an H point and the band gap of the semiconductor phase becomes indirect-when x is further increased the electronic phase is changed back to semimetal. The obtained results were compared with previously obtained theoretical and experimental results and were found in good agreement.

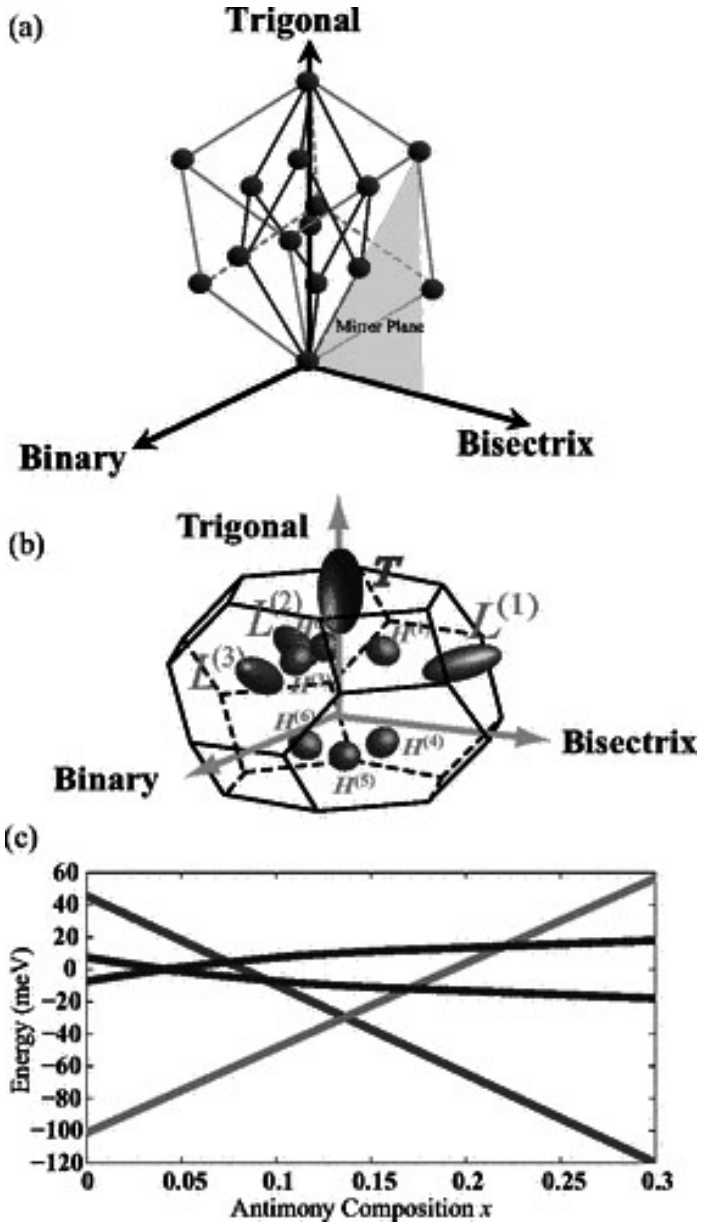

Fig. 1: Atomic and band structure of bulk bismuth antimony.

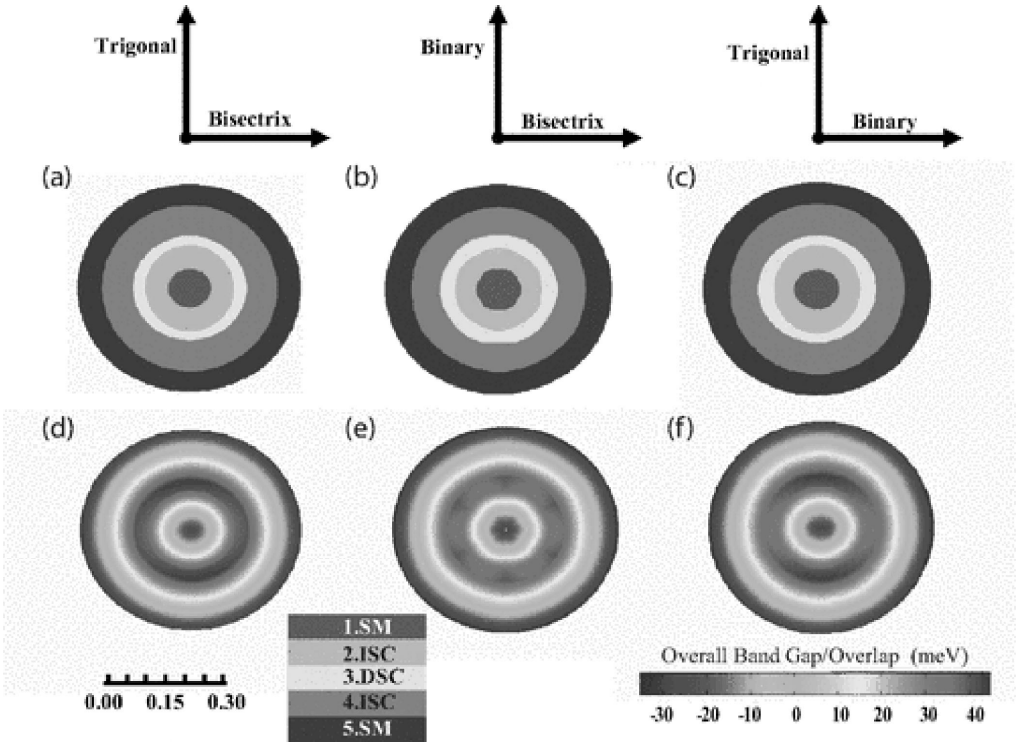

Fig. 2: The electronic phase diagrams (a) – (c), and the band-gap / overlap diagrams (d) – (f) of $Bi_{1-x}Sb_x$, nanowires of 100 nm wire width.

CONCLUSION

We have studied electronic band structure of bulk materials of bismuth antimony nanowires. We have studied the band edges and electronic phases as a function of growth orientation, wire diameter, stoichiometry, including the semimetal phases, the indirect and direct semiconductors phases. We also studied the band overlap the semimetal phases and the band gap of the semiconductor phases. The bulk materials of bismuth antimony and their alloys have the same symmetry with rohombohedral and lattice structure.

The band structure does not change with temperature. We have observed that bismuth antimony nanowires of larger wire width showed a much richer variation of electronic phases but of the anistropy for different growth orientation are less. The case of large values of antimony compositions turns to be similar with the case of small values, only the location of the top of the valence band edges for the semimetal phases and the indirect semiconductor phases are at the H. points for the median value of x = 0.13, instead of at the T point which applies to x = 0.05. When width of nanowire is large, the nontrivial quantum confinement effect near a L point shifts and band edge more quickly as the width decreases than does the trivial quantum confinement effect near an H or a T point. When the width of nanowire is very small, the direct band gap at an L point is larger enough to induce a significant reduction of the enterband coupling, which changes the nonparabolic dispersions at the L point into parabolic dispersions with larger mass components.

REFERENCES

1. Y.M. Lin, S. Cronin, O. Rabin, J.Y. Ying and M. Dresselnaus (2001), Appl. Phys. Lett. 79, 677.
2. O. Rabin, Y.M. Lin and M.S. Dresselhans, (2001), Appl. Phys. Lett. 79, 81.
3. A. Nikolaeva, L. Konopko, T. Huber, P. Bodiul, I.Popov and E. Moloshnik, (2012), J. Electron Mater, 41, 2313.
4. S. Tang and M.S. Dresselhans, (2012), Phys. Rev. B, 86, 075436.
5. A.W. Smith, (1911), Phys. Rev. (Ser I), 32, 178.
6. L.D. Hicks and M.S. Dresselhans, (1993), Phys. Rev. B, 47, 12727.
7. E. I. Rogacheva, A.A. Drozdova, O.N. Nashchekina, M.S. Dresselhaus and G. Dresselhaus, (2009), Appl. Phys. Lett. 94, 202111.