Optical Materials 136 (2023) 113430

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Growth and characterization of $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ crystals

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A R T I C L E I N F O

Keywords:
X-ray diffraction
Growth from melt
Band gap
Thermoelectric power

A B S T R A C T

Indium bismuthide is a well-known III-V group semi metallic compound. The compositions used were $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ crystals. The zone melting method used to grow the crystals. The zone-melting furnace has shown a temperature gradient of 45 °C/cm, and it has yielded the good quality crystals obtained, having a growth rate of 0.3 cm/h. The characterization of crystals was carried out using powdered X-ray technique. Using the FTIR spectra, the direct type band gap has been evaluated. The thermoelectric power measurement was carried out for $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ crystals. The Van der Pauw method has been employed for the Hall measurements at room temperature. This work report the detailed results of the above mentioned study and conclusions drawn therein.

1. Introduction

Semiconductors always offer wide scope of research due to its various applications. It is possible to manipulate their properties and hence functionality in devices. There is good amount of work done to develop materials for Infrared (IR) detectors using narrow gap semiconductors. Over the last few decades, MCT (mercury cadmium telluride) systems have been important materials for IR detector devices. However, these systems bear a drawback of thermal and lattice instabilities due to the weak Hg–Te bond. In this respect low band gap III-IV compound materials can prove to be more advantageous for IR technology.

In recent years, growth of III-IV group pseudo binary crystals has increasingly became a subject of significant research in view of demands of IR technology [1–4]. As a detector material InBi/InSb system is nonhazardous and suitable for narrow band gap applications as in IR optical devices. It has been observed that the materials studied so far in InBi:Te system are all Te rich quasi binary or ternary alloys. There are very few reports available on Indium rich alloy that too not related to the present investigation [4]. It is matter of great interest to investigate various narrow gap materials, such as, bismuth telluride based alloys including n-type $Bi_2(Te,Se)_3$ and p-type $(Bi,Sb)_2Te_3$. These materials are not only good thermoelectric devices that are available for near room temperature applications, but it is also useful for improving their figure of merit (ZT) values through structural and compositional modifications [5,6].

Among the pseudo binaries of interest in the present case, $InBi_{1\text{-}x}Te_x$ has been the least studied in this respect. This report is the first of its kind on InBi with Te as dopant. We have grown single crystals of $InBi_{1\text{-}x}Te_x$ ($x = 0.05$ and 0.1). The paper reports, band gap, thermoelectric power and Hall measurement of these grown crystals.

2. Experimental

In order to prepare the proposed composition material, the three elements (5 N purity) in their stoichiometric proportions were first mechanically mixed and then sealed in a quartz ampoule under residual pressure $\sim 10^{-5}$ Pa. The sealed mixture was melted at 150 °C in a furnace. The molten charge in an ampoule was rocked for 48 h, for effective homogeneous mixing and compound formation. The proportional controller has been used to measure temperature controller to an accuracy of ±5 °C, using Chromel-Alumel thermocouple. The zone melting technique of crystal growth has been employed to prepare $InBi_{0.9}Te_{0.1}$ ingot, ~60 mm × 8 mm crystals. The samples were processed and ten time's to-and-fro passes given for zone levelling at travel speed of 0.3 cm/h. The temperature gradient of ~45 °C/cm and having about 0.01 m zone length with zone temperature of about 150 °C. The plot of temperature versus distance of the zone melting furnace is given in Fig. 1.

The single crystal was obtained by using the zone levelled crystal, as described above, through self-nucleation process. Under optical microscope, freshly cleaved crystal surfaces as observed which is showing good crystal perfection.

Philips X-ray diffractometer (Model PM8203) have been used with

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https://doi.org/10.1016/j.optmat.2023.113430
Received 24 November 2021; Received in revised form 3 September 2022; Accepted 1 January 2023

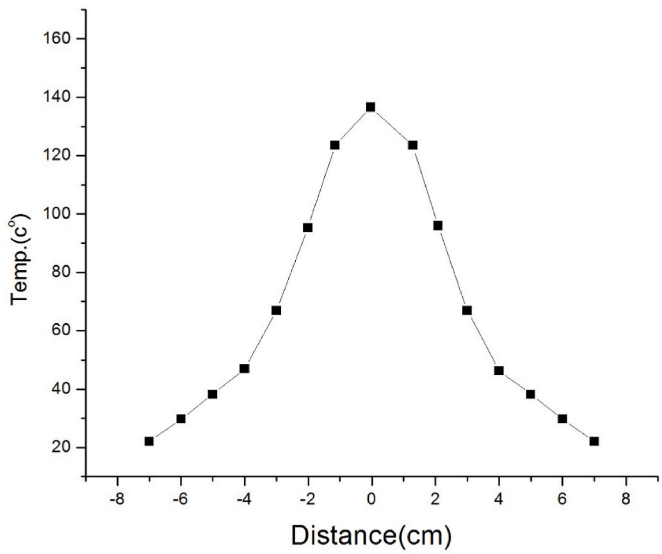

Fig. 1. Plot of the temperature versus distance used in the zone melting furnace.

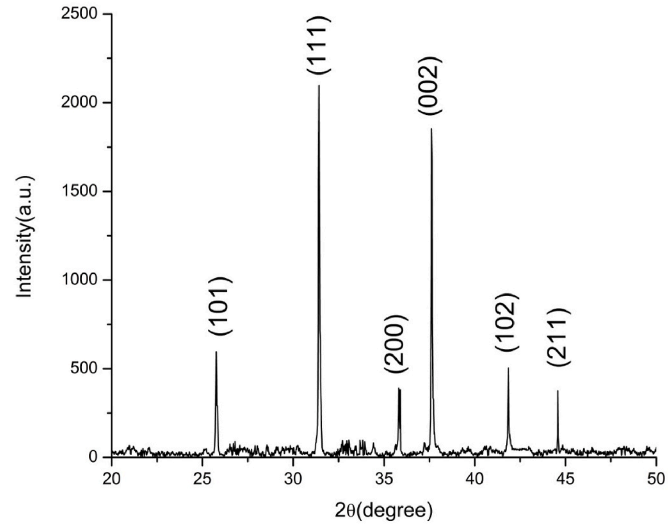

Fig. 4. The XRD plot of $InBi_{0.90}Te_{0.10.}$

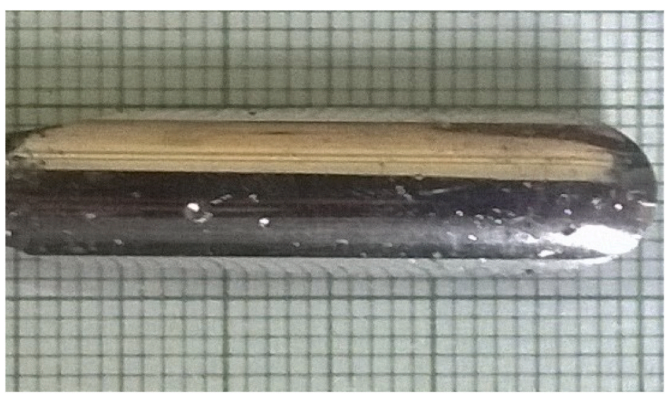

Fig. 2. As grown crystals of $InBi_{0.90}Te_{0.10.}$

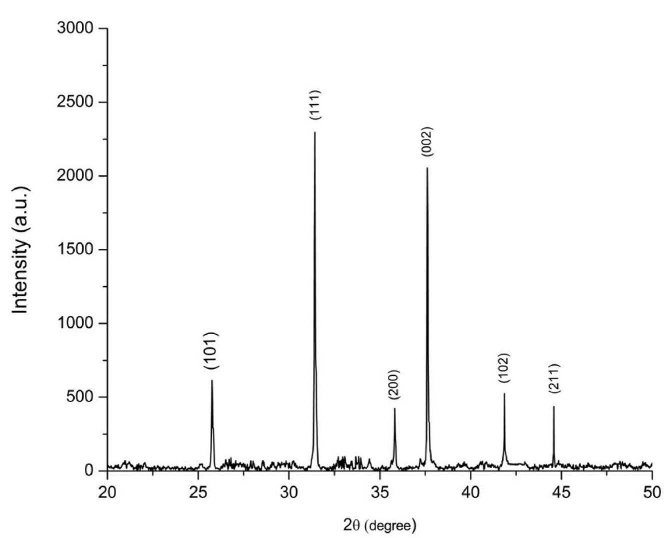

Fig. 3. The XRD plot of $InBi_{0.95}Te_{0.05.}$

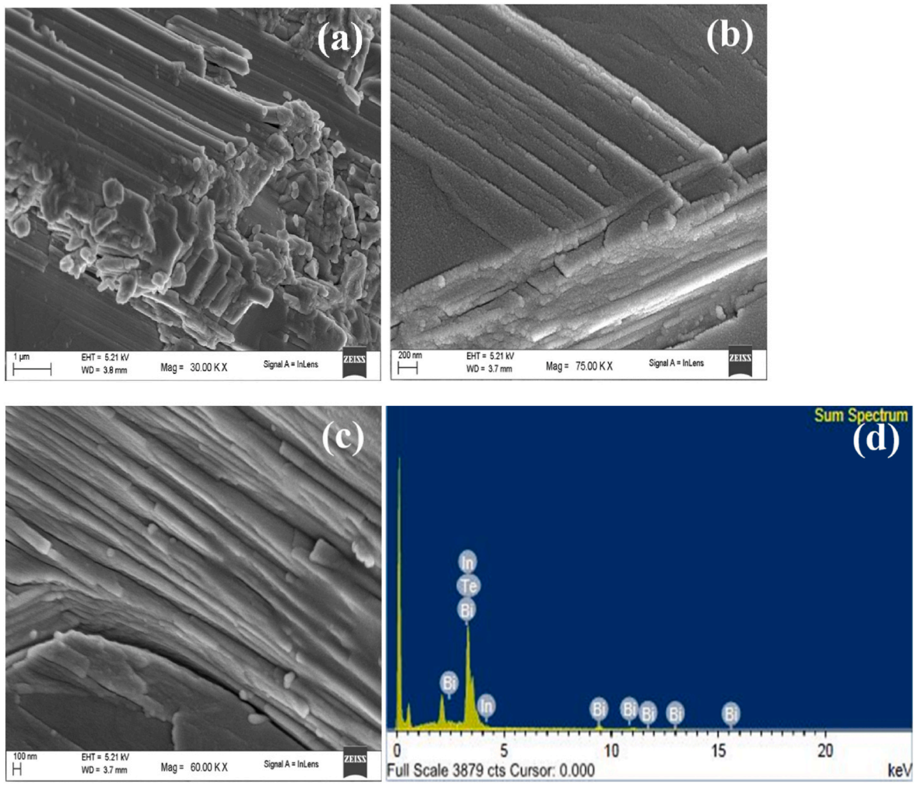

Fig. 5. (a–c) FESEM images and (d) Energy dispersive spectra of $InBi_{0.95}Te_{0.05}$ crystal, respectively.

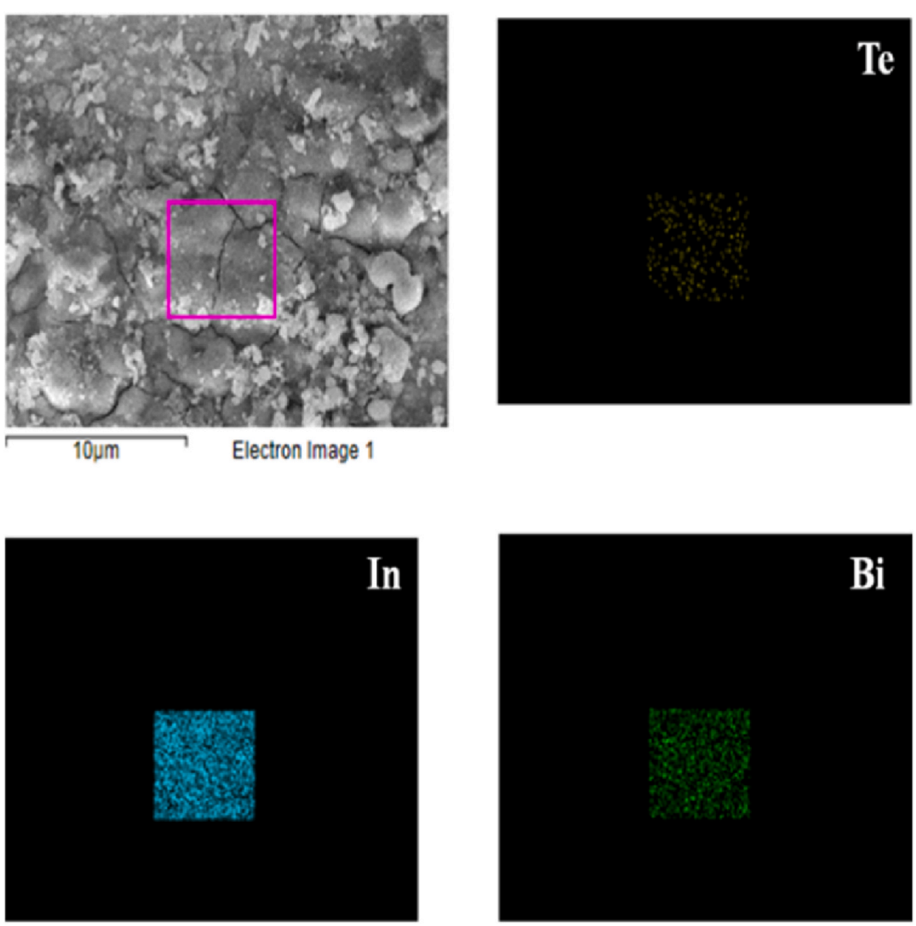

Fig. 6. Color mapping of $InBi_{0.95}Te_{0.05}$ crystal, respectively.

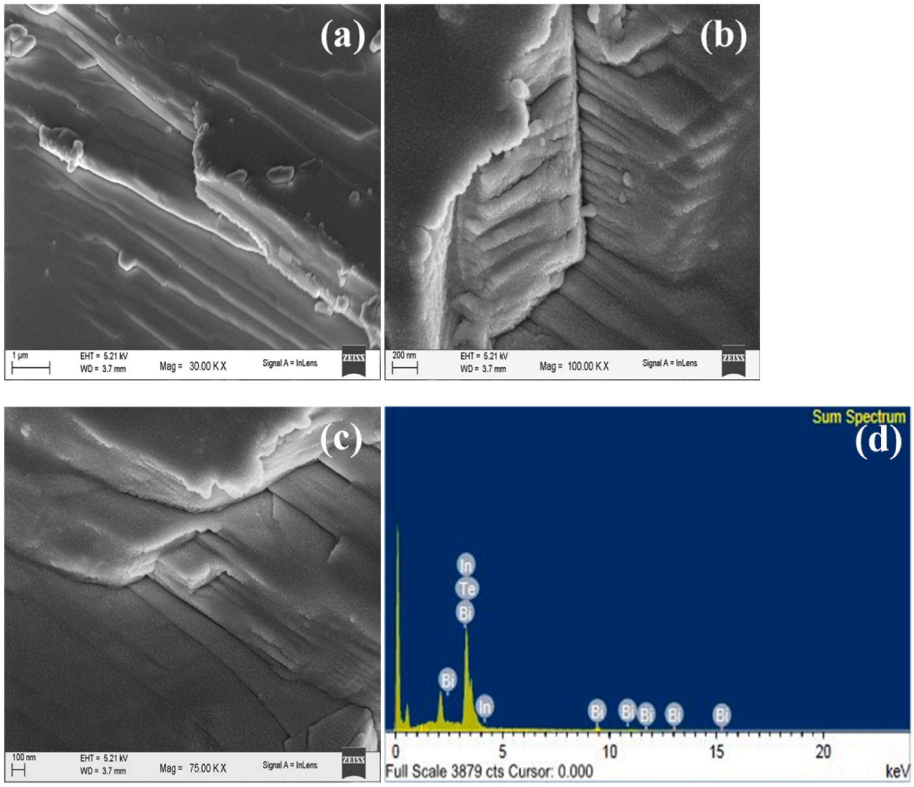

Fig. 7. (a–c) FESEM images and (d) Energy dispersive spectra of $InBi_{0.90}Te_{0.10,}$ crystal, respectively.

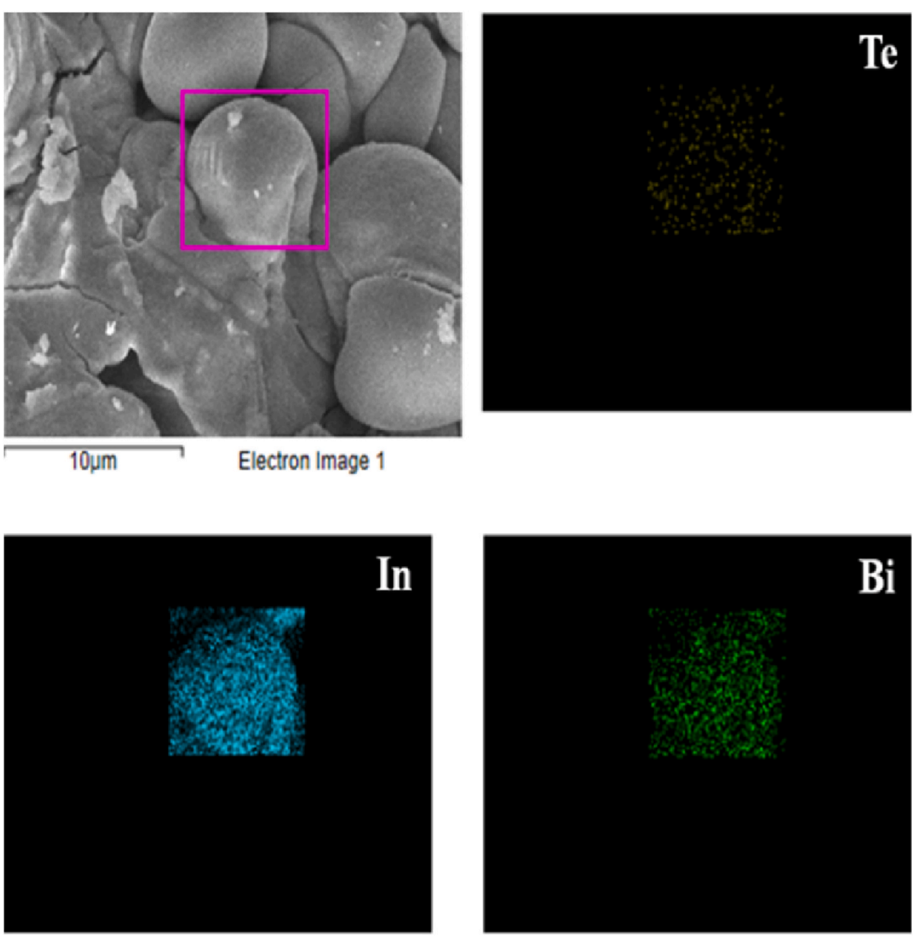

Fig. 8. Color mapping of $InBi_{0.90}Te_{0.10}$ crystal, respectively.

Table 1
The elemental compositions as analyzed in three different region of $InBi_{1\text{-}x}Te_x$ (x = 0.05 and 0.1) single crystal.

Crystal	Element Present			Atomic (%)
$InBi_{0.95}Te_{0.05}$	**In**	**Bi**	**Te**	**35.80** **62.73** **1.47**
$InBi_{0.90}Te_{0.10}$	**In**	**Bi**	**Te**	**36.42** **59.56** **4.02**

radiation $Cu_{k\alpha}$ ($\lambda = 1.5418$ Å), for acquiring XRD data from the ingot. The FTIR Spectrophotometer (Jasco 4100, Japan) have been employed, using the powdered crystal and mixed with KBr followed by preparation of pelleted samples to obtain the optical spectrum in the wave number range of 400–4000 cm^{-1}. The band gap of the respective crystals was analyzed with Tauc plots. The Scanning Electron Microscope of OXFORD Model was used to obtain the composition of the samples from the Energy Dispersive Analyzer by X-ray (EDAX) data.

The TEP Model-2000, supplied by Scientific Solutions, Mumbai, India has been used to measure the thermoelectric power (TEP). The samples used were in the forms of slices of dimensions of ~9 × 6 × .5 mm^3.Mica sheets were used for mounting the samples so as to make the two junctions smooth and at the same time, touch the samples. The temperature difference between the two junctions (ΔT) was controlled by using a suitable temperature controller. ΔT was kept constant at 5^0 throughout the temperature variation of the hot junction across the range from 308 K to 423 K.

3. Results and discussions

Fig. 2 shows a crystal grown having length of 60 mm and diameter 8 mm. The overall appearances of all the crystals grown were similar. The doped as well as pure crystals were observed to have fairly good lustre.

Figs. 3 and 4, show the powder X-ray diffraction plots obtained for $InBi_{1\text{-}x}Te_x$ with x = 0.05 and x = 0.1, respectively. The peaks observed in Fig. 4 at 25.75°, 31.45°, 35.85°, 37.65°, 41.85° and 44.56° corresponds to (101), (111),(200), (002), (102) and (211) InBi reflections, respectively, were in good agreement with ASTM-JCPDS card no. 32–0113.

Figs. 5 and 6 show the FESEM, EDAX, and the color mapping for $InBi_{0.95}Te_{0.05}$ sample, respectively. Similarly, Figs. 7 and 8 represent FESEM, EDAX, and the color mapping for $InBi_{0.90}Te_{0.10}$ crystals, respectively. Fig. 5(a–c) and 6 (a-c) shows the FESEM images of crystals

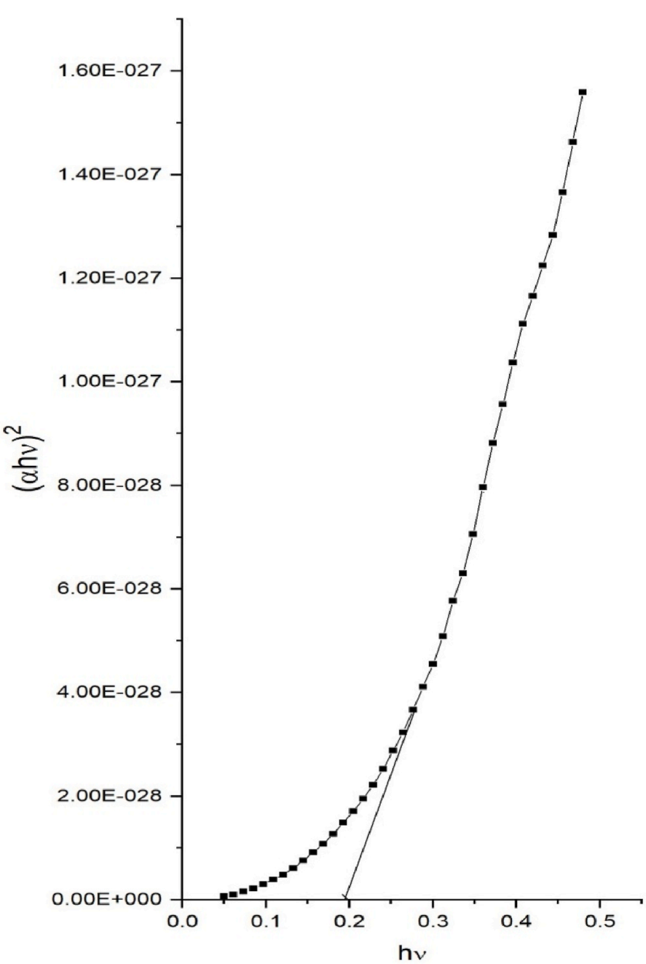

Fig. 9. Plots of $(\alpha h\nu)^2$ versus photon energy (hν) for $InBi_{0.95}Te_{0.05}$crystals.

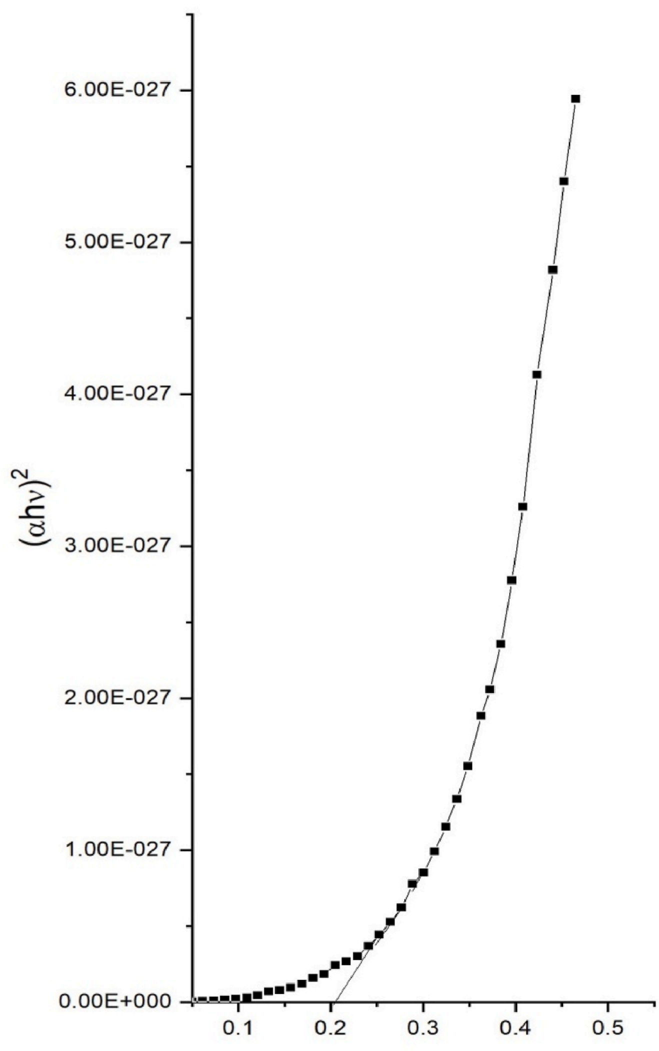

Fig. 10. Plots of $(\alpha h\nu)^2$ versus photon energy (hν) for $InBi_{0.90}Te_{0.10}$crystals.

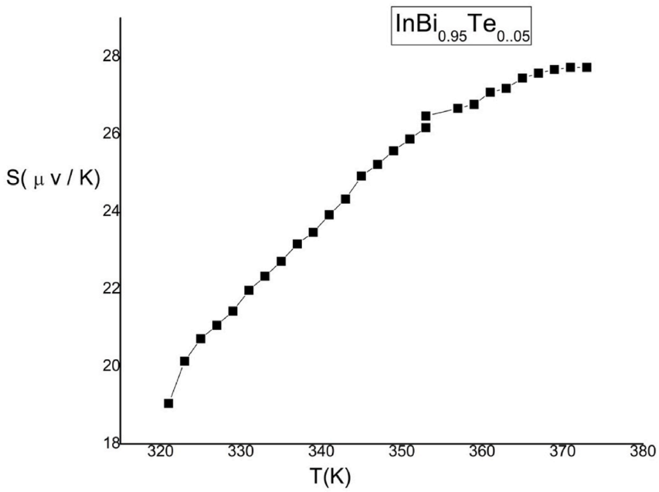

Fig. 11a. The plot of S (thermoelectric power) vs T (Temperature) for $InBi_{.95}Te_{.05}$ crystals.

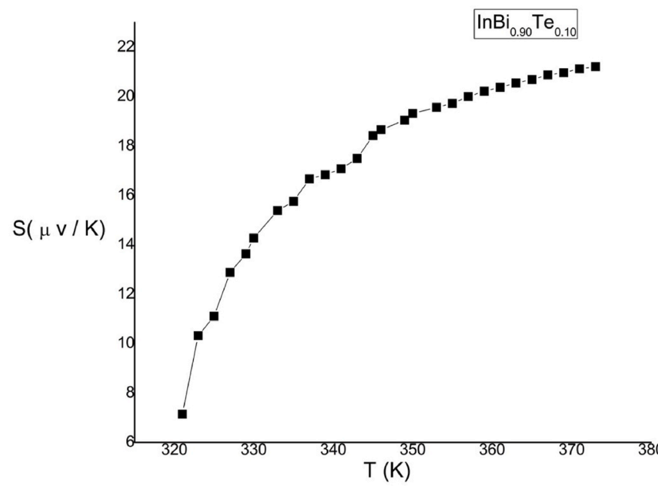

Fig. 11b. The plot of S (thermoelectric power) vs T (Temperature) for $InBi_{.90}Te_{10}$ crystals.

($InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$) implying the material growing into smooth layer growth mode with planar surfaces of good perfection. The EDAX spectra for both the crystals could provide a qualitative overview about the elemental composition. In support of EDAX, the color mapping of both the crystal was studied for better qualitative and quantitative evaluation of the elements. The atomic percentage of In, Bi, Te, in $InBi_{1-x}Te_x$ ($x = 0.05$ and 0.1) as obtained from EDAX are mentioned in Table 1. It can be observed that the samples have quite satisfactory stoichiometric composition.

In order to avoid the plastic strain, the freshly grown ingot was cleaved along the basal plane at 0 °C. The crystal has easy cleavage along the plane (001). The ingot obtained after zone-melting was cleaved at various places. It was found that the cleavage surface exhibits constant orientation along the length of the crystal, which indicates the ingot is a single crystal. The cleaved surface of the crystal did not exhibit any disorientation as observed under an optical microscope, implying very good macroscopic perfection.

Optical absorption and consequent inter-band transition at the absorption edge was governed by the absorption coefficient α, which can be used to analyze the band gap employing a Tauc plot $(\alpha h\upsilon)^2$ versus hυ in the case of allowed direct transition [7]. In the present case, the plot of $(\alpha h\upsilon)^2$ versus hυ would be linear at the absorption edge, as shown in Figs. 9 and 10.

The inter-band transition is responsible for the direct absorption. The band gaps, of $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ single crystals, obtained as intercepts of extrapolated linear nature of plot near absorption edge were found to be, 0.195 eV and 0.213 eV, respectively. Therefore, with increasing Tellurium content, the band gap shows an increasing trend.

Fig. 11(a) and (b) show plots of S (thermoelectric power) versus T (Temperature) for $InBi_{1-x}Te_x$with $x = 0.05$ and $x = 0.10$, respectively. Further thermoelectric power is found to increase with increasing temperature, confirming the typical degenerate semiconductor behaviour of $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ crystals [8]. In both the crystals, the sign of the thermo-emf and the results of the hot probe tests show that the all the crystals are of n-type.

The Van der Pauw method has been used for Hall measurements at room temperature. The Hall coefficient and carrier concentration of $InBi_{1-x}Te_x$ ($x = 0.05$ and 0.1) crystals are listed in Table 2. The Hall coefficient was found to be negative indicating that the charge carriers are electrons.

Table 2
The carrier concentration and Hall coefficient for different doping of $InBi_{1-x}Te_x$ crystals are shown below.

Crystals	Hall Co-efficient $(R)_H$ (Ωm/T)	Carrier concentration (N) (m^{-3})
InBi	0.66×10^{-6}	9.432×10^{24}
$InBi_{0.95}Te_{0.05}$	1.19×10^{-6}	5.251×10^{24}
$InBi_{0.90}Te_{0.10}$	3.13×10^{-6}	1.996×10^{24}

4. Conclusions

In the present study the growth and characterization of crystals of $InBi_{1-x}Te_x$ ($x = 0$ to 0.1) have been carried out. Following important conclusions can be drawn out of this investigation.

1. Zone-melting method can be successfully used to grow single crystals of $InBi_{1-x}Te_x$ ($x = 0$ to 0.1).
1. The EDAX analysis shows the stoichiometric composition of the grown crystals.
2. All direct type band gaps of $InBi_{0.95}Te_{0.05}$ and of $InBi_{0.90}Te_{0.10}$ single crystals are about 0.195eV and 0.213 eV, respectively. Addition of Te in InBi results in a semiconducting material (narrow band gap type) with the band gap increasing as Te content increases.
3. The sign of thermo-emf and the results of hot probe tests show that the $InBi_{0.95}Te_{0.05}$ and $InBi_{0.90}Te_{0.10}$ crystals are all of n-type in agreement with the Hall coefficient results. Further thermoelectric power increases with increasing temperature, confirming the typical degenerate semiconductor behaviour of $InBi_{1-x}$ Te_x ($x = 0.05$ to 0.1) crystals.

Author statement

The corresponding author is responsible for ensuring that the descriptions are accurate and agreed by all authors. Authors may have contributed in multiple roles as follows:

Nimesh Nanda - Conceptualization, Investigation, Writing-Original Draft, Dr. P. H. Soni – Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgements

The authors gratefully acknowledge Dr. Mukul Gupta (IUC-UGC-CSIR, Indore) for providing Powder X-ray diffraction facility. Thanks are also due to the Head, Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, for his kind help and for providing different research instruments in the department, which helped us to complete all of the characterization work efficiently and under one roof.

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