Crystal Growth and X-ray Diffraction Characterization of Sb_2Te_3 Single Crystal

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Abstract. We report the single crystal growth and X-ray diffraction characterization of bulk Sb_2Te_3 single crystal. Single crystal of Sb_2Te_3 was grown by modified Bridgman method. The diffraction peaks corresponding to {0, 0, 3} planesreveal the growth of crystal along the c-direction.X-ray diffraction analysis by rietveld refinement confirms and verifies the phase purity, rhombohedral structure and single crystalline nature of the prepared Sb_2Te_3 crystal .Unit cell structure of Sb_2Te_3 consist of three quintuple layers stacked one above the other.

INTRODUCTION

Discovery of topological insulators have drawn new interest in condensed matter physics because of their intriguing physical properties and novel device applications like spintronics, thermoelectric, and quantum computing [1–3]. Topological insulators possess bulk band gap like an ordinarybandinsulator but have topologically protected metallic surface states on their surface or edges [4–6]. The two factors responsible for these exotic surface states are spin-orbit interaction and time-reversal symmetry. The widely studied examples of topological insulators are Bi2Se3, Bi2Te3 and Sb2Te3 by various measurements.The fascinating physical properties in these topologically insulatingmaterials like large magnetoresistance, weakantilocalization (WAL), high mobilitymakes them suitable for technical applications [7–9].Most of the studies in literature on TIs are on thin films whereas the single crystals are comparatively less studied. The formation of single crystals of these TIs depends on the process followed during the preparation which highly determines the observed physical properties. For example the type of defects present in the Bi2Se3 crystals gives rise to various interesting properties like large linear magnetoresistance, π-berry phase and the observation of quantum hall effectetc [10–13].

Sb2Te3 is a well-known narrow-gap semiconductor with a band gap ~ 0.26ev which is demonstrated as a topological insulator experimentally by measurements like angle resolved photoemission spectroscopy (ARPES) [14]. Sb2Te3 is a p-type topological insulator due to the holes which is introduced by Sb/Te antisite defects [15]. It would be interesting to study the structural correlation with physical properties like in magneto-transport properties due to the inherent characteristics and defects/in-homogeneities created during the crystal formation. With this aim we have prepared the single crystal of Sb_2Te_3 and here we present its growth and structural characterization.

EXPERIMENTAL DETAILS

Single crystal of Sb2Te3 was grown by modified Bridgman method. The high purity elements of Sb (99.999%) and Te (99.999%) were accurately weighed in their stoichiometric ratio. The sample was melted at 850°Cfollowed by cooling and annealing at about 600°C for a couple of days. As grown crystal of Sb_2Te_3 was cleaved from which a smooth and shiny surface was found for structural characterization. X-ray diffraction of grown Sb_2Te_3 single crystal was carried out using the Bruker D8 Advance x-ray diffractometer that used the Cu k_α radiation having the wavelength 1.54Å.

RESULTS AND DISCUSSION

Structural characterization of as grown Sb_2Te_3 single crystal is carried out by X-ray diffraction measurement. **FIGURE 1** shows the powder XRD data along with its rietveld refinement. The x- axis indicates the 2θ values and y- axis represents the intensities corresponding to the 2θ values. The red circles are the observed data points and black lines show the fitted pattern obtained using Fullprof Suite software. The blue line indicates thedifference between the experimental and theoretical fit. The completeoverlap of the experimental and theoretical pattern obtained after the refinement and absence of any extra peaks in the calculated pattern confirms the single phase formation of the sample and its rhombohedral structure with R-3m (D5) space group. The green lines indicate the corresponding Bragg peaks.

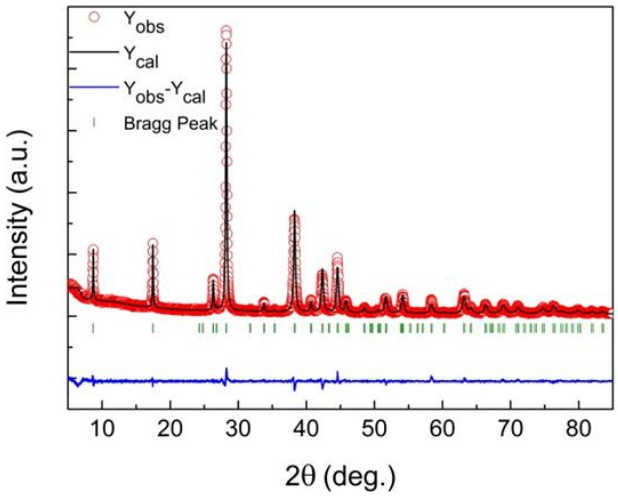

FIGURE 1: Room temperature powder X-ray diffraction data along with its Rietveld refinement fit.

The goodness of fit obtained from the refinement is 1.98 indicating the proper fit to the data. The fitting parameters obtained such as lattice constants, c/a ratio, volume etc. have been tabulated in **TABLE 1**. The lattice parameters obtained from therietveld refinement are in well agreement with the earlier reports in the literature [16]. The obtained Wyckoff positions for our crystal are as follows; Sb position 6c (0,0,0.3992); Te^1 position 3a (0,0,0) ; Te^2 position 6c (0,0,0.2122). The approximate occupancy for Sb (6c) is 2.373, Te^1(3a) is 1.1975 and Te^2(6c) is 2.380. **FIGURE 2** shows the crystal structure of Sb2Te3 generated using the VESTA software. The obtained unit cell structure of the grown Sb_2Te_3crystal exhibits the layered atomic arrangement in the rhombohedral structure which consists of three quintuple layers (QLs) and each quintuple layer contains five atoms in the order of (Te^1-Sb-Te^2-Sb-Te^1).These superscripts (1) and (2) represents the distinctly bonded tellurium atoms.Adjacent quintuple layers are bonded with each other by weak vander Walls (vdW) forces and shows the presence of vander wall gap in between the twoQLs, while atoms within the QLs are covalently bonded.

TABLE 1: Refined values of the parameters obtained from the Rietveld refinement

a = b (Å)	c (Å)	c/a	Volume(Å^3)	χ^2
4.264(3)	30.48(2)	7.143(2)	480.72(4)	1.98

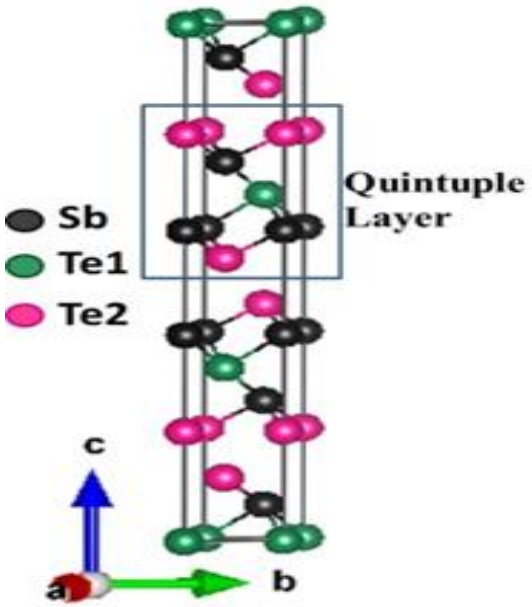

FIGURE 2: Crystal structure of $Sb_2Te_3$by VESTA software obtained by using parameters refined from rietveld refinement, showing quintuple layers.

Apart from powder X-ray diffraction of the obtained sample we performed the X-ray diffraction on the cleaved surface of the single crystal also the shiny flat surface is obtained after crystal cleaving. XRD pattern of cleaved surface of Sb_2Te_3 crystal suggests that growth is along c- direction which as shown in **FIGURE 3**. All the diffraction peaks of the grown Sb_2Te_3 single crystal were indexed with the help of standard JCPDS file for Sb_2Te_3.The large intensity of peaks corresponding to the {003} planes assures the single crystalline nature of the grown single crystal and the orientation of our crystal is along the c-axis.

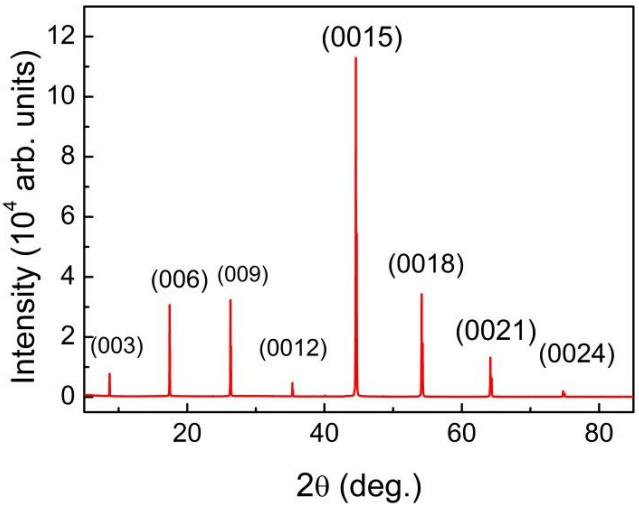

FIGURE 3: X-ray diffraction pattern for the cleaved crystal of Sb_2Te_3. The peaks corresponding to {003} planes indicate orientation of crystal planes along c-direction.

CONCLUSION

A successful attempt to grow a single crystal of Sb_2Te_3 by modified Bridgeman method was made. We confirm the single crystalline formation of Sb_2Te_3crystal, which is oriented along the c-axis. Rietveld refinement analysis confirmed the rhombohedral structure having (R-3m) space group and the occupancies of Sb, Te^1, and Te^2 atoms. The formation of quintuple layers stacked over one another in the Sb_2Te_3 crystal is visualized by using VESTA software. These layers are bound by vander Waals (vdW) forces having atom bonded by covalent bonds.

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