Hikami-Larkin-Nagaoka (HLN) Fitting of Magneto Transport of Bi₂Se₃ Single Crystal in Different Magnetic Field Ranges

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Abstract. We report the detailed study of structural/micro-structural and high magnetic field magneto transport properties of Bi₂Se₃ single crystal. Bi₂Se₃ single crystal is grown through conventional solid-state reaction route via the self-flux method. Rietveld analysis on Powder X-ray Diffraction (PXRD) showed that the studied Bi₂Se₃ crystal is crystallized in single-phase without any impurity. The surface morphology analyzed through Scanning Electron Microscopy (SEM) study which shows that as-grown single crystal exhibit layered type structure and the quantitative weight% of the atomic constituents (Bi and Se) are found to be close to the stoichiometric amount in energy-dispersive X-ray spectroscopy (EDS) analysis. Low temperature (2.5K) magneto-resistance (MR) exhibited a v-type cusp around origin at lower magnetic field, which is the sign of weak anti-localization (WAL) effect. Further, Bi₂Se₃ single crystal magneto conductivity data is fitted by well-known HLN equation in different magnetic field range of 2Tesla, 4Tesla and 6Tesla and the resultant found that the conduction mechanism of Bi₂Se₃ is dominated by WAL state.

INTRODUCTION

Topological Insulator (TI) is the new state of quantum matter having protected conducting surface states; on the other hand, the bulk is the insulator. These surface states are Time Reversal Symmetry (TRS) protected and do have strong Spin-Orbit Coupling (SOC). Bi₂Se₃ is the binary tetradymite compounds in which the strong SOC is present and is having single Dirac cone in their energy versus momentum diagram at Γ point [1-3]. Bi₂se₃ has attracted lot of attention due to their various quantum phenomenon as Weak Anti Localization (WAL), Aharonov-Bohm (AB) oscillation and high field linear Magneto Resistance (MR) associated with their conducting surface states [4, 5]. WAL is considered due to the suppression of back scattering of carriers by the π -Berry phase of topological surface states and helical spin momentum locking as reported earlier [4, 5].

In the present short article, we report the successful growth and structural/micro-structural details and high field (10 Tesla) magneto conductivity analysis by HLN fitting of Bi₂Se₃ single crystal.

EXPERIMENTAL DETAILS

High-quality Bi₂Se₃ single crystal has been synthesized by the self-flux method through the conventional solidstate reaction route [6]. High-purity (99.99%) bismuth (Bi) and selenium (Se) were weighed accurately in their stoichiometric ratio, well mixed and ground thoroughly inside a glove box under high-purity Ar (Argon) atmosphere to avoid oxidation of the any element. The homogeneously mixed powder then was pressed in form of a rectangular pellet using a hydraulic press under a pressure of 50 kg/cm² and then vacuum-sealed (10^{-5} Torr) into high quality

> 3rd International Conference on Condensed Matter and Applied Physics (ICC-2019) AIP Conf. Proc. 2220, 110028-1–110028-4; https://doi.org/10.1063/5.0001476 Published by AIP Publishing, 978-0-7354-1976-6/\$30.00

quartz tube. The sealed tube was then sintered inside a tube furnace with a rate of 2°C/min. up to 950°C, kept there for 24 h and then slowly cooled down to 650°C at a rate of 2°C/h. Further, the tube furnace was allowed to cool to room temperature naturally. The obtained sample was shiny and silver in color, which was mechanically cleaved for further characterizations.

XRD pattern had been performed using a Rigaku Made Mini Flex II X-ray diffractometer and SEM study followed by EDS were performed on Bruker made scanning electron microscope. Further, magneto resistance measurements were carried out by a conventional four-probe method on a Physical Property Measurement System (PPMS-10Tesla) using a close cycle refrigerator.

RESULT AND DISCUSSION

Figure 1(a) shows the Rietveld fitted room-temperature XRD pattern of a crushed piece of Bi₂Se₃ crystal. All peaks are well fitted confirms that the sample is crystallized in single phase having a rhombohedral structure within the R³m space group [7]. The lattice parameters as obtained from the Rietveld refinement are a = b = 4.15609(3) Å, and c = 28.73611(8) Å and the values of α , β and γ are 90°, 90°, and 120° respectively.

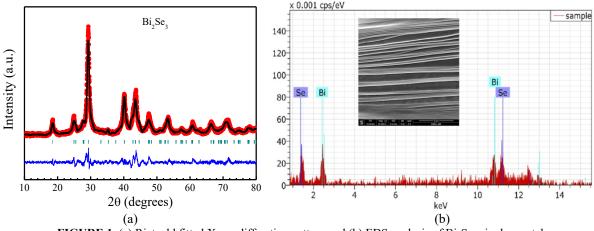


FIGURE 1. (a) Rietveld fitted X-ray diffraction pattern and (b) EDS analysis of Bi₂Se₃ single crystal and inset is SEM image of same.

SEM and EDS analyze the surface morphological characteristics, as well as the chemical composition of the as grown Bi_2Se_3 single crystal. Fig. 1(b) exhibits the EDS spectrum with SEM image in inset view of as grown Bi_2Se_3 single crystal. The SEM image of the studied single crystal exhibits layered type crystal morphology [8], and the quantitative weight% of the atomic constituents (Bi and Se) is found to be near the stoichiometric amount. Apparently, the studied crystal seems to be pure, composed of only Bi and Se atomic constituents present in the studied sample.

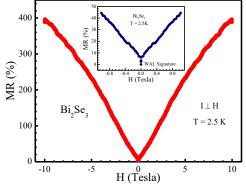


FIGURE 2. Magneto resistance (MR%) as a function of varying applied magnetic field from -10 Tesla to +10 Tesla for pure Bi₂Se₃ single crystal at 2.5K temperature, inset shows the zoomed part of same in low field range from -1Tesla to +1Tesla.

Figure 2 shows the magneto resistance (MR%) as a function of varying applied magnetic fields from ± 10 Tesla to ± 10 Tesla for Bi₂Se₃ single crystal at 2.5 K temperature. Almost a linear curve is found with increase in magnetic field. A clear v-type cusp around origin is seen at lower magnetic field. Thus, at lower magnetic field a sharp dip like positive MR is observed in absence of any magnetic scattering. This type of behavior is known for the signature of WAL effect in earlier reports [9, 10]. The inset of fig. 2 shows the closed view of MR% up to ± 1 Tesla applied magnetic field.

The surface states dominated conductivity of topological insulators is known to follow the HLN (Hikami-Larkin-Nagaoka) equation as below [11]

$$\Delta\sigma(H) = \sigma(H) - \sigma(0) = -\frac{\propto e^2}{\pi h} \left[\ln(\frac{B_{\phi}}{H}) - \Psi\left(\frac{1}{2} + \frac{B_{\phi}}{H}\right) \right]$$

Here, $\Delta\sigma(H)$ represents the change of magneto-conductivity, $\sigma(0)$ conductivity at zero magnetic field, α is a coefficient signifying the type of localization, \mathbf{e} denotes the electronic charge, \mathbf{h} represents the Planck's constant, Ψ is the digamma function, \mathbf{H} is the applied magnetic field, $B_{\varphi} = \frac{\mathbf{h}}{8e\pi(I_{\varphi}^2)}$ is the characteristic magnetic field and \mathbf{l}_{φ} is the phase scheme \mathbf{r}_{φ} by the scheme \mathbf{r}_{φ} is the characteristic magnetic field \mathbf{r}_{φ} is the characteristic magnetic field \mathbf{r}_{φ} .

is the phase coherence length. The HLN fitted magneto-conductivity plots for Bi₂Se₃ single crystal at 2.5 K in various field ranges of 2, 4 and 6 Tesla are shown in figure 3. The obtained values of α are -0.48, -0.45 and -0.41 at 2, 4 and 6 Tesla respectively. On the other hand the values of l_{ϕ} are 81.58, 88.42 and 99.44 nm at 2, 4 and 6 Tesla respectively. The value of α is associated with different types of localizations (WL, WAL or both WL and WAL). The overall value of α decides the type of spin-orbit interactions (SOI and magnetic scattering) [11]. In present case the value of α is close to -0.50, which is known to be a strong SOI case without any magnetic scattering [11]. As it is near to -0.50 indicates WAL contribution of Bi₂Se₃ crystal in conduction mechanism, which is in agreement with MR(%) measurement (shown in fig. 2). The HLN fitted values of α and l_{ϕ} are tabulated in Table 1. There is general trend that the value of pre-factor α increases with increase in fitting ranges of the field. As well, the values of phase coherence length (l_{ϕ}) increase with increase in fitting ranges of the magnetic field.

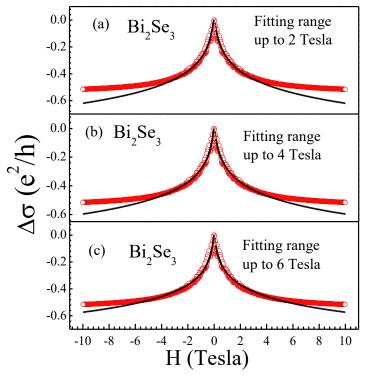


FIGURE 3. HLN fitting in the field range of (a) up to 2Tesla (b) up to 4Tesla (c) up to 6Tesla for Bi2Se3 crystal

Magnetic Field Range	pre-factor (α)	Phase coherence length (l _{\$\phi\$}) (nm)	Fitted parameter (R ²)
±2 Tesla	-0.48	81.58	0.9691
±4 Tesla	-0.45	88.42	0.9855
±6 Tesla	-0.41	99.44	0.9849

TABLE 1: HLN fitted values of the pre-factor (α), phase coherence length (l_{ϕ}) and fitted parameter (R^2) at 2.5K temperature for
Bi₂Se₃ single crystal in different magnetic field range.

CONCLUSION

The Bi₂Se₃ crystal has been grown successfully through the conventional solid-state reaction route. Rietveld fitting of PXRD confirms the phase purity of as grown crystal. The obtained results from SEM and EDS measurement confirm the growth of single crystal, which exhibits layered structure and the quantitative weight % of the atomic constituents (Bi and Se) are close to the stoichiometric amount. Magneto-transport measurement is carried out up to ± 10 Tesla, a v-type cusp around origin is seen at lower magnetic field, which shows the signature of WAL effect, in the Bi₂Se₃ sample at temperature around 2.5 K. The change in magneto-conductivity has been estimated with the HLN fitting, the values of α (type of localization) and l_{ϕ} (Phase coherence length) obtained which validate the WAL state in conduction mechanism of Bi₂Se₃ crystal.

ACKNOWLEDGMENT

The authors would like to thank Director NPL, India for his keen interest in the present work. Author would like to thanks CSIR, India for research fellowship and AcSIR-NPL for Ph.D. registration.

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