Study of local structure around Bi in Topological insulating materials $(Bi_{1-x}Sb_x)_2Te_3$ using extended x-ray absorption fine structure technique

Rajashri R. Urkude* and Umesh A. Palikundwar
X-ray Research Laboratory, Department of Physics, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur, India.
rajashriurkude@gmail.com* uapali@nagpuruniversity.nic.in

Abstract

Topological insulators (TIs) are new and interesting class of materials (A_2B_3 type i.e. Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3) attracting a great attention in condensed-matter physics, due to their high potential technological applications and physical properties. In TIs, the bulk energy band gap is comparable to that of an ordinary insulator while the surface exhibits conducting type of behaviour. This suggests the different kind of electronic and local structures in bulk and at the surface. Bi_2Te_3 is a well-known example of three-dimensional TIs with the gapped bulk band structure and topologically protected surface states with Dirac-like energy-momentum dispersion and spin-momentum locking. The surface states are protected by time-reversal symmetry and are immune to surface impurities and backscattering.
In this work, we have carried out a systematic study of local structure around Bi in Topological insulating materials $(Bi_{1-x}Sb_x)_2Te_3$ ($0 < x < 0.9$). Samples have been prepared by precipitation method and characterized by powder x-ray diffraction (XRD) method. Extended x-ray absorption fine structure (EXAFS) measurements were carried to get the local structure around Bi. The crystal structure of the samples were found to be rhombohedral with R-3m symmetry. The XRD data were analyzed via the Rietveld refinement method. The lattice parameters and the atomic coordinates obtained from the refinements were used as inputs for the powder cell program to visualize the crystal structure of the samples. The atoms are arranged within quintuple layer, in the sequence of Te2-Bi/Sb-Te1-Bi/Sb-Te2 stacked along the c-axis of the unit cell. A systematic study of the local structure around Bi in the bulk level have been carried out by EXAFS measurements associated with the Bi L_{III} edge in transmission and fluorescence modes. EXAFS experiment was performed at Beamline BL-09 Scanning EXAFS of Indus-2 synchrotron source at Raja Ramanna Centre for Advanced Technology (RRCAT), India. Analysis of EXAFS data reveals that, Sb atoms are substituted for Bi sites within the quintuple layers, which shows a trivalent character. EXAFS measurements have provided the local structure parameters in term of the bond distances and coordination number for the different shells. This information is useful in understanding and correlating the bulk topological insulating states with structural parameters in these compounds.

Keywords: topological insulators, time-reversal symmetry, quintuple layer, EXAFS

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