Se K edge EXAFS study of 3d transition metal doped Topological insulator $Bi_{2-x}Mn_xSe_3$

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Topological insulators (TIs) attracted a lot of attention in recent years. While in the bulk they behave like ordinary insulators, their surface states are quite extraordinary. The 2D topological surface states have a conical energy momentum dispersion and spins of electrons are locked to their momentum. Such properties promise many applications in spintronics and quantum computing. Doping of topological insulators by magnetic ions breaks the time reversal symmetry and opens a gap in the energetic structure. This allows a long range magnetic order, which may lead to a number of striking topological phenomena. Recently, transition metal (TM) doped TIs have been the focus for the studies due to the exotic quantum and magneto-electric effects exhibited by them, and their expected high potential technological applications.
In this work, we have carried out a systematic study on 3d TM doped Topological insulator $Bi_{2-x}Mn_xSe_3$ ($0 < x < 0.9$). The samples of $Bi_{2-x}Mn_xSe_3$ have been successfully synthesized by precipitation method. The crystal structure of the samples were found to be rhombohedral with R-3m symmetry. The powder X-ray diffraction 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 unit cell consists of 15 atomic layers grouped in three quintuplets with Se–Bi–Se–Bi–Se order. The quintuplets are van der Waals bonded to each other by a double layer of Se atoms. This gap is larger than other interlayer distances in the structure and it is expected to host extrinsic atoms in the case of Mn doping. There are two possible symmetric positions within the gap – distorted octahedral and distorted tetrahedral. Both the positions are surrounded by Se atoms. Other possibility is that extrinsic Mn atoms can substitute Bi atoms. Here we report a systematic study of the local structural environment surrounding Se in the materials $Bi_{2-x}Mn_xSe_3$. EXAFS measurements were carried out on the Se K edge in transmission mode at Beamline BL-09 Scanning EXAFS of Indus-2 synchrotron source at Raja Ramanna Centre for Advanced Technology (RRCAT), India.
Analysis of the Se K edge EXAFS reveals a change in local environment around Se due to doping of Mn in the compound. This may be due to substitutional as well interstitial positions occupied by Mn atoms in the basic Bi_2Se_3 crystal structure. Our results point towards strengthening of covalent character of the Mn-Se bond. This information will be helpful in understanding the exotic physical properties of magnetic impurity doped topological insulators.

Keywords: Topological Insulators, EXAFS, Time Reversal Symmetry, Doped Topological Insulators

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