Distribution of Mn dopants in Bi_2Se_3 single crystals

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Bi_2Se_3 single crystals belong to the class of materials called Topological Insulators (TI). These are insulators in the bulk with surface states protected by time reversal symmetry, that is resistant to non-magnetic impurities, defects and geometry deformations. Although magnetic dopants are expected to destroy these unique properties, thin films of TI doped with V and Cr reveal robust ferromagnetic ordering and quantum anomalous Hall effect, a prerequisite of non-trivial topology. This opens up a possibility to externally control magnetic properties of TI, which is important both for fundamental and technological interest, particularly in view of recent developments in magnetoelectrics and spintronics.

Among crystalline TI the long range magnetic order is established only in the Mn doped Bi_2Te_3 in the temperature range $T_C < 12$ K [1,2]. On the other hand, the ordering temperature of Mn doped Bi_2Se_3 is significantly lower [3]. Magnetic susceptibility of this system depends strongly on stoichiometry that is tentatively ascribed to the differences in relative distribution of Mn dopants between Bi sites and interstitial position within quintuple layers (QL) and van der Walls (vdW) gap.

We performed systematic studies of the distribution of Mn dopants in single crystalline Bi_2Se_3 by means of Extended X-ray Absorption Fine Structure (EXAFS) analysis, supported by Density Functional Theory (DFT) calculations. It revealed that substitution sites and O_h vdW interstitials are occupied by Mn dopants, as observed in thin films [4]. However, the other kind of interstitials, i.e. O_h QL and T_d vdW, although less abundant, are recognized as well. The latter were rationalised by the cohesive energy of different Mn interstitials in Bi_2Se_3 structure provided from *ab initio* calculations and related to the results of bulk magnetic measurements.

References:

[1] J. Choi, S. Choi, J. Choi, *et al.*, *physica status solidi (b)*, 2004, **241**, 1541–1544.
[2] Y. S. Hor, P. Roushan, H. Beidenkopf, *et al.*, *Phys. Rev. B*, 2010, **81**, 195203.
[3] L. J. Collins-McIntyre, M. D. Watson, A. A. Baker, *et al.*, *AIP Advances*, 2014, **4**, 127136.
[4] A. I. Figueroa, G. v.d. Laan, L. J. Collins-McIntyre, *et al.*, *J. Phys. Chem. C*, 2015, **119**, 17344.