Occupancy disorder and magnetism in tetradymite based topological insulators

Laura Christina Folkers[1,2,3] , Anna Isaeva[3,4]

[1]*Technical University Dresden, Dresden, Germany;*
[2]*Institute for Solid State and Materials Physics, TU Dresden, Germany;*
[3]*Leibniz Institute for Solid State and Materials Research, Dresden, Germany;*
[4]*University of Amsterdam, Amsterdam, The Netherlands*

laura_christina.folkers1@tu-dresden.de

Magnetic topological insulators (MTIs) are a hot topic of materials science, promising future availability of spintronics with low energy consumption, quantum computing and phenomena like the Quantized Anomalous Hall Effect (QAHE) [1-2]. MTIs are chemically and structurally akin to the original non-magnetic topological insulators. Of those, the tetradymites Bi_2Te_3 and Sb_2Te_3 have recently proven to allow the introduction of a third magnetic element resulting in magnetically active, topologically non-trivial compounds. A magnetic element can be incorporated either via substitution on the Bi/Sb position in $(Bi, Sb)_2Te_3$, or by adding a third element which introduces a new crystallographic site, resulting for example in $MnBi_2Te_4$. $(Bi, Sb)_2Te_3$ itself and all members of its family exhibit the rhombohedral $R\bar{3}m1$ space group (No. 166) [2]. Therein interchanging sheets of Mn, (Bi, Sb) and Te build septuple layers with the central sheet being Mn (Wyckoff position 3a). Situated between the respective layers is a van der Waals gap (Fig. 1).

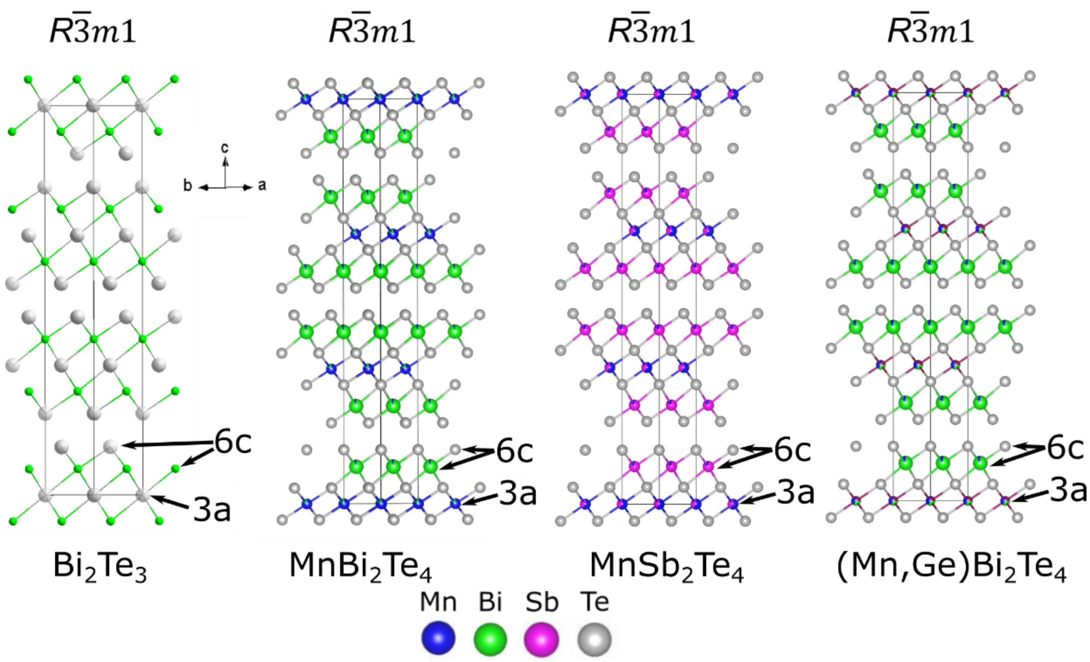

Figure 1: The structure of Bi_2Te_3 [3], $MnBi_2Te_4$, $MnSb_2Te_4$ and $(Mn, Ge)Bi_2Te_4$. All of those compounds are classified as topological insulators and are currently being investigated by us.

Our group was the first to successfully grow single crystals and conduct an in depth study of the physical properties of $MnBi_2Te_4$ [4-5]. Single crystal diffraction experiments reported in that study showed intermixing of Mn and Bi and since then several studies have reported intermixing of the two elements ($MnBi_{2.14}Te_{3.96}$ [6], $Mn_{1.01}Bi_{1.99}Te_4$ and $Mn_{0.98}Bi_{2.05}Te_4$ [7]). While a lot of attention has been given to $MnBi_2Te_4$, $MnSb_2Te_4$ proved to be synthetically achievable too. Similar to $MnBi_2Te_4$, $MnSb_2Te_4$ features intermixing of Mn and Sb ($Mn_{0.852}Sb_{2.296}Te_4$ [8]). For $MnSb_2Te_4$, a recent study by Murakami et al. uncovers the impact of finding a certain amount of the magnetic Mn on the position of the non-magnetic Sb [9]. According to their discoveries, this changes the magnetic order from antiferromagnetic to ferrimagnetic.

These compounds are known to react sensitively to synthesis procedure and tempering history. Hence, our studies aim at understanding the greater connection between synthesis aspects and the resulting structural and physical properties. More precisely we studied $MnBi_2Te_4$ and $MnSb_2Te_4$ containing various amounts of Mn and other analogues of these systems. In these studies we uncovered, that the magnetism in $MnSb_2Te_4$ is even more sensitive to annealing procedures than previously expected.

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