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# How Occupancy Disorder Impacts Magnetism in Topological Insulators

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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 Bi2Te3 and Sb2Te3 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)2Te3, or by adding a third element which introduces a new crystallographic site, resulting for example in (MnBi2Te4)(Bi2Te3)m (m = 0, 1, 2). (Bi, Sb)2Te3 itself and all members of its family exhibit the rhombohedral *R* -3 *m* 1 space group (No. 166) [2]. Therein interchanging sheets of (Bi, Sb) and Te build (Bi, Sb)2Te3 quintuple layers and 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) and depending on m, various stacking orders can be observed.
Our group was the first to successfully grow single crystals, and conduct an in depth study of the physical properties of MnBi2Te4, the m = 0 member of the above discussed MTI family [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 (MnBi2.14Te3.96 [6], Mn1.01Bi1.99Te4 and Mn0.98Bi2.05Te4 [7]). While a lot of attention has been given to MnBi2Te4 and its higher order relatives, MnSb2Te4 proved to be synthetically achievable too. Similar to MnBi2Te4, MnSb2Te4 features intermixing of Mn and Sb (Mn0.852Sb2.296Te4 [8]). For MnSb2Te4, 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 MnBi2Te4 and MnSb2Te4 containing various amounts of Mn and other analogues of these systems.

Figure 1: The structure of Bi2Te3 [3] and the stacking variants (MnBi2Te4)(Bi2Te3)m (m = 0 - 2). For clarity, only 1/3 of the unit cell of MnBi6Te10 is displayed.

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