ESRF	**Experiment title:** Probing the Mn incorporation and magnetic anisotropy in magnetically doped topological insulators Bi_2Se_3 and Bi_2Te_3 using XLD and XMCD	**Experiment number**: HC-2077
Beamline: ID 12	**Date of experiment**: from: 25.11.2015 to: 02.12.2015	**Date of report**: 26.02.2016
Shifts: 21	**Local contact(s)**: F. Wilhelm	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

A. Ney*, V. Ney, G. Bauer, G. Springholz* (JKU Linz), T. Hesjedal (Univ. Oxford), O. Caha* (Univ. Brno)

Report:

The aim of the proposal is to study incorporation of Mn into the two topological insulators (TIs) Bi_2Se_3 and Bi_2Te_3 by x-ray linear dichroism (XLD) and to determine the associated magnetic properties using x-ray magnetic circular dichroism (XMCD) up to high magnetic fields. During the beamtime range of Mn-doped Bi_2Se_3 Bi_2Te_3 samples grown on $BaF_2(111)$ or sapphire substrates were investigated, in addition two bulk samples were also available. For all samples the Mn K-edge XANES and associated XLD were measured as well as the XANES of the Se K- and Te L_1-edges, respectively. The samples grown on sapphire were all thin layers and thus the signal was rather noisy, see for example M2-0171 in Fig. 1. The bulk samples suffered from a variety of Bragg peaks so that in the following only the 1-2 micron thick lavers on $BaF_2(111)$ were studied in more detail. Figure 1 compiles the XANES and associated XLD at the Mn K-edge of the Bi_2Se_3 sample series while Figure 2 shows the Bi_2Te_3 series. Compared to the previous experiment (see report HC-1225) the film thickness was now sufficient to yield a satisfying signal-to-noise ratio and the main findings regarding the spectral shape of the selenide could be confirmed. The XANES and XLD of the telluride series show consistent differences compared to the selenide, namely a more pronounced second peak in the XAENS as well as an altered shape of the XLD spectrum. Simulations of the spectra using the FDMNES code can only reproduce one peak in the XANES which may be indicative that the second peak in the XANES stems from Mn interstitials in the van-der-Waals gap which would be consistent with other findings by EXAFS. IN addition, the XLD of the tellurides shows discrepancies in the first negative peak which seems to be related with the sample series being indicative of some preparation or diffusion-related issues in this class of material. These differences between the selenide and telluride are then further investigated using XMCD.

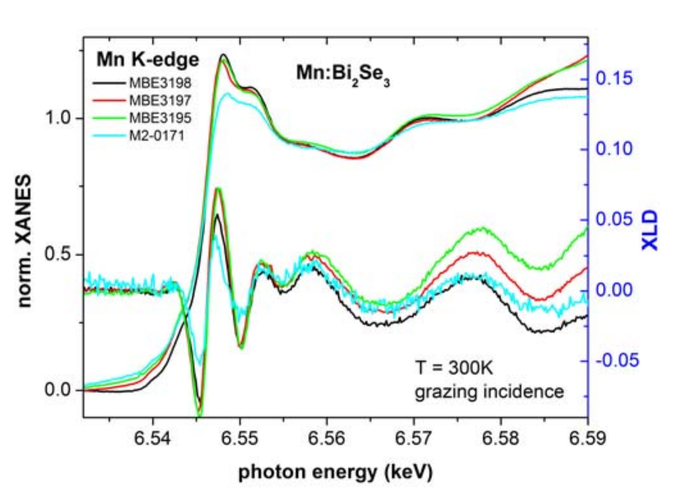

Figure 1: XANES/ XLD at the Mn K-edge for the selenides.

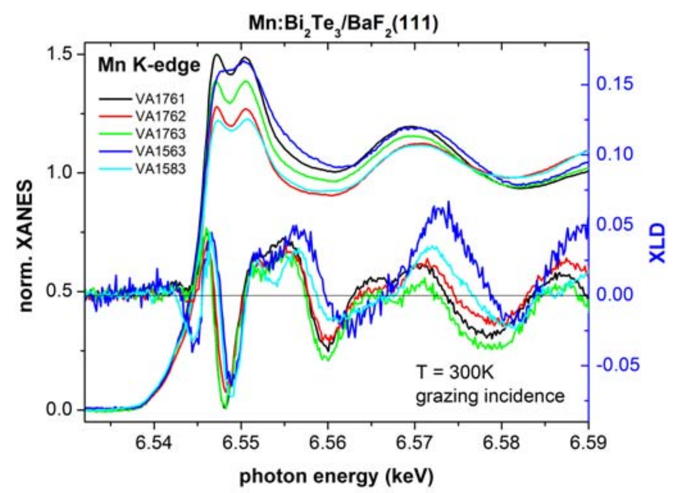

Figure 2: XANES/ XLD at the Mn K-edge for the tellurides.

One sample of the selenide and telluride has been selected for a detailed investigation using XMCD at 2K and up to 17T for both principal orientations of the film. SQUID measurements in the forefield have already revealed that the selenide has a weak in-plane (IP) easy axis while the telluride has a strong out-of-plane (OOP) easy axis. Therefore the XMCD at the Mn K-edge has been measured IP as well as OOP for the selenide (Fig.3, top) and the telluride (Fig.4, top). These reveal that the spectral shape of the XMCD is quite different for the selenide compared to the telluride. Also, the double excitation feature 47eV above the edge is visible in both samples and orientations (see HC-1225). The XMCD(H) curves indicate that the magnetization increases abruptly from remanence and then it only slightly increases up to about 9 T above which it is constant within the noise level of the XMCD. Antiferromagnetic interactions as discussed in HC-1225 are therefore only very weak if present at all. At present it is not straightforward to correlate the different spectral shapes of the Mn K-edge XMCD os the selenide and the telluride with the altered magnetic anisotropy or the opening of the Dirac cone, which is only seen in the selenide. To further shed light onto the magnetic properties also the magnetic polarization at the Se K-edge (Fig.3, bottom) as well as the Te L_1-edge (Fig. 4, bottom) was recorded. While a rather clear XMCD at the Se K-edge together with a clear XMCD(H) trace could be measured here, the weak XMCD at the Te L_1-edge is rather noisy and the XMCD(H) could not be measured any more. This is because the thick film started to delaminate from the substrate and also the second sample piece could not be measured with sufficient statistics any more. Therefore, the important test, whether the weak XMCD signal at the Te L_1-edge is a credible indication of magnetic polarization, could not be made and only the finite magnetic polarization of the Se sublattice can be demonstrated. Nonetheless the magnetic measurements have revealed quite clear differences between the Mn specific magnetic properties of the two topological insulator materials.

In summary, we were able to record many XANES, XLD and XMCD spectra for a large set of samples Mn doped Bi_2Se_3 and Bi_2Te_3 samples. For the selenide we could corroborate the basic findings of HC-1225 now with the absence of severe background issues. Some indications for secondary phase formation remain, in particular the second peak in the Mn K-edge XANES. The comparison to the tellurides revealed some significant differences. The magnetic polarization of the host material was only convincingly measured for the selenide, while the telluride XMCD is too weak to be held of significance.

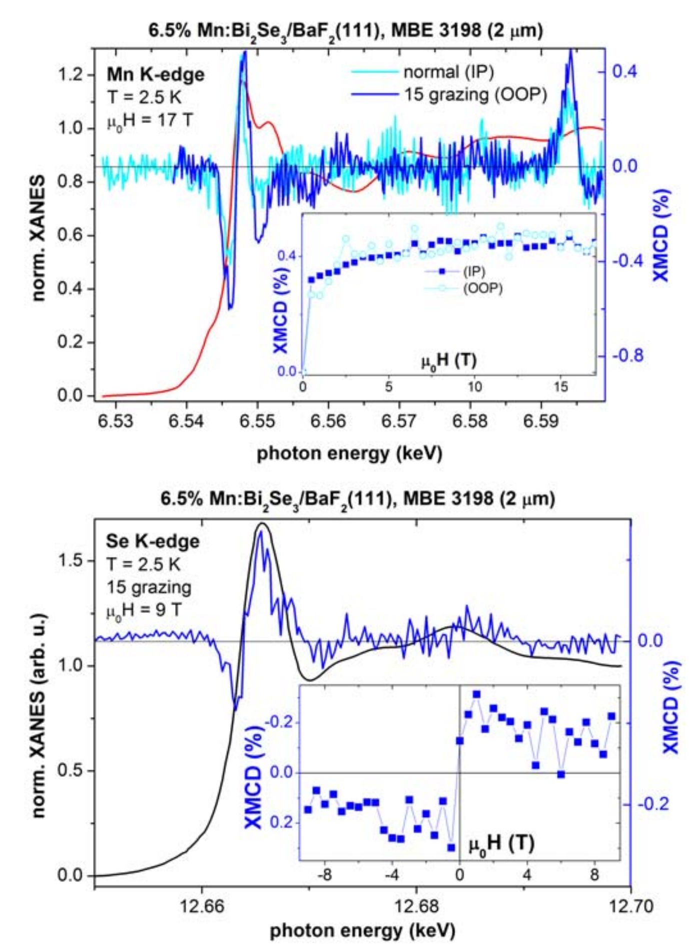

Figure 3: XANES, XMCD and field dependence (insets) at the Mn and Se K-edges of the selenide.

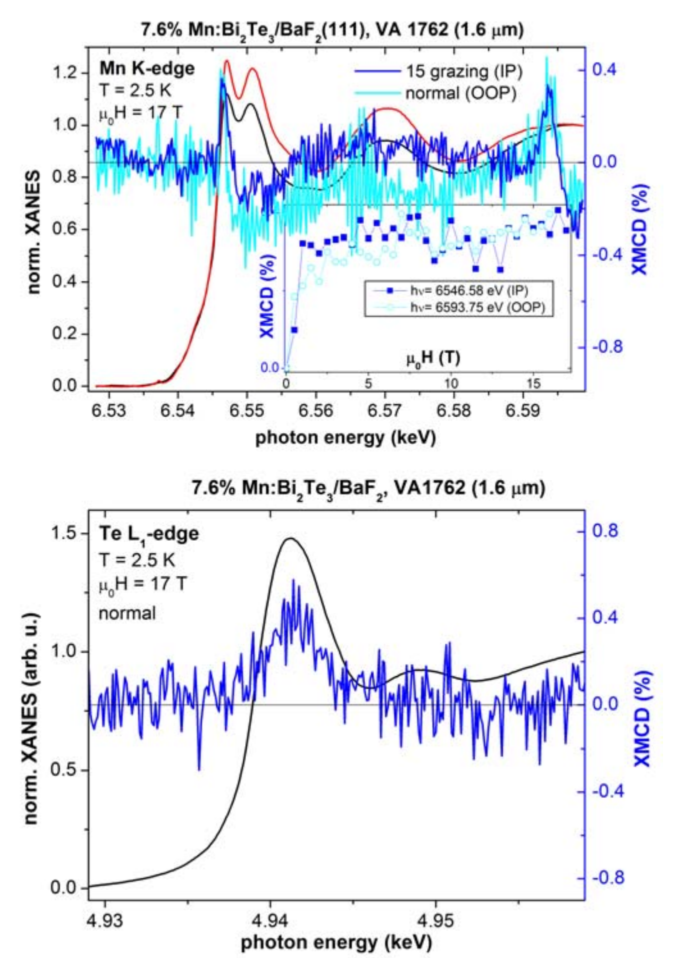

Figure 4: XANES, XMCD and field dependence (insets) at the Mn K and Te L_1-edges of the telluride..