Surface and bulk properties of topological insulators

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The discovery of the quantum spin Hall effect in HgTe [1] has induced extensive investigations of topological phases in three-dimensional (3D) insulators with spin-polarized topological surface states [2, 3]. In particular, Bi-based materials with strong spin-orbit coupling [4], such as Bi_2Te_2Se, and even strongly correlated $4f$ compounds, such as SmB_6 [5], are attracting considerable attention. We have studied the bulk and surface electronic properties of these two topological materials using photoemission spectroscopy in the soft and hard x-ray photon energy regime.

Topological surface states (TSS) in chalcogeniode semiconductors [4], such as Bi_2Te_2Se, have been thoroughly studied by angle-resolved photoemission spectroscopy (ARPES) in the (extreme) ultraviolet photon (UV) energy range (ca. 6–100 eV). Using the ASPHERE III endstation at the P04 beamline of PETRA III we have explored the possibility to probe TSS by ARPES at higher energies above 260 eV. In general, ARPES in the soft x-ray regime is expected to bear a number of conceptual advantages as compared to the UV regime, such as a better justification of the free electron final state assumption and a more bulk-sensitive probing depth going along with a suppression of unwanted influences of surface roughness or contamination [6, 7]. Fig. 1 (left panel) shows an ARPES data set for Bi_2Te_2Se taken at $h\nu = 265$ eV. The TSS near the Fermi energy is clearly discernable in the spectrum with its Dirac-point located at the $\overline{\Gamma}$ point. The dispersion of the TSS shows the typical linear behavior [4]. At higher binding energies we observe a complex band structure which is attributed to the bulk valence states. The present results indicate that TSS can be probed at elevated photon energies above the UV regime. The increased bulk sensitivity of these measurements might be useful e.g. for investigations of heterostructures involving topological materials. Further studies are required to explore whether final state effects in photoemission of TSS are reduced in the soft x-ray as compared to the UV regime [8].

In SmB_6 the opening of a hybridization gap between an f-band with odd-parity and a conduction band with even-parity may lead to the emergence of a topological mixed-valence insulator [9]. The precise nature of the gap in SmB_6 is expected to be related to the f density of states (DOS) near the Fermi energy that, in turn, is determined by the bulk valence of the Sm ion. However, the valences of the Sm ion near the surface and in the bulk and, in particular, their temperature dependence have not been investigated in detail yet. Sm valences of sputtered and annealed surfaces of SmB_6 single crystals show different valences on the surface and in the bulk that were detected by angle-dependent x-ray photoemission measurements using Al Kα radiation ($h\nu = 1486.6$ eV) [10]. In order to support these results by excluding the effect of Ar ion bombardment, we measured the Sm $3d$ core level for cleaved surfaces using photon energies of $h\nu = 2$ keV (surface sensitive) and 6 keV (bulk sensitive) at the beamlines P04 and P09 of PETRA III, respectively.

The photoemission spectra in Fig. 1 (right panel) are normalized to the peak intensity of the $3d_{3/2}$ component of the Sm^{3+} signal. Similar as for sputtered and annealed surfaces [10], the Sm valence near the surface is larger than that in the bulk, i.e. the spectral weight ratio between the Sm^{3+} and the Sm^{2+} contribution is larger for $h\nu = 2$ keV than for 6 keV. The estimated valences are $\sim$2.77 and $\sim$2.62 by using $h\nu = 2$ keV and 6 keV at $T \sim 100$ K, respectively, and $\sim$2.75 and $\sim$2.59 at $T \sim 30$ K, respectively. Thus, the overall temperature dependence of the Sm valence is consistent with the results from x-ray absorption (XAS) experiments [11], which show a decrease in the Sm valence with decreasing temperature. However, our obtained Sm valences show 4% higher values

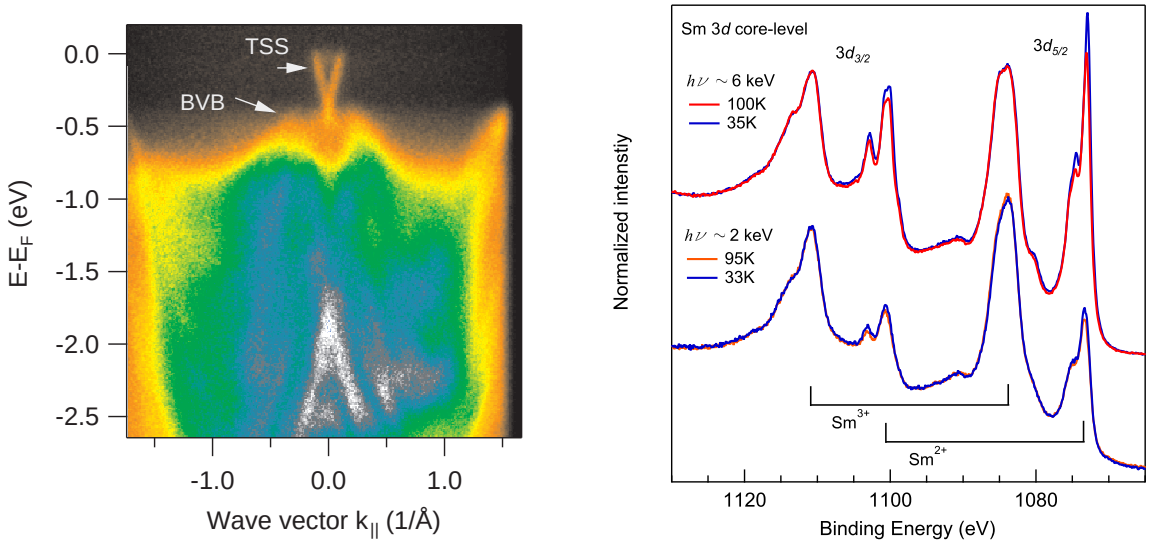

Figure 1: Left Panel: Angle-resolved photoemission data set along the $\overline{\Gamma\mathrm{M}}$ direction obtained at a photon energy of $h\nu = 265\,\mathrm{eV}$ for the topological insulator Bi_2Te_2Se (ASPHERE III endstation at beamline P04). Near the Fermi energy a topological surface state (TSS) with linear dispersion is observed. At higher binding energies the spectrum is dominated by the bulk valence band (BVB). Right panel: Temperature-dependent Sm $3d$ core-level spectra for the topological mixed-valent insulator SmB_6 measured with $h\nu \sim 6\,\mathrm{keV}$ (HAXPES endstation at beamline P09) and $h\nu \sim 2\,\mathrm{keV}$ (ASPHERE III endstation at beamline P04). The spectra were normalized to the $3d_{3/2}$ level of the Sm^{3+} signal. The spectral ratio of Sm^{3+} to Sm^{2+} for $h\nu \sim 2\,\mathrm{keV}$ is larger than for $h\nu \sim 6\,\mathrm{keV}$, indicating an increased Sm valence near the surface.

as compared to the XAS results. Our studies indicate a rather complex behavior of the Sm valence in SmB_6 that should be taken into account in theorectical descriptions of its electronic structure, e.g. based on density functional theory methods [12].

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