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THE RASHBA SPLITTING IN SmB_6

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The present article highlights two aspects at the intersection between Rashba physics and topological matter. This is firstly the importance of the Rashba splitting for the question whether a topological insulator driven by strong electron correlation has been identified in SmB_6. Secondly, the unique nature of the Rashba-split surface state on SmB_6 is revealed by comparison to other experimentally investigated cases.

In 1959, Rashba and Sheka noted that in the inversion asymmetric wurtzite structure under spin-orbit coupling the spin splitting perpendicular to the c axis is linear in momentum k causing a ring of extrema in the band dispersion $E(k)$ [1], the observation that is most commonly associated with the Rashba effect. In 1984, Bychkov and Rashba extended the work to quasi two-dimensional systems [2] extending the scientific field further to heterostructures and surfaces [3–5].

Spin-orbit coupling plays a major role in topologically nontrivial matter [6, 7]. Topological insulators are characterized by topological invariants which leads to symmetry protected surface states. These surface states appear as Dirac cones with a helical spin texture and spin-momentum locking which are known from Rashba-split surface states. The Dirac-cone surface states bridge an inverted bulk band gap and provide in this way surface metallicity in a bulk insulating system, provided the Fermi level is situated in the bulk band gap. The presence or absence of topological surface states can directly be checked by angle-resolved photoelectron spectroscopy (ARPES). The strong topological insulator has an odd number of Dirac-cone surface states per surface Brillouin zone (topological invariant $\nu_0 = 1$), whereas this number is even for trivial materials ($\nu_0 = 0$).

As mentioned above, spin-momentum locking leads to a spin texture that Rashba-type surface states have in common with Dirac-type topological surface states and can be verified by spin-resolved ARPES [3–5]. Another connection between Rashba physics and topologically nontrivial matter is that the topological insulator was at first predicted in a two-dimensional form (where the topologically protected surface states take the form of one-dimensional dissipationless edge states) for graphene under the presence of a sizeable intrinsic spin-orbit interaction [8]. Although carbon is very light, it is in principle possible to impose in the experiment a formally intrinsic spin-orbit interaction in a two-

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dimensional material such as graphene, however, the creation of a Rashba-type spin-orbit interaction is also likely in this geometry [9]. Intercalation of an atomic layer of Au leads indeed to the observation of a giant Rashba splitting in the Dirac cone of graphene [10]. Another aspect where Rashba physics becomes important in topological matter deals with the properties of SmB_6.

Topological insulators are a band structure effect, and an interesting question is whether a topological insulator exists that is caused by strong electron correlation. The material class that has attracted most interest are topological Kondo insulators [11, 12] and in particular SmB_6 [13]. A Kondo insulator has a small band gap due to the Kondo effect, i. e., in this case the hybridization of itinerant conduction electrons and localized f electrons. It was understood that the odd parity of the f states together with the even parity of d states can lead to an inverted bulk band gap and a topological insulator phase [12]. In calculations for the (100) surface of SmB_6, e. g., in Ref. [13], an odd number of Dirac cone surface states per surface Brillouin zone, as required for a strong topological insulator, was predicted. Several groups obverved in ARPES these surface states. In Fig. 1 we show the main features of these data. Four Fermi surface ellipses appear centered at the $\bar{\boldsymbol{X}}$ point (two per surface Brillouin zone) and a surface state at the center $\bar{\Gamma}$, which give an odd number of Dirac cone surface states per surface Brillouin zone, corresponding to a strong topological insulator.

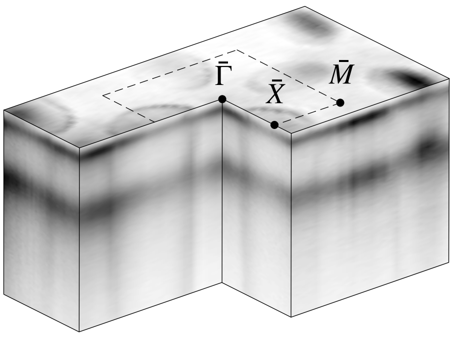

Fig. 1. ARPES data of the Fermi surface of SmB_6(100) showing surface-state contours at the $\bar{\boldsymbol{X}}$ points. An additional surface state is observed at the center $\bar{\Gamma}$

Practically all ARPES studies agreed and have been interpreted in favor of a topologically nontrivial character of of SmB_6, although no Dirac-cone dispersion appears in the data, as can also be seen in Fig. 1. The high quality of our SmB_6 crystals enabled us to observe the dispersion of the $\bar{\Gamma}$ surface state in detail for the first time [14]. For SmB_6 crystals with a B termination of the cleaved surface, the $\bar{\Gamma}$ surface state shows a Rashba splitting [14]. This means that it is not possible anymore to reach an odd number of Dirac cones in the surface Brillouin zone, no matter whether the two ellipses at $\bar{\boldsymbol{X}}$ in the surface Brillouin zone are part of the prediced Dirac-cone surface states or not. New data show the behavior of the Rashba splitting with different light polarization and with surface contamination. Upon surface contamination, the state at $\bar{\Gamma}$ vanishes which is not expected from a robust topological surface state. The $\bar{\boldsymbol{X}}$ state, on the other hand, is robust. We find that this robustness is due to the fact that the state stems from the hybridization of f and d bulk states which are surface-shifted by 10 meV [14]. Because the bulk gap is smaller than 10 meV, the $\bar{\boldsymbol{X}}$ surface state renders the surface metallic, this is the case for B and Sm termination and even more so for surfaces exposed to air [14]. The 10 meV-shift appears also in scanning tunneling spectroscopy [15] and is consistent with published scanning tunneling spectroscopy data.

We determine a Rashba parameter α_R of only $(3.5 \pm 0.1) \cdot 10^{-12}$ eV · m. Because the Rashba splitting is proportional to the effective mass,

$$\Delta k_{\parallel} = \frac{m^* \alpha_R}{\hbar^2}, \quad (1)$$

which has a large value $m^* \approx 17 m_e$ (with electron mass m_e) due to the strong $4f$ character, we are able to observe the Rashba splitting in the ARPES experiment. This peculiarity of f-derived surface states is highlighted in Fig. 2, which also shows that the Rashba splitting in momentum space of SmB_6 is of record size as compared to other surfaces. A large Rashba splitting in momentum space is important in spintronics since it allows for a small channel length in a spin field effect transistor.

In conclusion, the Rashba splitting of the $\bar{\Gamma}$ surface state of SmB_6(100) has been investigated. Because of its very large effective mass it has a record momentum offset at a rather small Rashba parameter. Only for this reason, it was possible to observe its splitting which is essential to characterize the surface electronic structure of SmB_6 as trivial. The reason for the robust surface metallicity of SmB_6 lies in the surface state at $\bar{\boldsymbol{X}}$. The state is a surface shifted $5d$–$4f$ hybrid and trivial where the very small surface shift of 10 meV is sufficient to bridge the bulk band gap.

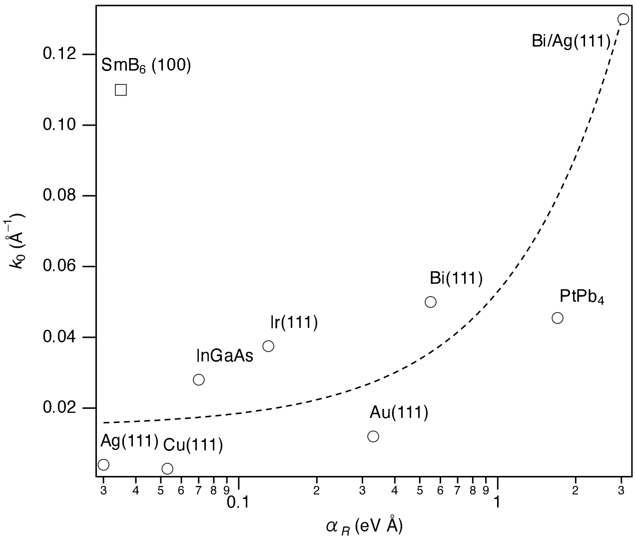

Fig. 2. Rashba splittings in momentum space for different systems. The case of SmB_6 is unique due to the strong $4f$ character and high effective mass

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