Three-Dimensional Spin Rotations at the Fermi Surface of a Strongly Spin-Orbit Coupled Surface System

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Abstract: The spin texture of the metallic two-dimensional electron system (√3×√3)-Au/Ge(111) is revealed by fully three-dimensional spin-resolved photoemission, as well as by density functional calculations. The large hexagonal Fermi surface, generated by the Au atoms, shows a significant splitting due to spin-orbit interactions. The planar components of the spin exhibit a helical character, accompanied by a strong out-of-plane spin component with alternating signs along the six Fermi surface sections. Moreover, in-plane spin rotations toward a radial direction are observed close to the hexagon corners. Such a threefold-symmetric spin pattern is not described by the conventional Rashba model. Instead, it reveals an interplay with Dresselhaus-like spin-orbit effects as a result of the crystalline anisotropies.

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Supplemental Material

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This supplemental material provides details of the band-structure modeling according to Eq. (3):

\[
H(k) = \left( \frac{\hbar^2 k^2}{2m^*} - C + c_h (k_+^6 + k_-^6) \right) \sigma_0 + v(k_x \sigma_y - k_y \sigma_x) + \lambda (k_+^3 + k_-^3) \sigma_z + i \zeta (k_+^5 \sigma_+ - k_-^5 \sigma_-),
\]

where \(\sigma_0\) is the 2 \(\times\) 2 identity matrix, \(\sigma_x, \sigma_y\) and \(\sigma_z\) are Pauli matrices, \(\sigma_\pm = \sigma_x \pm i \sigma_y\), and \(k_\pm = k_x \pm ik_y\). This Hamiltonian is invariant with respect to symmetry operations of the \(C_{3v}\) group and time-reversal symmetry. For the following choice of parameters, the \(E = 0\) energy surface of this model Hamiltonian reproduces well both, the Fermi contour and the spin structure of the metallic surface band in \((\sqrt{3} \times \sqrt{3})\)-Au/Ge(111): \(m^* = 0.4 m_e, C = 0.77 \text{ eV}, c_h = 70 \text{ eV \AA}^{-6}, v = -0.1 \text{ eV \AA}^{-1}, \lambda = -7 \text{ eV \AA}^{-3}, \zeta = 5.5 \text{ eV \AA}^{-5}\).

The first part of the Hamiltonian, proportional to \(\sigma_0\), is the spinless part, giving rise to spin doubly degenerate states. The sixth-order in \(k\) term in the parentheses is responsible for the hexagonal warping of the constant energy contours. This term reproduces well the Fermi contour of our \textit{ab-initio} calculations, before including the spin-orbit interaction.

The second part of the Hamiltonian, \(v(k_x \sigma_y - k_y \sigma_x)\), is the well-known Rashba term. It has full \(O(2)\) symmetry and produces an isotropic spin splitting. The two resulting constant-energy contours (corresponding to \(S_1^A\) and \(S_1^B\)) have a spin texture being fully planar, vortical (clockwise for \(S_1^B\) and counter-clockwise for \(S_1^A\)) and perpendicular to the surface momentum vector \((k_x, k_y)\).

The third part of the Hamiltonian, of third-order in \(k\), was proposed by L. Fu in Ref. 24 in order to explain the hexagonal warping of the Dirac-fermion band at the surface of the topological insulator \(\text{Bi}_2\text{Te}_3\). Apart from affecting the shape of energy contours, it generates a \(z\)-component in the spin vector. This vertical part of the spin exhibits an alternating sign (\(up\) or \(down\)) between neighboring hexagonal sheets of the energy contours. The in-plane part of the spin vector remains, however, perpendicular to the momentum vector \((k_x, k_y)\). Along the \(\Gamma - K\) azimuth, there is no \(z\)-component of spin due to symmetry reasons.

The last term, of fifth-order in \(k\); \(i \zeta (k_+^5 \sigma_+ - k_-^5 \sigma_-)\), was recently proposed by S. Basak \textit{et al.} [25]. This term is needed to explain the \textit{ab-initio} results showing radial rotations of the in-plane spin components for the Dirac-fermion bands at the surface of the topological insulator \(\text{Bi}_2\text{Te}_3\). Similarly as the third-order term, it contributes to the hexagonal warping of the energy contours, but its main function is the rotation of in-plane spin components towards a radial direction. This happens in close vicinity to the \(\Gamma - K\) azimuth.
Figure S1: $E = 0$ energy contours derived from the model Hamiltonian with the in-plane spin texture of the spin-split states (a) $S_{1A}$ and (b) $S_{1B}$. The spin arrows are red for spins directed out-of-plane and blue for an orientation into the plane. Green color signifies fully in-plane spin alignment.

Figure S1 displays the energy contours and spin texture of the model Hamiltonian (Eq. (3)) for the choice of parameters listed above. For better clarity each spin-split state ($S_{1A}$ and $S_{1B}$) is shown in a separate plot.