Berry phase engineering at oxide interfaces

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(Received 15 January 2020; revised manuscript received 3 April 2020; accepted 11 May 2020; published 25 June 2020)

Three-dimensional strontium ruthenate (SrRuO3) is an itinerant ferromagnet that features Weyl points acting as sources of emergent magnetic fields, anomalous Hall conductivity, and unconventional spin dynamics. Integrating SrRuO3 in oxide heterostructures is potentially a novel route to engineer emergent electrodynamics, but its electronic band topology in the two-dimensional limit remains unknown. Here we show that ultrathin SrRuO3 exhibits spin-polarized topologically nontrivial bands at the Fermi energy. Their band anticrossings show an enhanced Berry curvature and act as competing sources of emergent magnetic fields. We control their balance by designing heterostructures with symmetric (SrTiO3/SrRuO3/SrTiO3) and asymmetric interfaces (SrTiO3/SrRuO3/SrIrO3). Symmetric structures exhibit an interface-tunable single-channel anomalous Hall effect, while ultrathin SrRuO3 embedded in asymmetric structures shows humplike features consistent with multiple Hall contributions. The band topology of two-dimensional SrRuO3 proposed here naturally accounts for these observations and harmonizes a large body of experimental results.

DOI: 10.1103/PhysRevResearch.2.023404

I. INTRODUCTION

In topologically nontrivial band structures, electrons acquire an additional phase factor when their wave functions traverse a closed loop in momentum space [1]. Although this concept is now commonly referred to as the Berry phase mechanism, Karplus and Luttinger already demonstrated decades earlier that the anomalous Hall effect—which is prevalent in itinerant ferromagnets—finds its origins in the nontrivial geometry of the band structure and acts as an effective magnetic flux, which generally underlies topological transport phenomena such as the quantum, spin, and anomalous Hall effect (AHE) [1–5]. The anomalous velocity is transverse to the electric field and gives rise to a Hall current, with a sign and magnitude that depend sensitively on the band structure topology. In systems with ferromagnetic order and sizable spin-orbit coupling (SOC), the Berry curvature is strongly enhanced near avoided band crossings, which act as a source or sink of the emergent magnetic field [6]. A prototypical system is the transition-metal oxide SrRuO3 (SRO), a 4d itinerant ferromagnet [7]. Its anomalous Hall conductivity in the bulk depends sensitively on the magnetization and on the position of the Fermi energy with respect to the Weyl points in the three-dimensional (3D) electronic spectra [5,8–10]. Extrinsic (scattering) mechanisms are known to contribute to the AHE in SRO [11–13]. However, when the Weyl points are in close proximity to the Fermi energy the intrinsic Berry curvature mechanism becomes dominant [10], particularly at temperatures far below the Curie point [5,11]. The Berry curvature is particularly sensitive to electronic reconstructions. Accordingly, integrating ultrathin SRO within heterostructures is a promising route to engineer topological transport phenomena. A suitable material for this purpose is SrIrO3 (SIO), a 5d paramagnetic semimetal with strong atomic SOC (∼0.4 eV) [14–18] and excellent structural compatibility with SRO.

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Recently, the behavior and control of the AHE in SRO ultrathin films and heterostructures have been at the center of intense research [19–28], fueled by the observation of humplike features in the transverse resistivity [29]. Such features are generally considered to be a manifestation of the topological Hall effect (THE). In this scenario, noncollinear spin textures give rise to Berry curvature sources in real space [30–32]. Embedding SRO in SrTiO$_3$ (STO) and SrIrO$_3$ (SIO) heterostructures (SIO/SRO/STO) sets a favorable environment for nontrivial spin textures (e.g., skyrmions) because of the strong SOC present in SIO and the breaking of inversion symmetry [19,29]. Moreover, humplike features in the Hall response have also been observed in SRO thin films interfaced with STO and vacuum [33–37], pointing to an important role played by asymmetric boundary conditions and momentum-space sources of Berry curvature. Despite a number of seminal contributions, a unifying scheme is still lacking. In this work we perform a theoretical analysis of the low-energy electronic structure and band topology of SRO in the two-dimensional limit. We reveal spin-polarized topologically nontrivial bands at the Fermi energy, associated with sources of Berry curvature, bringing about competing contributions to the anomalous Hall response. We subsequently use these insights to investigate theoretically and experimentally the AHE in ultrathin SRO films with (a)symmetric boundary conditions. Our results highlight the importance of momentum-space Berry curvature contributions, in addition to the real-space sources discussed so far.

The remainder of the article is organized as follows: in Sec. II we present the methodology regarding the density function theory (DFT) calculations, sample fabrication, and the structural and magnetotransport characterization. Section III is devoted to the main results; (1) the Hall effect measurements in symmetric and asymmetric heterostructures (SRO interfaced with SIO and STO) and (2) the theoretical calculations of the Hall conductivity, combining DFT and effective tight-binding modeling for the designed heterostructures. Section IV contains a discussion and concluding paragraph.

II. METHODS

A. Density functional theory calculations

First-principles DFT calculations were performed using the VASP [38] package based on plane-wave basis set and projector augmented wave method [39]. A plane-wave energy cutoff of 500 eV was used. For the treatment of the exchange-correlation, the LSDA (local spin density approximation) with the Perdew-Zunger [40] parametrization of the Ceperly-Alder data [41] for the exchange-correlation functional was considered. The choice of the LSDA exchange functional is suggested by Etz et al. [42], where it was shown that the LSDA is a better approximation than the generalized gradient approximation for bulk SRO and its heterostructures [43,44]. In our simulations, the STO/SRO/SIO heterostructure was constructed using a lateral supercell of $\sqrt{2}a \times \sqrt{2}a$, where the phases without rotations were contracted using a lateral supercell of $a \times a$. The in-plane lattice parameter was fixed to the STO substrate, while for the out-of-plane lattice parameters the experimental values of the single unit cell of SRO and SIO were used. The hopping parameters were estimated from the electronic structure of the nonmagnetic SRO/SIO and SRO/STO interfaces without Coulomb repulsion. After obtaining the Bloch wave functions from DFT, the maximally localized Wannier functions [45,46] were constructed using the WANNIER90 code [47]. Starting from an initial projection of atomic $d$-basis functions belonging to the $t_{2g}$ manifold and centered on metal sites, the $t_{2g}$-like Wannier functions were obtained. To extract the hopping parameters from the electronic bands at low energies, the Slater-Koster interpolation, as implemented in WANNIER90, was used. This approach is applied to determine the real space Hamiltonian matrix elements in the $t_{2g}$-like Wannier function basis for the SRO/SIO and SRO/STO interfaces.

B. Sample fabrication

SRO/STO, SRO/SIO/STO, and SIO/SRO/SIO/STO heterostructures were prepared by pulsed laser deposition on TiO$_2$-terminated STO(001) substrates. The films were deposited at 600°C in an oxygen pressure of 0.1 mbar. The laser fluence was 1.2 $J/cm^2$ and the repetition rate was 1 Hz. The samples were annealed at 550°C in an oxygen pressure of 300 mbar and cooled down in the same pressure at a rate of 20°C/min. The growth was monitored by reflection high-energy electron diffraction (RHEED), indicating a layer-by-layer growth mode for all three materials.

C. Structural and magnetotransport characterization

Atomic scale characterization of the lattice structure was performed on an aberration corrected STEM. The FEI Titan 80-300 microscope was operated at 300 kV and the samples were prepared in a vacuum transfer box and analyzed in a Gatan vacuum transfer holder to avoid any influence of air on the film [48,49]. Collection angles for HAADF imaging, ABF imaging, and EELS were 44–190, 8–17, and 47 mrad, respectively. The STEM-EELS measurements show that there is negligible diffusion of Ru and Ti, whereas there is a measurable diffusion of Ir into the top RuO$_2$ layer. The heterostructures were further investigated by synchrotron x-ray diffraction measurements and atomic force microscopy (see Sec. I A of the Supplemental Material [50]). Hall bars were patterned by e-beam lithography and the heterostructure was contacted by Ar milling and in situ deposition of Pd and Au, resulting in low resistance Ohmic contacts. An STO capping layer was used to impose symmetric boundary conditions or to prevent degradation of the SIO layer [17,18,51]. Transport measurements were performed in a He flow cryostat with a 10 T superconducting magnet and a base temperature of 1.5 K. Measurements in current-bias configuration were performed by sourcing a low frequency (~17 Hz) 10 $\mu$A current and measuring the resulting (longitudinal and transverse) voltage drop with a lock-in amplifier.

III. RESULTS

We first analyze theoretically the properties of ultrathin SRO, starting from the Ru-based $t_{2g}$ electronic structure close to the Fermi level. Our ab initio derived tight-binding
Evolution of the intrinsic contribution to $\sigma$ the nontrivial bands, which have a predominantly $dxz$ polarizations ary conditions, shown in Figs. 1(e)–1(g). We consider het-
(h) Chern number sector there are two topologically nontrivial bands carrying a presence of SOC. We first focus on the monolayer SRO Fig.1(b) have a nontrivial Chern number, the Berry curvature the avoided bands crossings. Since the lowest energy bands in avoided crossings and causes the bands with opposite Berry sign changes when considering the averaged Berry curvature. leads to a dominance of one of the contributions, including electron occupation. Their splitting and relative occupation changes in the Fermi level or, in general, of the corresponding information regarding the synthesis and characterization of all samples is provided in the Supplemental Material [50].

A complete compensation is improbable and can only occur by electronic fine tuning. SOC influences the character of the hybridization of the Ir $t_{2g}$ bands depends sensitively on the electronic and magnetic reconstruction at the interface. This behavior can be qualitatively captured by modeling Ru/Ti and Ru/Ir bilayers, i.e., systems with a single u.c. of SRO coupled to a single u.c. of STO or SIO. As shown in Fig. 1(h), for small/intermediate amplitude of the Ru magnetization the AH conductivity is negative for the Ru/Ti bilayer, while it is positive for the Ru/Ir bilayer. In the former, only the Ru $d_{xz}$ contribute since the STO is electronically inert, while for the latter, the intrinsic competition of the topological Ru bands is modified through the hybridization of the Ir/Ru $d_{xz}$ orbitals, and interfacial magnetic canting/reconstruction.

To study the effect of asymmetric boundary conditions, we now investigate the tricolor STO/SRO/SIO system (Fig. 2). Given the different trends observed in the symmetric systems, we expect competition in the total $R_{xy}$ in this case. The atomic arrangement at the interfaces is investigated by high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) [Fig 2(b)]. Chemical analysis by electron
energy loss spectroscopy (EELS) shows that the Ti/Ru and Ti/Ir interfaces are atomically sharp, while at the Ru/Ir interface there is a diffusion of Ir into the topmost RuO$_2$ layer. In addition, the thicknesses of both the SRO and SIO layers are 4 u.c. as designed (see also Sec. I C of the Supplemental Material [50]). After quantifying atomic column positions in the HAADF-STEM image using StatSTEM [52], a detailed analysis of the atomic positions shows that octahedral tilts are suppressed and both the SRO and SIO tend to a tetragonal rather than an orthorhombic symmetry as in their bulk form. In addition, we find that the tetragonality ($c/a$ ratio) of the unit cell varies strongly across the SRO and SIO layers [Fig. 2(a)]. Since the magnetic anisotropy of SRO is known to be sensitive to strain and tetragonality [53–55], this affects the local magnetization of the Ru atoms. Theoretical calculations with multilayer configurations corresponding to the designed heterostructures show that the temperature dependent sign change of the AHE is well reproduced by the combined ab initio and tight-binding modeling (see Sec. V D of the Supplemental Material [50]). Furthermore, we demonstrate that the reversal temperature and amplitude of the AH conductance with multilayer configurations corresponding to the designed heterostructures can be considered as a superposition of AH channels with opposite sign and suitable weights [56–58]. Indeed, the data are well described by two such channels, each having a slightly different coercive field [see Fig. 3(a)]. When a current is applied in the plane of the heterostructure and an out-of-plane magnetic field is varied in the range [0, $B$, $-B$, 0], the total AHE is given by the sum of the AHE of the two contributions (this assumption is valid for small Hall angles, which is appropriate for SRO [28], see also Sec. II F of the Supplemental Material [50]). Depending on their relative magnitudes, three different behaviors can be discerned for $B_{ext} < B_{crit}$. In Fig. 3(b) we present a sketch of the corresponding real-space picture. For opposite signs of the anomalous amplitude, majority spin is accumulated on opposite terminals, resulting in opposite Hall voltages. When the anomalous amplitudes are equal in magnitude, the total AHE reduces to zero. In Fig. 3(c) the ordinary Hall component has been subtracted and the remaining anomalous Hall component ($R_{AH}$) is presented. As the temperature is increased from 46 K towards 51 K, the behavior of the total AHE evolves from the leftmost scenario in Fig. 3(a) to the rightmost scenario, with the middle scenario emerging at $T_R = 48$ K. Accordingly, we fit the experimental data with two oppositely oriented AHE loops, as $R_{AH} = R_{AH,||} \text{tanh}[\omega(B - B_{crit,||})] + R_{AH,\perp} \text{tanh}[\omega(B - B_{crit,\perp})]$, where $\omega$ is a parameter describing the slope at $B_{crit}$. An excellent agreement is obtained between this model [dashed black lines in Fig. 3(b)] and the data, enabling us to extract the individual AH components as a function of temperature [Fig. 3(d)]. The corresponding $R_{AH}$ values are shown in Fig. 3(e); both

![Figure 2](image-url)
FIG. 3. Double AHE model. (a) Addition of two AHE contributions with opposite sign of $R_{\text{AH}}$. (b) Illustration showing the opposite spin accumulation of the two individual contributions. (c) Measured total AHE curves with the ordinary Hall component subtracted. The black dashed lines represent a fit to two individual loops. (d) The two anomalous Hall components that add up to the total accumulation of the two individual contributions. (e) Measured total AHE curves with the ordinary Hall component subtracted. The black dashed lines illustrate a possible temperature dependence of $R_{\text{AH}}^0$, and the extracted $R_{\text{AH}}^0$ from the two anomalous Hall components as a function of temperature. The dashed lines illustrate a possible temperature dependence of $R_{\text{AH}}^0$. (f) In- and out-of-plane magnetization for an (green) STO/SRO/STO and (purple) STO/SRO/SIO heterostructure, measured by SQUID.

components show a smooth evolution in temperature, with one disappearing above 58 K (green) and the other below 35 K (purple). At 48 K the two components are equal, leading to the fully compensated case. The dashed lines illustrate a possible dependence of $R_{\text{AH}}^0(T)$ at higher and lower temperatures, which suggests that $R_{\text{AH}}^0$ and $B_0$ of the two contributions follow a qualitatively similar temperature dependence, shifted by 23 K. This implies that, for $T < 35$ K and $T > 58$ K, $R_{\text{AH}}^0$ of the two contributions are of the same sign or the opposite contribution is below the detection limit of our experiment, rendering the total AHE indistinguishable from that of a single spin-polarized contribution (see Sec. II D of the Supplemental Material [50]). We note that any two curves that add up to the total $R_{\text{AH}}$ are in principle possible.

There are various observations to be made concerning the relationship between the emergence of two opposite sign AH channels and the role of (in- and out-of-plane) inhomogeneities in the magnetization. First, we point out that the magnetic anisotropy is strongly affected by asymmetric boundary conditions. Figure 3(f) compares the in- and out-of-plane magnetization for an STO/SRO/STO and STO/SRO/SIO heterostructure. We observe that at STO/SRO interfaces, the out-of-plane component of the magnetization is reduced and an in-plane component emerges. Considering the tetragonality profile discussed in Fig. 2(a), a nonuniform magnetization along the growth axis is expected, giving rise to the emergence of two opposite AH channels as two effective layers. The impact of an inhomogeneous magnetic anisotropy is also deduced from the theoretical calculations performed for an asymmetric STO/SRO/SIO heterostructure with 4 u.c. SRO (see Fig. S20 in the Supplemental Material [50]). Second, we note that an in-plane distribution of coercive fields may also play a role. In this scenario, the plane would be broken up into various domains with different switching fields and different AHE amplitudes. The agreement of the data with the double AHE model then suggests a bimodal distribution of switching fields [Figs. 4(a) and 4(b)]. Such a scenario arises naturally at asymmetric heterostructures, where intermixing with the top layer (SIO) or an incomplete surface termination (vacuum) is common. For the employed phenomenological model, the choice of two AH loops with slightly different coercive fields is generally nonlinear and not equivalent for the electronic
states having opposite sign Berry curvatures, then one can, in general, produce an imbalance with a humplike profile of the Hall response close to the magnetization switching point (see Sec. II E of the Supplemental Material [50]). The two-channel AH model should also be of relevance to other systems displaying the topological Hall effect, provided that a sign inversion is enabled by a temperature-dependent Hall response. It has also been proposed in the context of magnetically doped topological insulators [59].

**IV. CONCLUSION**

Finally, we discuss the scenario proposed here in the context of recent studies performed on SRO thin films and heterostructures, where similar anomalous Hall characteristics were observed and attributed to the topological Hall effect due to a skyrmion phase [19,29,60]. Although within this picture the topological Hall effect would be enhanced in the SIO/SRO/SIO case due to Dzyaloshinskii-Moriya interaction at both interfaces (contrary to our observation), our data cannot exclude contributions from real-space Berry curvature effects due to noncollinear spin textures forming in a specific range of temperature and magnetic fields. Our analysis highlights robust topological effects due to nontrivial Berry curvature in reciprocal space and that this scenario explains the superposition of AH components in asymmetric structures. We remark that, due to the strong connection between the magnetization and AHE, there is likely an interplay between noncollinear magnetism and the momentum-space Berry curvature. Hence, SRO-based heterostructures represent a unique platform to exploit and investigate the interplay of Berry curvature effects in both real and momentum space. The evolution of 3D Weyl points to pairs of topological bands in the 2D limit is a phenomenon that is not limited to ruthenates, but extends to magnetic $t_{2g}$ systems in general. The same holds for the sensitivity of the total Berry curvature to interface effects and thus we expect that similar phenomenology would arise in other heterostructures based on ferromagnetic $t_{2g}$ systems. In this respect, transition-metal oxides are an ideal platform owing to a delicate interplay between spin, charge, and lattice degrees of freedom. Our results establish that oxide interfaces host tunable topological phenomena, thereby providing new perspectives in the field of oxide electronics.

The data that support the findings of this study are available from the corresponding author upon reasonable request.

**ACKNOWLEDGMENTS**

The authors thank Y. Blanter, G. Koster, M. Golden, A. M. R. V. L. Monteiro, I. Lindfors-Vrejoiu, M. Gabay, J.-M. Triscone, S. Gariglio, and M. Kawasaki for discussions. The authors thank M. Gibert for experimental support. This work was supported by The Netherlands Organisation for Scientific Research (NWO/OCW) as part of the Frontiers of Nanoscience (NanoFront) and VIDI program, by the Research Foundation Flanders (FWO, Belgium), and by the European Research Council under the European Union’s Horizon 2020 programme/ERC Grant Agreements No. 677458, No. 770887, and No. 731473 (Quantox of QuantERA).
ERA-NET Cofund in Quantum Technologies). C.A. and S.P. acknowledge financial support from Fondazione Cariplo via the project Magister (Project No. 2013-0726) and from CNR-SPIN via the Seed Project “CAMEO.” C.A. acknowledges the CINECA award under the ISCRA initiative IsC54 “CAMEO” Grant, for the availability of high performance computing resources and support. W.B. acknowledges support by Narodowe Centrum Nauki (NCN, National Science Centre, Poland) Project No. 2016/23/B/ST3/00839. The work is supported by the Foundation for Polish Science through the IRA Programme co-financed by the European Union within SG OP. N.G. and J.V. acknowledge support from the GOA project “Solarpaint” of the University of Antwerp. The Qu-Ant-EM microscope was partly funded by the Hercules fund from the Flemish Government.

The authors declare no competing financial interests.

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