Surface conductivity in antiferromagnetic semiconductor CrSb₂Qianheng Du,^{1,2,*} Huixia Fu,³ Junzhang Ma,⁴ A. Chikina,^{4,†} M. Radovic,⁴ Binghai Yan,³ and C. Petrovic^{1,2,‡}¹Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA²Department of Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, New York 11790, USA³Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel⁴Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

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The contribution of bulk and surface to the electrical resistance along crystallographic b and c axes as a function of crystal thickness gives evidence for temperature-independent surface states in an antiferromagnetic narrow-gap semiconductor CrSb₂. Angle-resolved photoemission spectroscopy shows a clear electronlike pocket in the Γ -Z direction which is absent in the bulk band structure. First-principles calculations also confirm the existence of metallic surface states inside the bulk gap. Whereas combined experimental probes point to enhanced surface conduction similar to topological insulators, surface states are trivial since CrSb₂ exhibits no band inversion.

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Topological states on surfaces of topological insulators (TIs) are of high interest in quantum information and spintronics alike [1,2]. Such conducting states are immune to backscattering-induced localization and exhibit high mobility and electron diffusion length [3,4]. Moreover, they also show efficient spin filtering, strong spin-momentum locking, and a highly efficient and Fermi-level-dependent charge-to-spin current conversion [5–8]. Topological surface states in correlated electron materials were theoretically predicted within the topological Kondo insulator (TKI) framework and experimentally verified on the surfaces of SmB₆ crystals [9–13]. TKIs arise when the bulk insulating gap opens due to the hybridization of $4f$ with conduction electron orbitals of different parities via a band inversion mechanism at the high-symmetry point in the Brillouin zone, and are the embodiment of interacting topological phases of matter [14]. Kondo insulator physics with a reduced Coulomb repulsion has also been proposed for FeSi by Aeppli and Fisk [15]. This was supported by neutron scattering and thermodynamic measurements [16,17]. Interestingly, conducting surface states have also been observed in FeSi [18].

FeSb₂ and CrSb₂ crystallize in an identical marcasite crystal structure and both are FeSi-like narrow-gap semiconductors with a dominant $3d$ character of the electronic states near the valence- and conduction-band edges [19–22].

Whereas the former compound features temperature-induced paramagnetism [19,23], the latter hosts relatively high-temperature antiferromagnetic (AFM) order below $T_N = 273$ K and quasi-one-dimensional (1D) magnons [20,24]. The relation to Kondo insulator physics and surface conducting states has been discussed in FeSb₂ [19,25–29]. In this paper, we demonstrate the existence of the conducting states on CrSb₂; in contrast to SmB₆, topological states are trivial and are formed by Cr $3d$ orbitals.

Single crystals of CrSb₂ were grown as described previously [30]. Electrical transport was measured in a Quantum Design physical property measurement system (PPMS-9). Resistivity was measured by a standard four-probe method. The Hall effect was measured with current along the b axis and magnetic field along the a axis. Angle-resolved photoemission spectroscopy (ARPES) data were taken on *in situ* cleaved crystals along the ac plane at the PSI SIS beamline. The vacuum was better than 5×10^{-11} mbar throughout the measurements.

Figures 1(a) and 1(b) present the temperature dependence of the resistivity $\rho(T)$ for a single crystal as a function of size reduction; the crystal was oriented using a Laue camera and cut along the b and c axis for the resistivity measurement. In order to study the size-dependent resistivity, a bar-shaped sample was cut from a big single crystal along the specific axes and the sample size was varied by polishing. For the current path along the b axis, the crystal was reduced along both orthogonal directions in five steps B1–B5 as the cross section decreased, whereas for the c -axis current path the crystal cross section was reduced in a single orthogonal direction in four steps C1–C4 (Fig. 1 inset). There is a decrease in $\rho(T)$ values down to 20 K, as expected for a semiconductor in all investigated samples. For B1–B5 crystals $\rho(T)$ increases about five times for the sample size decrease from B1 ($360 \mu\text{m} \times 750 \mu\text{m}$) to B5 ($330 \mu\text{m} \times 525 \mu\text{m}$), whereas $\rho(T)$ doubles from C1 ($400 \mu\text{m}$) to C4 ($216 \mu\text{m}$). Below 20 K

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FIG. 1. In both directions, $R(T)$ is well described by a thermally activated semiconducting bulk contribution with a surface contribution. Size dependence of the electrical resistivity for current flow along the (a) b axis and (b) c axis. The resistivities along both axes have a size-dependent plateau from 50 to 80 K (red arrows). The insets show the definition of the sample dimensions. Temperature dependence of the normalized electrical resistance along the (c) b axis and (d) c axis. Solid lines represent fitting using a two-channel conductance model which gives the conductivity for each conducting channel. (e) and (f) show the relationship between the normalized crystal sizes and the ratio of surface contribution to conductance along the b and c axes at different temperatures.

there is no monotonic increase; the c -axis resistivity shows a decrease in $\rho(T)$ with size reduction.

First, we discuss the high-temperature behavior. To eliminate uncertainty in the geometric factor arising from a varying contact geometry, we plot the resistance ratio $R_b/R_b(300\text{ K})$ and $R_c/R_c(120\text{ K})$ for crystals with a current path along the b and c axis, respectively, i.e., the $R(T)$ is normalized to resistance values at 300 and 120 K, respectively [Figs. 1(c) and 1(d)]. The resistance curves show similar qualitative behavior. The change from high-temperature thermally activated behavior to a plateau in $R(T)$ around (80–100) K has been attributed to a strong electron-phonon interaction [20]. This is inconsistent with the thickness dependence of the electrical resistance presented in Figs. 1(c) and 1(d), which shows a clear separation of normalized resistance curves from a single trace at higher temperatures to distinct plateau values for each thickness at that temperature.

A simple parallel conductance model, with a total conductance described by $G = G_S + G_B$, is used to extract the contribution from the bulk and surface. Here, $G_S = 1/R_S$ is the surface contribution, which is assumed to be independent on T . The $G_B = 1/R_B$ is the bulk contribution assumed to be

thermally activated due to a bulk energy gap Δ . Therefore, $R_S = 1/G_S$ and $R_B = 1/G_B \propto e^{\Delta/2k_B T}$, where k_B is the Boltzmann constant, are geometry-dependent resistances. Then $R_b/R_b(300\text{ K})$ and $R_c/R_c(120\text{ K})$ are dimensionless and size-independent resistance ratios,

$$r = \left[\frac{R(T)}{R(T_0)} \right]^{-1} = [r_S]^{-1} + [r_B e^{\frac{\Delta}{2k_B T}}]^{-1}, \quad (1)$$

where $r_S \equiv R_S/R(T_0)$ and $r_B \equiv R_B/R(T_0)$ are dimensionless, normalized surface and bulk resistance ratios ($T_0 = 300$ and 120 K for the b and c axes, respectively) [13].

Fitting results to this model using r_S , r_B , and Δ as free parameters are shown as solid lines in Figs. 1(c) and 1(d). We obtain a size-independent energy gap of $101.9(1) \pm 0.4\text{ meV}$, consistent with our electrical transport measurement and a former report [20]. The calculated ratio of contribution from the surface state G_S/G using the fitted parameters for the size reduction and current paths along the b and c axes are presented in Figs. 1(e) and 1(f), respectively. The values show a clear relation to crystal sizes: For a current path along the b axis where the crystal size was reduced in two orthogonal directions, the ratio G_S^b/G^b exhibits a quadratic dependence on the cross section. For a current path along the c axis where the crystal size was varied along one orthogonal direction, the G_S^c/G^c shows a linear trend with thickness change. This indicates a decreasing relative contribution of the surface conductance relative to the bulk conductance with increasing sample thickness. Conversely, at 65 K, the extrapolated values of $G_S/G \approx 1$ at the zero-thickness (or zero-cross-section) limit denote zero electrical conductance through the bulk, as expected in the bulk-surface model. In the plateau region, the contribution of the surface increases as temperature decreases. This confirms the presence of a surface state in the formation of the $\rho(T)$ plateau.

ARPES measurements [Fig. 2(a)] do not indicate an obvious characteristic of electron-phonon coupling. Hence, it is unlikely that the electron-phonon interaction contributes to the formation of the plateau in temperature-dependent resistivity. There is also a clear electronlike pocket along the Γ_0 - Z_0 direction. This state is absent in the bulk band-structure calculations [22]. It shows a two-dimensional character on the corresponding Fermi surface map and appears in the gap of the bulk band structure, which is consistent with the surface nature of this state. The fitted value of the electron effective mass is $2.18m_e$, where m_e is the electron mass. The corresponding carrier density and Fermi velocity are $1.59 \times 10^{17}\text{ m}^{-2}$ and $2.84 \times 10^5\text{ m/s}$, respectively.

The Hall effect offers further insight into the surface contribution to electronic transport. We used three crystals with different thicknesses: S1 (450 μm), S2 (345 μm), and S3 (156 μm). The Hall resistivity ρ_{xy} at 20 K [Fig. 2(b)] shows a transition from linear one-band behavior (S1) to two-band behavior (S2 and S3) with a thickness reduction. Figure 2(c) shows the Hall coefficient $R_H (= \rho_{xy}/B)$ for S1 and the high-field R_H for S2 and S3. As the high-field limit of R_H is determined only by the number and type of carriers, these can be used to estimate the apparent carrier concentration about 10^{25} m^{-3} . Below 20 K, the Hall coefficients R_H are similar for

FIG. 2. (a) ARPES spectra at the Γ_0 - Z_0 cut in the Brillouin zone measured at 20 K show an electron pocket which is absent in the bulk band-structure calculations. (b) Hall resistivity at 20 K for different samples. Solid lines are fittings. (c) Hall effect measurements show a transition from one-band to two-band behavior with decreasing sample sizes, which confirms the increasing contribution from the surface state with decreasing sample size. Temperature dependence of the R_H (S1) and high-field R_H (S2 and S3).

all crystals, whereas above 20 K the Hall coefficients follow a similar trend but the values for S1, S2, and S3 are different.

All experimental observations above indicate the increase in contribution from the surface states as the thickness decreases. The surface electron concentration in the ARPES measurement is $1.59 \times 10^{17} \text{ m}^{-2}$. This corresponds to effective 3D Hall coefficients of $-1.76 \times 10^{-4} \text{ m}^3/\text{C}$ (S1), $-1.35 \times 10^{-4} \text{ m}^3/\text{C}$ (S2), and $-6.13 \times 10^{-5} \text{ m}^3/\text{C}$ (S3), much larger than the observed value. Hence, both bulk and surface electronic states account for the R_H in S2 and S3 whereas the thick S1 crystal shows single-band behavior since the signal from the surface electrons is dwarfed by bulk electronic states. The two-band electronic transport model

$$\rho_{xy} = \frac{(R_s \rho_n^2 + R_n \rho_s^2)B + R_s R_n (R_s + R_n)B^3}{(\rho_s + \rho_n)^2 + (R_s + R_n)^2 B^2} \quad (2)$$

fits the whole $\rho_{xy}(B)$ curve well [Fig. 2(b)] [31]. Here, R_n and ρ_n are the Hall coefficient and resistivity of the bulk state. $R_s = t/(eN_s)$ and $\rho_s = \rho_{\square}t$ are the Hall coefficient and resistivity of the surface state with $\rho_{\square}$ the surface sheet resistance and t the sample thickness. For S2, the fitting results are the surface mobility $\mu_s = 0.12 \text{ m}^2/\text{V s}$ and the bulk mobility $\mu_n = 7 \times 10^{-4} \text{ m}^2/\text{V s}$, along with the surface carrier concentration $N_s = 1.59 \times 10^{17} \text{ m}^{-2}$ and the bulk carrier concentration $n = 3.7 \times 10^{25} \text{ m}^{-3}$. For S3, the corresponding values are $\mu_s = 0.11 \text{ m}^2/\text{V s}$, $\mu_n = 1 \times 10^{-3} \text{ m}^2/\text{V s}$, $N_s = 1.59 \times 10^{17} \text{ m}^{-2}$, and $n = 4.8 \times 10^{25} \text{ m}^{-3}$, which are quite similar to the results of S2. This confirms the existence of a thickness-independent surface state.

In order to analyze the individual conductivity of the surface and bulk states, we consider the conductivity ten-

FIG. 3. (a) Conductivity vs temperature below 20 K. The sample labels are described in the text. Solid lines are two-band model fitting. (b) Conductivity of the surface (solid) and bulk state (open symbols).

sor $\sigma = \rho^{-1}$, where σ is the sum of surface and bulk contributions [32],

$$\sigma_{xx} = \frac{\sigma_{xx}^s}{t} + \sigma_{xx}^b, \quad (3)$$

and t is the crystal thickness [31]. From the Drude model,

$$\sigma_{xx} = \frac{2n_s|e|}{t} \frac{\mu_s(T)}{1 + \mu_s^2(T)B^2} + n_b(T)|e| \frac{\mu_b}{1 + \mu_b^2 B^2}, \quad (4)$$

where e is the electron charge and n and μ are the carrier density and mobility, respectively. We use the subscripts s and b to denote the surface and bulk contributions. According to the Matthiessen's rule [33] for the electron mobility, the μ_s is treated as $\frac{1}{\mu_s(T)} = \frac{1}{\mu_{s0}}(1 + cT^\gamma)$. The possible temperature dependence of μ_b was neglected since the thermal activation of $n_b(T) = n_{b0} \exp(-\Delta_{bt}/T)$ dominates. The n_s , μ_{s0} , c , γ , n_{b0} , Δ_{bt} , and μ_b are free parameters in a fit to this two-band model of electrical conductivity.

Two crystals were polished to four different samples labeled as R_{ij} where $i = 1, 2$ represents the crystal number and $j = 1, 2$ represents different thicknesses. A larger j value means a thinner sample. The low-temperature conductivities of these samples are shown in Fig. 3(a). The solid lines

FIG. 4. Surface band structures. (a)–(c) Surface structures of CrSb_2 for ac , ab , and bc planes, respectively. The red dots highlight the surface states. Surface states correspond to the AFM magnetic configuration. The Fermi energy is set to zero.

represent the fit of the two-band conductivity model. The two-band model explains the low-temperature conductivity well. From the fitting results, we calculated the surface and bulk contributions [Fig. 3(b)]. The conductivity of the bulk is nearly identical for all samples, which is associated with similar amounts of defects and imperfections. The contribution of the surface state is independent of the temperature, which also confirms the validity of the model used to analyze resistivity at higher temperatures. It is of interest to note that there is a crossover in the conductivity around 15 K. This crossover explains the low-temperature behavior shown in Fig. 1(b). Below the crossover temperature, the conductivity of the surface state is higher than that of the bulk state. As the sample thickness decreases, the contribution of the surface state increases and the total conductivity increases. Above the crossover temperature the trend is opposite due to the higher conductivity of the bulk states.

CrSb₂ surface states feature an enhanced effective mass over the bare electron mass and also a smaller surface mobility when compared to canonical topological insulators [34–36]. However, surface states are 5–20 times smaller when compared to the massive ones observed in SmB₆ [37]. Electronic correlations and AFM order could play important roles in the mass enhancement of the surface state; in that context it is of interest to note that conducting surface states have been observed in FeSi in transport measurements but ARPES data failed to detect such states, possibly due to their location well above the Fermi level [18,38].

We performed density-functional theory (DFT) calculations within the local density approximation [39] using the VASP package [40]. We considered the experimentally reported AFM configuration [20] and obtained an insulating bulk band structure, similar to previous reports [30]. In the AFM bulk structure, the lattice parameters are $a = 6.008$ Å, $b = 13.726$ Å, and $c = 6.536$ Å. The bulk phase is likely a trivial insulator since we do not find a clear topological feature. To simulate the surface states, we constructed slab models for the ac , ab , and bc planes. The slab models inherit the bulk AFM configuration. Then we calculated the surface band structures by including the spin-orbit coupling (SOC).

Figure 4 shows the surface band structure. For different surfaces, there are metallic surface states inside the bulk gap, which exhibit strong SOC splitting. We take the ac plane, for example [Fig. 4(a)]. The ac surface forms a chainlike structure along the c axis. In the momentum space, surface bands follow this anisotropy and are more dispersive along

the Γ -Z direction, compared to the Γ -X direction. Corresponding surface bands are dominantly contributed by the surface Cr 3d orbitals. We note that slab models have atomically flat terminations. In reality, the surface atomic configuration may be strongly disordered, leading to the blurred surface bands, as shown in Fig. 2(a) along the Γ_0 -Z₀ line. When comparing the calculation and the ARPES data, it should be noted that the Brillouin zone is folded along the Γ_0 -Z₀ direction in the calculation with the AFM phase. The surface states entered at the $\tilde{Z}$ point, which is located between Γ_0 and Z₀ in Fig. 2(a); that indicates good agreement between the calculation and experiment. On the other hand, for the bulk band, the ARPES data do not show any band folding between Γ_0 and Z₀, most probably because the AFM-induced magnetic field is not strong enough to dramatically change the electronic structure. Thus, the spectral weight of the folded bands can be too weak to be observed. In brief, both calculations and ARPES show the existence of metallic surface states inside the bulk energy gap, which is consistent with the transport measurement.

In summary, we have presented evidence that CrSb₂ hosts surface conducting states. The thickness-dependent resistivity and the transition from the one-band to two-band Hall effect come from the increased contribution from the surface state as the sample size decreases. The crossover in the conductivity of the bulk and surface states explains the plateau and low-temperature behavior in resistivity. The surface states are also observed in ARPES measurements, in good agreement with electronic transport. First-principles calculations indicate that surface states in the bulk energy gap are topologically trivial.

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APPENDIX

Text regarding tables in appendix.

TABLE I. Fitted parameters r_b , r_s and Delta used in formula (1) for the current path along the b axis. B1-B4 denote crystals in Fig. 1(a).

	B1	B2	B3	B4	B5
$r_b (\times 10^{-2})$	6.1 ± 0.4	6.8 ± 0.4	4.9 ± 0.3	4.5 ± 0.2	4.8 ± 0.2
r_s	31.4 ± 0.2	37.2 ± 0.3	54.4 ± 0.3	72.8 ± 0.3	78.3 ± 0.3
Δ (meV)	50.9 ± 0.2	51.2 ± 0.2	51.1 ± 0.2	50.8 ± 0.2	50.9 ± 0.2

TABLE II. Fitted parameters r_b , r_s and Delta used in formula (1) for the current path along the c axis. C1-C4 denote crystals in Fig. 1(b).

	C1	C2	C3	C4
$r_b (\times 10^{-3})$	3.2 ± 0.4	5.7 ± 0.8	3.5 ± 0.3	2.6 ± 0.2
r_s	6.45 ± 0.05	5.82 ± 0.07	7.01 ± 0.04	7.61 ± 0.04
Δ (meV)	50.8 ± 0.2	49.9 ± 0.2	50.1 ± 0.2	53.1 ± 0.2

TABLE III. Fitted parameters used in formula (4). The R11-R22 denote crystals in Fig. 3. The n_s is fixed to the value obtained from ARPES ($1.59 \times 10^{17} \text{ m}^{-2}$) and the γ is fixed to be 0.

Sample	$\mu_{s0} (\text{m}^2/\text{V s})$	c	$n_{b0} (\times 10^{26} \text{ m}^{-3})$	$\mu_b (\times 10^{-2} \text{ m}^2/\text{V s})$	Δ (K)
R11	0.47 ± 0.05	4.8 ± 0.3	1.0 ± 0.1	1.0 ± 0.2	115.4 ± 3.3
R12	0.40 ± 0.03	1.5 ± 0.1	0.8 ± 0.1	0.8 ± 0.1	112.6 ± 2.1
R21	0.63 ± 0.03	4.2 ± 0.2	1.3 ± 0.2	1.4 ± 0.2	117.9 ± 1.9
R22	0.52 ± 0.04	3.1 ± 0.3	1.2 ± 0.2	1.2 ± 0.1	115.1 ± 1.8

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