de Haas-van Alphen effect and the first-principles study of the possible topological stannide Cu₃Sn

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The quest for quantum materials with diverse symmetry-protected topological states has been the focus of recent research interest, primarily due to their fascinating physical properties and the potential technological utility. In this work, we report on the magnetotransport, de Haas-van Alphen (dHvA) oscillations, and the first-principles calculations of the stannide Cu₃Sn that is isostuctural with the recently reported topological semimetal Ag₂Sn. The magnetoresistance was found to vary quasi-linearly in field. Clear dHvA oscillations were observed under a field as low as 1 Tesla at 2 K, with three major oscillation frequencies $F_\alpha=8.74$ T, $F_\beta=150.19$ T and $F_\gamma=229.66$ T and extremely small effective masses. The analysis of dHvA quantum oscillations revealed a possible nonzero Berry phase, suggestive of the nontrivial band topology. The corroborating evidence for the nontrivial electronic topology also comes from the first-principles calculations which yield a nonzero $Z_2$ topological index. These results collectively suggest that Cu₃Sn, in analogy to its homologue Ag₂Sn, may be another intermetallic stannide hosting topological Dirac fermions.

INTRODUCTION

In recent years, there has been mounting research interest in topological semimetals, such as Dirac semimetals, Weyl semimetals or nodel-line semimetals, ever since the materials classification based on their symmetry and topology was extended from insulators to metals or semimetals [1, 2]. The relativistic fermions in these materials manifest themselves in a plethora of exotic physical phenomena, such as unsaturated linear magnetoresistance (MR) [3], the chiral anomaly effect [4–6], nontrivial quantum oscillations [7, 8] and the anomalous Hall effect [9], etc., thereby opening up the avenue for vast material functionalities and applications in future devices and technologies. Among these topological semimetals, the class of binary stannides has attracted growing attention owing to their intriguing physical properties. For example, inspired by the observation of ultrahigh MR in the binary PtSn₄ [10], the angle-resolved photoemission spectroscopy (ARPES) studies subsequently revealed a novel type of topological phase, namely, the surface-derived Dirac nodes that formed open arcs (rather than a closed loop) in reciprocal space [11]. More interestingly, its sister compound PdSn₄ was reported to possess topological carriers that were significantly enhanced in the effective mass, possibly due to the the vanishing density of states near the Fermi level and the resultant weaker screening of the Coulomb interaction [12]. Remarkably, in some extreme settings, the topological carriers in some stannides may undergo superconducting transitions at low temperatures, thereby raising the possibility to realize the highly sought topological superconductivity in the family of stannides [13, 14].

In this broad context, the topological nodal-line semimetal AuSn₄ was recently reported to host peculiar two dimensional superconductivity with a transition temperature $T_c \sim 2.40$ K arising from its Dirac surface state, leading to the speculation that the topological su-
perconductivity may exist on its surface [13]. In parallel, another stannide Ag₃Sn was also found to exhibit a nontrivial Berry phase in the Shubnikov-de Haas (SdH) oscillations and display a strange angle-dependent magnetoresistance, placing this binary alloy in the shrine of topological materials [15]. A natural question arises as to the topological property of Cu-Sn alloys, since the elements of Au, Ag and Cu reside in the same group in the periodic table. In this work, we address this question in the affirmative.

Here, we report the synthesis of Cu-Sn alloy Cu₃Sn by the solid-state reaction method. Cu₃Sn grown in this way is found to crystallize in the same space group as the previously reported Ag₃Sn [15]. Additionally, quantum dHvA oscillations suggest the nontrivial Berry phase of its underlying carriers; the nontrivial Z₂ index and the Dirac-like surface spectrum revealed by the first-principles calculations are also consistent with the topologically nontrivial states in this material. Taken together, our results suggest that, similar to its analogues AuSn₄ and Ag₃Sn, the Pmmn phase of Cu₃Sn may be another stannide that hosts topological Dirac fermions and therefore merits the in-depth investigations in the future.

**METHODS**

High-quality Cu₃Sn single crystals were synthesized by the self-flux method. Starting materials Copper (Cu, 99.99 %) powder and Tin (Sn, 99.99 %) shots were mixed together in a molar ratio of Cu : Sn = 6 : 5 in a glove box filled with highly pure argon gas (O₂ and H₂O < 0.1 ppm). The mixture was then sealed in an evacuated quartz tube. The quartz tube was heated to 1173 K and kept at this temperature for 10 hours to ensure that the mixture was melt thoroughly. The tube was subsequently cooled to 673 K at a rate of 2 K/h, followed by a furnace-cooling to room temperature. The shiny platelet-shaped Cu₃Sn crystals were finally obtained [see the photographic image shown in Fig. 1]. The X-ray diffraction (XRD) data acquisition was performed at room temperature with a monochromatic Cu Kα radiation using a PANalytical x-ray diffractometer (Model EMPIREAN) radiation by a conventional θ-2θ scan for a crystal mounted on the sample holder. Energy-dispersive x-ray spectroscopy (EDS) was carried out by the Hitachi S-3400 instrument to get the chemical composition of the as-grown crystals. The EDS analysis was performed on the fresh surface of the selected crystals, which gives the average composition of Cu₃.00Sn₃.97, very close to the stoichiometric Cu₃Sn. The detailed results are tabulated in Table S1 of the Supplemental Material (SM). The crystal structure was plotted with the software VESTA [16]. The Laue diffraction was carried out to confirm the crystal structure and the orientations of the crystals. The typical EDS spectrum for the crystal was shown in Fig. 1(d).

**RESULTS AND DISCUSSION**

As reported in the literature, Cu₃Sn can crystallize in several distinct structures, including the space groups of Pmmm [21], F43m [22], Pnma [23], and P6₃/mmc [24]. The XRD pattern of the crystals with the plate-like facet lying on the sample holder at 298 K is shown in Fig. 1(c). A set of diffraction peaks from (00l) can be observed. The interplanar spacing is calculated to be 4.78 Å, very close to the reported lattice parameter of c = 4.74 Å for the orthorhombic Pmmm phase [21]. The full width at half-maximum of the diffraction is only 0.049°, e.g., for the (002) peak, indicating high quality of our crystals. The Laue diffraction photograph along this axis, as shown in the lower panel of Fig. 1(b), further indicates the single crystalline nature of the crystals. Meanwhile, we simulated the Laue diffraction patterns for all possible space groups quoted above in which Cu₃Sn can crystallize. As summarized in the SM, the simulated pattern for the Pmmm phase shows the best consistency with the experimental one on the same scale, thereby corroborating the structural type of our crystals to be Pmmm, isostructural to the intermetallic stannide (IMS) Ag₃Sn [15]. As noted, on the shiny plate-like surface of the crystals, we can observe some striped lines [the left inset of Fig. 1(c)] and striped boundaries [the upper panel of Fig. 1(b)]. Our Laue diffraction measurements indicate those striped lines or boundaries are actually aligned along the crystal...
lographic b axis, which suggests the chemical bonding is much stronger along this direction. The crystallographic structure of Cu₃Sn is displayed in Fig. 1(a), from which we see each unit cell comprised of six Cu atoms and two Sn atoms.

Having determined the a-axis and b-axis of the crystals (see the insets of Fig. 2(a) and (d)), we turn to measure the electrical resistivity along these two directions. The temperature (T) dependence of electrical resistivity ρₐ and ρₜ is shown in Fig. 2(a) and (d), respectively. As seen, Cu₃Sn displays a high degree of metallicity in the whole temperature range studied and has a remarkably low resistivity, i.e., ρₛ = 7.09 μΩ·cm (ρₜ = 9.03 μΩ·cm) at room temperature, falling to 0.11 μΩ·cm (0.21 μΩ·cm) at 1.8 K, yielding an residual resistivity ratio RRR = ρₜ(300K)/ρₜ(1.8K) = 64 (ρₜ(300K)/ρₜ(1.8K) = 43). At low temperatures, ρₐ and ρₜ show a power-law dependence on temperature (see the insets in Fig. 2(a) and (d)), indicating the dominant electron-electron scattering. At high temperatures (e.g., T ≥ 50 K), the resistivity shows quasi-linear behaviors in temperature due to dominant electron-phonon scattering, which can be further modelled with the Bloch-Grüneisen (BG) formula [25]:

$$\rho(T) = \rho_0 + A \left( \frac{T}{\Theta_D} \right)^5 \int_0^{\Theta_D} \frac{x^5}{(e^x - 1)(1 - e^{-x})} \, dx,$$

where ρ₀, A and Θ_D are the residual resistivity, electron-phonon interaction constant, Debye temperature respectively. The red solid lines in Fig. 2(a) and Fig. 2(d) represent the fits with the above equation. The fitting yields ρ₀ = 0.17 ± 0.01 μΩ·cm, A = 22.68 ± 0.02 μΩ·cm, Θ_D

![FIG. 1. (Color online) Crystallographic structure and sample characterizations of Cu₃Sn. (a) The crystallographic structure of Cu₃Sn with an orthorhombic unit cell plotted using VESTA software. (b) Laue picture along the [001] axis (lower panel) and the as-grown crystal (upper panel) on which the Laue picture was taken. (c) Single-crystal x-ray diffraction pattern at room temperature. The right inset enlarges the second reflection in the x-ray diffraction pattern. The left inset is a photograph of the as-grown Cu₃Sn crystals. (d) A typical energy-dispersive x-ray spectrum with electron beams focused on the selected area (marked in the inset).]
\(\frac{\Delta \rho}{\rho_0} = 235 \pm 2 \text{ K for } \rho_b \) and \(\rho_0 = 0.34 \pm 0.01 \mu\Omega\text{ cm, } A = 26.63 \pm 0.02 \mu\Omega\text{ cm, } \Theta_D = 220 \pm 2 \text{ K for } \rho_a.\)

With the magnetic field applied along the c axis, both \(\rho_b\) and \(\rho_a\) show nearly identical \(T\) dependence with that in zero magnetic field, as shown in the insets of Fig. 2(a) and (d), i.e., with no field-induced resistivity upturns. We also measured the field-dependent MR with the magnetic field applied along the c axis at fixed temperatures below 100 K, defined as \(\Delta \rho / \rho(0 \text{ T}) [\Delta \rho = \rho - \rho(0 \text{ T})].\) As shown in Fig. 2(b), the transverse MR of \(\rho_b\) reaches only 154\% at 1.8 K and 9 T and varies quasi-linearly in field without saturation. This quasi-linear MR is more clearly seen in \(\rho_a\) (Fig. 2(e)). In the same setting, the MR in \(\rho_a\) is approximately a factor of 4 larger than in \(\rho_b\) (\(\Delta \rho_b / \rho_a\) reaching a magnitude as high as 642\% at 2 K and 9 T), reflecting the anisotropy in the a-axis and b-axis transport. The nonsaturating quasi-linear MR has been observed in many topological semimetals including WTe\(_2\) [26], PtSn\(_4\) [12], TaPdTe\(_5\) [27] and was invoked as evidence for the existence of topological carriers. For topological materials hosting Dirac fermions with a linear energy dispersion, the linear MR could generically arise due to the small quantum limit in magnetic field [12].

In the framework of the Boltzmann theory, the Kohler’s rule describes the form of MR in magnetic field [28] and has been found to be well obeyed in a large number of standard metals, including the single-band and multiband systems [29, 30]. Generally, the Kohler’s rule simply dictates \(\Delta \rho / \rho_0 = f(H/\rho_0)\) so that the MR at different temperatures will collapse onto a single curve when it is plotted as a function of \(H/\rho_0\). Here \(\rho_0\) is the zero-field resistivity. The violation of this rule implies either the change of carrier density with temperature or the anisotropic electron scattering \(\tau(k)\) that changes the form with temperature [28, 31]. By the same token, the validity of the Kohler’s rule indicates the carrier density does not change significantly with temperature or there is no strange electron scattering of the underlying Fermi surface (FS). The Kohler’s rule in Cu\(_3\)Sn, as plotted in Fig. 2(c) and Fig. 2(f), is overall obeyed, indicating that there is neither strange scattering nor the prominent change of carrier density with temperature. This is conceivable in this Cu\(_3\)Sn system from the Hall measurement. The Hall resistivity \(\rho_{xy}\) as a function of field, measured with the electrical current flowing along the b axis and the magnetic field applied along the c axis, at several fixed temperatures below 200 K, is shown in Fig. 2(g). As seen, \(\rho_{xy}\) varies nearly linearly in field. The linear Hall resistivity in a multiband system indicates either the perfectly compensated electrons and holes, or the dominant one type of charge carriers. From the calculations shown below, the electron pockets dominate in
$\Delta M(10^{-2}\text{ emu/g})$

Cu$_3$Sn. The negative values of $\rho_{xy}$ in the whole temperature range also indicate the dominance of electron-type carriers, consistent with the calculations. The Hall coefficient $R_H$ can be extracted from the linear fitting of $\rho_{xy}$ and was plotted in Fig. 2(h). We find that $R_H$ is only weakly temperature dependent. Since electron-type carriers dominate, the back-of-envelope calculation gives its carrier density and the Hall mobility by

$$n = 1/R_{He} \text{ and } \mu_H = R_H/\rho_0$$

at 5 K, yielding $n \sim 2.68 \times 10^{22}$ cm$^{-3}$ and $\mu_H \sim 4.91 \times 10^6$ cm$^2$/V$\cdot$s$^{-1}$. Because of this high carrier density (comparable to many other systems in which the Kohler’s rule was reported to be valid [31]), it makes the thermally induced changes in the carrier density irrelevant, therefore justifies the validity of the Kohler’s rule in this system.

The isothermal magnetization measured up to 7 T under $B \parallel c$ for Cu$_3$Sn is shown in Fig. 3(a). The dHvA quantum oscillations can be clearly observed when the magnetic field exceeding 1 T at 2 K, and can sustain up to 20 K. The subtraction of the third-order polynomial background results in the oscillatory components of magnetization at corresponding temperatures, presented in Fig. 3(b). From the fast Fourier transform (FFT) analyses of the oscillatory magnetization, we derive three major oscillation frequencies $F_\alpha$, $F_\beta$, $F_\gamma$.

In order to obtain the effective mass $m^*$ for each orbit, the oscillatory dHvA magnetization is further analyzed by the Lifshitz-Kosevich (LK) formula [32], which takes
the Berry phase into account for a Dirac system [33]:

\[ \Delta M \propto -R_T \cdot R_D \cdot R_S \cdot \sin[2\pi \left( \frac{F}{B} + \frac{1}{2} - \frac{\varphi_B}{2\pi} - \delta \right)], \] (2)

where \( R_T = \frac{2\pi^2 k_B m^* T/\hbar B}{\sinh(2\pi^2 k_B m^* T/\hbar B)} \), \( R_D = \exp(-2\pi^2 k_B T_D m^*/\hbar B) \), and \( R_S = \cos(\pi g m^*/2m_e) \) are the thermal damping factor, Dingle damping term, and a spin-related damping term, respectively. \( T_D \) is the Dingle temperature and \( \varphi_B \) is the Berry phase. The oscillation of \( \Delta M \) is described by the sine term with the phase factor \( \frac{1}{2} - \frac{\varphi_B}{2\pi} - \delta \). The additional phase shift \( \delta \) is determined by the dimensionality of the FS, and is equal to 0 for a two-dimensional FS and \( \pm 1/8 \) for a 3D FS. The fitting of the temperature-dependent FFT amplitude to the thermal damping factor \( R_T \), as shown in Fig. 3(d), yields effective masses corresponding to three fundamental frequencies \( m_{\alpha}^* = 0.029(5)m_e \), \( m_{\beta}^* = 0.030(1)m_e \), and \( m_{\gamma}^* = 0.033(6)m_e \) (\( m_e \) is the bare electron mass), all of which are extremely small. With the fixed parameters of three fundamental frequencies and corresponding effective masses, the oscillation pattern can be well fitted by using the LK formula directly. The extracted single-frequency oscillatory signals are plotted separately in Fig. 3(e), and the LK formula well reproduces the oscillations at 2 K. The quantum relaxation time \( \tau_\text{q} \) can be obtained from the Dingle temperature by \( \tau_\text{q} = \hbar/(2\pi k_B T_D) \). The corresponding values for \( T_D \), \( \tau_\text{q} \) and \( m^* \) for different bands are also listed in Table I. The phase factors are fitted to be 1.06 \( (F_\alpha) \), 1.02 \( (F_\beta) \), and 1.29 \( (F_\gamma) \), from which the Berry phases \( \varphi_B \) are derived to be 0.12\( \pi \), 0.37\( \pi \) and 0.13\( \pi \) \( (F_\alpha) \), 0.04\( \pi \), 0.33\( \pi \) and 0.17\( \pi \) \( (F_\beta) \) and 0.58\( \pi \), 1.41\( \pi \) and 0.91\( \pi \) \( (F_\gamma) \) for \( \delta = 0, \pm 1/8 \) and \( \pm 1/8 \), respectively. In general, the Berry phase is zero for a parabolic energy dispersion and \( \pi \) for a linear energy dispersion. A finite Berry phase, deviating from the exact \( \pi \) value, is also possible due to the deviation of the dispersion relation \( E(k) \) from an ideal linear dispersion [34]. In addition,
the Berry phase can be further evaluated using the Landau level (LL) fan diagram [35]. The minima of $\Delta M$ should be assigned to a LL index of $n - 1/4$ [36]. The established LL fan diagram is shown in Fig. 3(f) and (g). The linear extrapolation in the fan diagram yields three intercepts $n_0 = 0.91 \left( F_x \right)$, $n_0 = 0.76 \left( F_\beta \right)$ and $n_0 = 0.68 \left( F_\gamma \right)$, corresponding to a nontrivial Berry phases of $\varphi_B = 2\pi(0.91 + \delta) \left( F_x \right)$, $\varphi_B = 2\pi(0.76 + \delta) \left( F_\beta \right)$ and $\varphi_B = 2\pi(0.68 + \delta) \left( F_\gamma \right)$. The slopes of the LL fan diagram are 8.78 T, 151.19 T and 229.85 T for the $F_x$, $F_\beta$ and $F_\gamma$ bands, respectively, in excellent agreement with the oscillation frequencies identified through the FFT analysis.

In order to gain more insights into the topological properties of Cu$_3$Sn, we investigate, based on the first-principles calculations, the bulk band structures along the high-symmetry lines as shown in Fig. 4(a). Here the spin-orbit coupling is considered. One can observe that Cu$_3$Sn exhibits the metal character. Several bands around the Fermi level cross each other, which in fact open small band-gaps owing to the same double irreducible representation ($\Gamma_2$). Furthermore, as the system respects the inversion symmetry, $\mathbb{Z}_2$ invariant of this system can be evaluated using the Fu-Kane formula as shown in Ref. [37]. We find $\mathbb{Z}_2$=1 by calculating the parities for all the occupied bands at 8 time-reversal invariant momenta [37], suggesting the strong topological state in Cu$_3$Sn. Furthermore, in Fig. 4(b), we show the results of the surface state along $\bar{X} - \bar{\Gamma} - \bar{Y}$ for the (001) surface by combining the Wannier-basis tight-binding model with the surface Green’s function method [38–40]. It is clear to see that there exists nontrivial Dirac-cone-like surface state located at the $\bar{\Gamma}$ point, further supporting the calculation of $\mathbb{Z}_2$=1.

There are four bands crossing the Fermi level $E_F$ and their individual FSs are shown in the SM, which demonstrates strong 3D characteristics. Band 1 and 2 are hole-like while Band 3 and 4 are electron-like. The resultant FSs show strong similarity between two hole(electron)-like pockets and signify the dominance of the electron-like carriers, consistent with the Hall measurements.

**SUMMARY**

In summary, we have successfully grown the high-quality single crystals of an IMS Cu$_3$Sn that is isostructural with the topological semimetal Ag$_3$Sn. The quasi-linear MR and the quantum dHvA oscillations, featuring extremely small effective masses and the possible nonzero Berry phases, suggest that Cu$_3$Sn may be another topologically nontrivial stannide, in common with its analogues Ag$_3$Sn and Au$_3$Sn$_4$. Our first-principles calculations further corroborate its nontrivial band topology. More experiments, such as the angle dependent dHvA oscillations, ARPES, are highly desirable to provide further evidence for its Fermiology and the putative topological states proposed in this study.

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