SPECIAL TOPIC—Superconductivity in vanadium-based kagome materials

A density-wave-like transition in the polycrystalline V$_3$Sb$_2$ sample with bilayer kagome lattice

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Recently, transition-metal-based kagome metals have aroused much research interest as a novel platform to explore exotic topological quantum phenomena. Here we report on the synthesis, structure, and physical properties of a bilayer kagome lattice compound V$_3$Sb$_2$. The polycrystalline V$_3$Sb$_2$ samples were synthesized by conventional solid-state-reaction method in a sealed quartz tube at temperatures below 850 °C. Measurements of magnetic susceptibility and resistivity revealed consistently a density-wave-like transition at $T_{dw}$ ≈ 160 K with a large thermal hysteresis, even though some sample-dependent behaviors were observed presumably due to the different preparation conditions. Upon cooling through $T_{dw}$, no strong anomaly in lattice parameters and no indication of symmetry lowering were detected in powder x-ray diffraction measurements. This transition can be suppressed completely by applying hydrostatic pressures of about 1.8 GPa, around which no sign of superconductivity was observed down to 1.5 K. Specific-heat measurements revealed a relatively large Sommerfeld coefficient $\gamma = 18.5$ mJ mol$^{-1}$ K$^{-2}$, confirming the metallic ground state with moderate electronic correlations. Density functional theory calculations indicate that V$_3$Sb$_2$ shows a non-trivial topological crystalline property. Thus, our study makes V$_3$Sb$_2$ a new candidate of metallic kagome compound to study the interplay between density-wave-order, nontrivial band topology, and possible superconductivity.

Keywords: V$_3$Sb$_2$, kagome metal, charge density wave, pressure effect

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1. Introduction

The kagome lattice compounds consisting of corner-shared triangular network have been the focus of extensive investigations over last decades because they can host fascinating physical phenomena ranging from geometrically frustrated magnetism to nontrivial band topology [1–13]. When the localized moments are situated on the kagome lattice, frustrated spin interactions can lead to exotic magnetic ground states such as the quantum spin liquid state extensively studied in the herbertsmithite ZnCu$_3$(OH)$_6$Cl$_2$. [14–19] On the other hand, when the itinerant electrons are present, the metallic kagome lattice compounds hold the gene to achieve nontrivial electronic band structure containing Dirac cones, flat band, and van Hove singularities. [20–24] Upon proper electron filling, these features can promote novel correlated and/or topological states, such as bond wave order, [23,25] valence-bond state, [26] chiral spin-density-wave (SDW) order, [21] nontrivial charge-density-wave (CDW) order, [1,27–29] exotic superconductivity, [12,23,30] etc. Thus, much experimental effort has been devoted to the metallic 3d transition-metal-based kagome systems.

For the correlated magnetic kagome metals, the coexistence of spin and charge degrees of freedom leads to the emergence of many novel quantum phenomena with nontrivial electronic behaviors. For example, large anomalous Hall effect (AHE) and Dirac fermions have been realized in the ferromagnetic Fe$_3$Sn$_2$ with flat-band dominated electronic band structure [7,31,32] and the quantum-limit Chern ferromagnet TbMn$_6$Sb$_{12}$. [13] Large intrinsic AHE has been observed in ferromagnetic Weyl semimetal Co$_3$Sb$_2$Te$_2$ [6,33,34] and noncollinear antiferromagnetic Mn$_3$Sn$_2$. [35] Dirac fermions have also been revealed in the antiferromagnetic FeSn. [10,36] For the recently discovered AV$_3$Sb$_2$ ($A = K$, Rb, Cs) family with quasi-2D ideal kagome layers of V ions, no static magnetic order was observed but they exhibit the coexistence and complex competition between superconductivity and chiral CDW in addition to giant AHE and pair density wave state. [12,27–29,37–54] For this latter class of materials, there are still many open issues, such as the nature of superconductivity and the mechanism of chiral CDW order.

Since the materials’ realizations are scarce, it is indispensable to find more metallic kagome lattice compounds. To this end, we focus our attention on a simple binary compound V$_3$Sb$_2$, which is isostructural to Fe$_3$Sn$_2$ and contains bilayer...
kagome lattice of V ions. This material has been known to exist at temperatures below $875 \pm 25$ °C in the V–Sb phase diagram, but its physical properties have not been studied in detail to the best of our knowledge. In this work, we successfully synthesized nearly pure V$_3$Sb$_2$ polycrystalline sample and then characterized its structure, electrical transport, magnetic, and thermodynamics properties at ambient or high pressures. Our results reveal a density-wave-like transition at $T_{\text{dw}} \approx 160$ K, which is evidenced by a clear anomaly in both magnetic susceptibility and resistivity. This compound shows no long-range magnetic order and superconductivity down to 1.5 K even after the density-wave-like transition being suppressed completely by hydrostatic pressure. Since our density-functional-theory (DFT) calculations show that V$_3$Sb$_2$ has a non-trivial topological crystalline property, the present study indicates that it may serve as a new metallic kagome system to study the interplay between density-wave-order, nontrivial band topology and possible superconductivity.

2. Experimental and calculation details

Polycrystalline samples of V$_3$Sb$_2$ were synthesized by the traditional solid-state-reaction method. The powders of V (99.99%) and Sb (99.99%) in the molar ratio 3 : 2 were thoroughly mixed and pressed into a pellet, which was then placed into a quartz tube and sealed under high vacuum ($\sim 5 \times 10^{-4}$ Pa). The sealed ampoule was slowly heated to 700 °C and held for 48 hours, and then sintered again at 750–850 °C for 48 hours several times with intermediate grinding and pelletizing. According to the V–Sb phase diagram, the LT-phase of V$_3$Sb$_2$ with the Fe$_3$Sn$_2$-type structure is stable below the peritectoid temperature of $875 \pm 25$ °C, above which the V-deficient V$_3$–Sb phase is more stable. Thus, we have kept the highest sintering temperatures below 850 °C in order to obtain the LT-V$_3$Sb$_2$ with the Fe$_3$Sn$_2$-type structure in the present study. Phase purity of the obtained V$_3$Sb$_2$ polycrystalline samples was examined by powder x-ray diffraction (XRD) at room temperature with a Cu $K_{\alpha1}$ radiation. In order to extract the structural parameters, the refinements of the crystal structure were performed by the Rietveld method, using the FULLPROF program. Low-temperature XRD data in the temperature range 25–300 K were collected using an Oxford Phenix cryostat and a PANalytical X’Pert Pro MPD diffractometer (Cu $K_{\alpha1}$ radiation). The powder was mounted on an aluminum sample holder using Apiezon N-grease. Highscore Plus was used for Rietveld analysis of the XRD patterns from V$_3$Sb$_2$.

The magnetic properties were measured with a Quantum Design magnetic property measurement system (MPMS-III). Heat capacity and electrical transport measurements were carried out by using a Quantum Design physical property measurement system (PPMS, 14 T). High-pressure resistivity was measured by using a self-clamped piston-cylinder cell under various hydrostatic pressures up to 1.81 GPa. Daphne 7373 was used as the pressure transmitting medium and the pressure values were determined from the relative shift of the superconducting transition temperature of Pb.

Our DFT calculations employ the Vienna ab initio simulation package (VASP) code with the projector augmented wave (PAW) method. The Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional is used in our calculations. The kinetic energy cutoff is set to be 600 eV for expanding the wave functions into a plane-wave basis in VASP calculations while the energy convergence criterion is $10^{-6}$ eV. The $\Gamma$-centered $k$-mesh is $8 \times 8 \times 8$. The spin–orbital coupling is included in our DFT calculations. The calculation of topological indices employs vasp2trace program on Bilbao Crystallographic Server.

3. Results and discussion

We have attempted to prepare pure V$_3$Sb$_2$ samples by varying the final sintering temperatures between 750 °C and 850 °C. After tries and errors, we eventually obtained two V$_3$Sb$_2$ polycrystalline samples with relatively high purity as examined by XRD. Hereafter, these two samples sintered at 780 °C and 830 °C are labeled as S1 and S2, respectively. Since their physical properties show some different behaviors, in the following we present the experimental results of both samples comparatively so as to underline the fact that the physical properties of V$_3$Sb$_2$ are sensitive to the preparation conditions.

Figure 1 shows the XRD pattern of these two V$_3$Sb$_2$ samples after Rietveld refinement. It confirms that the obtained samples are nearly single phase with a small amount of impurity, which can be identified as V$_3$Sb for S1. The impurity phase is too weak to be identified for S2. The main phase of the XRD pattern can be refined by considering the hexagonal Fe$_3$Sn$_2$-type structure model (space group R-3m, No. 166) with one V position at the 18h ($x$, $y$, $z$) and two Sb positions at 6c ($0$, $0$, $z$), respectively. As illustrated in Fig. 1, the refinements converge well with reliable factors $R_p = 2.66\%$, $R_{\text{exp}} = 2.48\%$, and $\chi^2 = 2.28$ for S1, and $R_p = 2.98\%$, $R_{\text{exp}} = 2.26\%$, and $\chi^2 = 3.78$ for S2. According to the scaling factors, the amount of V$_3$Sb impurity in S1 was estimated to be $\sim 1.2$ wt%, which is consistent with the observed weak main peak of V$_3$Sb as shown by asterisk in Fig. 1(a). The obtained structural parameters for both samples are listed in Table 1 for comparison. As can be seen, the sample S1 has a shorter $a$ but a longer $c$, leading to a slightly smaller $V$ in comparison with those of sample S2. However, the differences are quite small, with the relative difference being smaller than 0.3%. These lattice parameters are also consistent with those reported in literature for LT-V$_3$Sb$_2$. In contrary, the positions of the atoms, especially along the $z$-axis, show a relatively large difference. Taking the V site as an example, the difference of the...
The crystal structure of V₃Sb₂ is schematically shown in Fig. 2 by taking the refined structural information of S1. As seen in Fig. 2(a), the crystal structure of V₃Sb₂ is composed of Sb₁ single layer and V–Sb₂ bilayer that are stacked alternatively along the c-axis. The Sb₁ atoms in the single layer form a 2D graphene-like honeycomb lattice, Fig. 2(b), while the V–Sb₂ bilayer consists of two V kagome layers with Sb₂ atoms embedded in the center of the V hexagons, Fig. 2(c). For each V kagome layer, there are two kinds of equilateral triangles with different V–V bond lengths, i.e., 2.8600(19) Å and 2.6839(19) Å for S₁ [2.864(4) Å and 2.691(4) Å for S₂], as shown in purple and blue in Fig. 2(d). This means that the kagome lattice is not ideal, different from that in AV₃Sb₅.

The obtained lattice parameters for both samples are also given in the figure.

### Table 1. Lattice parameters, atomic coordinates, and isotropic thermal factors Biso for V₃Sb₂ samples from powder XRD data at 295 K.

| Sample | Space group, Z | a (Å) | c (Å) | V (Å³) | Vₓ | Vᵧ | Vz | Biso, V (Å²) | Sb₁z | Biso, Sb₁ (Å²) | Sb₂z | Biso, Sb₂ (Å²) | Rp (%) | Rexp (%) | χ² | RBragg (%) |
|--------|---------------|-------|-------|--------|-----|-----|-----|-----------|-------|-------------|-------|-------------|--------|----------|----|-----------|
| S₁ (780 °C) | R-3m, Z = 6 | 5.5440(1) | 20.3529(4) | 541.76(2) | 0.49470(15) | 0.50530(11) | 0.11018(11) | 2.65(5) | 0.33189(4) | 2.72(3) | 3.49(4) | 2.66 | 2.48 | 2.28 | 4.35 |
| S₂ (830 °C) | | 5.5545(1) | 20.3374(6) | 543.40(2) | 0.49480(25) | 0.50520(25) | 0.10734(15) | 2.32(3) | 0.33281(5) | 2.41(3) | 0.10908(08) | 2.98 | 2.26 | 3.78 | 4.20 |

Fig. 1. Observed (cross), calculated (solid line), and difference (bottom line) XRD profiles of the polycrystalline V₃Sb₂ samples: (a) S₁ and (b) S₂ after Rietveld refinements. Bragg positions of the main phase V₃Sb₂ and the impurity phase V₃Sb are indicated by the two rows of tick marks in (a), while only the position of V₃Sb is shown in (b). The main peak of the V₃Sb impurity phase is marked by an asterisk in (a).

Fig. 2. (a) A schematic view of the layered structure of V₃Sb₂ (side view) stacked by Sb₁ and V–Sb₂ layers along the c-axis. The unit cell is enclosed by the dashed lines. (b) The Sb₁ atoms form a honeycomb sublattice below and above each V–Sb₂ bilayer with Sb₁–Sb₁ bond length of 3.20 Å. (c) The structure of the V–Sb₂ layer. The V atoms form bilayer kagome lattice and the Sb₂ atoms sit in the centers of the V hexagons in each V kagome layer. (d) Single V–Sb₂ kagome layer made of two kinds of equilateral triangles with the side lengths of 2.8602 Å and 2.6839 Å for S₁ [2.864(4) Å and 2.691(4) Å for S₂], as shown in purple and blue in Fig. 2(d). This means that the kagome lattice is not ideal, different from that in AV₃Sb₅.
As shown in Fig. 2(e), the V atoms of the smaller V triangles in two adjacent layers can be viewed to form a V5 octahedra with an interlayer V–V distance of 2.773(4) Å for S1 [2.870(6) Å for S2]. For S1, this value is equal to the average of two intralayer nearest-neighbor V–V bond lengths. Such a small interlayer distance should produce a relatively strong interlayer interaction. However, the interlayer V–V bond length for S2 is found to be $\sim 3\%$ longer than the average in the $ab$ plane, which might result in weaker interlayer interactions.

Figures 3(a) and 3(b) show the temperature-dependent magnetic susceptibility $\chi(T)$ of these two V3Sb2 samples measured in the temperature range 1.8–300 K under an external magnetic field of $\mu H = 1$ T. The experimental procedure is following: we first cooled the sample under zero field from room temperature to the lowest temperature, then applied 1 T field and recorded $\chi(T)$ upon heating up to room temperature, followed by measuring $\chi(T)$ upon cooling down to the lowest temperature under 1 T. They are thus denoted as the ZFCw- and FCCc-$\chi(T)$, respectively. As seen in Fig. 3(a), the ZFCw- and FCCc-$\chi(T)$ curves of S1 exhibit a step-like anomaly around 160 K, below which the magnetic susceptibility is reduced. In addition, an obvious thermal hysteresis is evidenced around the transition, implying a first-order nature of this transition. The transition temperatures, $T_{dw}$, defined as the maximum of $d\chi/dT$, are $\sim 159$ K and $\sim 165$ K for S1 in the cooling and heating processes, respectively, as shown in the top of Fig. 3(a). The $\chi(T)$ curves of S2 are basically similar to those of S1, but the transition is much wide and the thermal hysteresis becomes very weak, Fig. 3(b). In addition, the transition temperatures, $T_{dw}$ $\approx 154$ K and 158 K for the cooling and heating processes, are lower than those of S1. These comparisons indicate that the quality of S1 is better than that of S2. We note that the observed feature in the magnetic susceptibility is very similar to those seen in some typical CDW materials, such as 1T-TaS2,$^{64}$ NbSe2,$^{65}$ CuIr2Te4,$^{66}$ IrTe2,$^{67}$ and AV3Sb5.$^{12,37,39}$

Except for the transition region, the ZFCw- and FCCc-$\chi(T)$ curves are almost overlapped with each other in the whole temperature range, and show a paramagnetic behavior at high temperature and a low-temperature upturn without long-range magnetic order down to 1.8 K. As shown in Fig. 3(a), the susceptibility $\chi$ of S1 in the low-temperature range 2–10 K can be fitted by a modified Curie–Weiss (CW) model, $\chi(T) = \chi_0 + C/(T - \theta_{cw})$. Here, the obtained effective moment of $\mu_{eff} = 0.52 \mu_B/V$ and a CW temperature of $\theta_{cw} = -34.3$ K are similar to 0.22 $\mu_B/V$ and $-47.2$ K in KV3Sb5.$^{37}$ Noted that the presence of impurities and/or defects should dominate the low-temperature upturn in $\chi(T)$, especially considering the polycrystalline nature of the studied sample. The $\chi^{-1}(T)$ in the high temperature range 200–300 K, Fig. 3(c), seems to follow a linear behavior, and a CW fitting yields $\mu_{eff} = 3.07 \mu_B/V$ and $\theta_{cw} = -4820$ K. Such a large $\theta_{cw}$ is not physically meaningful and is consistent with a Pauli paramagnetism.

![Figure 3](https://example.com/fig3.png)

Fig. 3. Temperature dependence of the dc magnetic susceptibility $\chi(T)$ and its derivative $d\chi/dT$ for V3Sb2 samples: (a) S1 and (b) S2, measured in the ZFCw and FCCc modes under an external magnetic field of 1 T. The transition temperature $T_{dw}$ was defined as the peak of the $d\chi/dT$. (c) Temperature dependence of the inverse susceptibility $\chi^{-1}(T)$ for sample S1. The CW fitting curves are shown by the solid lines in (a) and (c). (d) The isothermal magnetization $M(H)$ curves for sample S1 measured between $+7$ T and $-7$ T at various temperatures.

Figure 3(d) presents the field dependence of magnetization $M(H)$ for S1 between $-7$ T and $+7$ T at various temperatures. The $M(H)$ curves at all temperatures except for 1.8 K exhibit a linear dependence on the external field with no hysteresis, confirming the absence of ferromagnetic contributions to the magnetism. The magnetic moment of $\sim 0.003 \mu_B/V$ at 7 T is small. These results make it significantly different from Fe$_3$Sn$_2$, but similar with the AV3Sb5 family where no magnetic order or even local moment of V ion was found. In the isostructural compound Fe$_3$Sn$_2$, the Fe atoms in the kagome plane exhibit strong frustrated magnetic interactions, undergoing complex magnetic phase transitions upon cooling down from a paramagnetic to a collinear ferromagnetic state.
at 640 K, then to a non-collinear ferromagnetic state at 350 K, and finally to a re-entrant spin glass phase at 70 K. In addition, we find that the magnitudes of $\chi(T)$ and $M(H)$ for $V_3Sb_2$ are very close to those of KV$_3$Sb$_3$, further indicating the similarity of magnetic states in these two V-based kagome systems.

The presence of a density-wave-like transition in $V_3Sb_2$ is further confirmed by the resistivity measurement. Figure 4(a) shows the temperature-dependent resistivity $\rho(T)$ of S1 measured in a thermal cycle under 0 T. As can be seen, it displays a metallic behavior in the whole temperature range and exhibits a clear hump-like anomaly around $T_{dw}^0 \approx 157$ K and 165 K in the cooling and heating processes. These transition temperatures defined from the dip of the $d\rho/dT$ curve are in good agreement with those determined from the $\chi(T)$ data shown in Fig. 3(a). In addition, a similar thermal hysteresis is evidenced around $T_{dw}^0$ in $\rho(T)$. We find that the application of 10 T external magnetic field has a negligible influence on the $\rho(T)$ near $T_{dw}^0$ (data not shown). This result indicates that the transition is most likely due to the formation of CDW rather than SDW. A small positive magnetoresistance (MR) was evidenced at low temperatures. The inset of Fig. 4(a) displays the $\rho(0) \times 100\%$ at 2 K in the field range from −14 T to 14 T. As can be seen, the MR is only $\sim 1.2\%$ at 2 K and 14 T, but it is non-saturating and can be well described by the expression $MR \propto H^n$ with $n = 1.35$.

Interestingly, the $\rho(T)$ of S2 is quite different with respect to that of S1 as seen in Fig. 4(b). Nonetheless, it also exhibits a pronounced anomaly centered around 150–160 K, and the transition temperatures determined from the minimum of $d\rho/dT$ are 152 K and 160 K in the cooling and heating processes, respectively. These temperatures are also consistent with those determined from the $\chi(T)$ data shown in Fig. 3(b). In comparison with S1, the transition is much stronger and extended over a wider temperature range. In addition, the resistivity below $T_{dw}$ becomes higher than that above the transition and displays a clear upturn at low temperatures. These comparisons highlight a better quality of sample S1 than that of S2, and the observed differences might be attributed to the fact that the final sintering temperature of $830\,^\circ C$ for S2 is closer to the peritectoid temperature. In the following we thus focus our attention on sample S1. Despite of these differences, the occurrence of density-wave-like transition, most likely a CDW one, around $T_{dw} \approx 160$ K in $V_3Sb_2$ should be an intrinsic and bulk behavior.

We have performed variable-temperature powder XRD on S1 from room temperature down to 25 K in order to check if the CDW order is accompanied by obvious structural transition. Within the resolution of our instrument, no obvious peak splitting or satellite peaks are observed in the XRD patterns over the whole temperature range, as illustrated in Fig. 5(a) for a portion of the XRD patterns measured at 25 K and 300 K. This indicates that the structural modification, if exists around $T_{dw}$, should be too weak to be detected by our lab XRD, and may await for verification with high-resolution synchrotron XRD or transmission electron microscope at low temperatures. Interestingly, we find that the lattice parameter $c(T)$ exhibits a negative thermal expansion over the whole temperature range, while both $a(T)$ and $V(T)$ display normal contraction upon cooling down as shown in Fig. 5(b). The smooth evolution of the lattice parameters across $T_{dw}$ is also consistent with the absence of structural transition in $V_3Sb_2$.

To further characterize the paramagnetic and metallic ground state of $V_3Sb_2$ with a possible CDW-like transition, we performed specific-heat measurements on S1 in the wide temperature range. Figure 6 displays the $C/T$ vs. $T$ of S1 from 2 K to 250 K under zero field. There is no obvious specific-heat anomaly near the CDW-like transition, suggesting that the thermodynamic signature of this transition is too weak to be observed. For the absence of specific-heat anomaly around $T_{dw}$ in $V_3Sb_2$ to the polycrystalline nature of the studied sample. In comparison with the single crystal, the relatively poor crystallization and the presence of grain boundaries in the polycrystalline samples would diminish considerably the specific-heat anomaly around a phase transition. This is well demonstrated in AV$_3$Sb$_3$[12,37–39] the specific-heat anomaly around the first-order transition can be barely
observed in the polycrystalline KV₃Sb₃[37] while it becomes clearer in the single-crystal KV₃Sb₃[38] and is much stronger in the CsV₃Sb₅ crystal[12] with a better quality than KV₃Sb₅. We also noticed that the density-wave-like transition in resistivity and susceptibility of our polycrystalline V₃Sb₂ sample is relatively broad, which can further obscure the thermodynamic signature. The inset of Fig. 6 shows the plot of C/T vs. T^2 at the low-temperature range, and a linear fit to C/T = γ + βT^2 considering the electronic and lattice contributions yields the Sommerfeld coefficient γ = 18.5(1) mJ·mol⁻¹·K⁻² and β = 0.73(1) mJ·mol⁻¹·K⁻⁴. The Debye temperature Θ_D ≈ 237 K can be calculated according to the relation Θ_D = (12π²nR/5β)¹/³, where R = 8.314 J·mol⁻¹·K⁻¹ is the ideal gas constant and n = 5 is the number of atoms per formula unit. The obtained γ is relatively large compared with elemental metal and is close to that of KV₃Sb₃[37] implying the moderate enhancement of the effective electron mass and the presence of electronic correlations.

Fig. 5. (a) A portion of the XRD patterns measured at 25 K and 300 K. (b) Temperature dependences of the normalized lattice parameters of V₃Sb₂ sample S1.

From the above characterizations, we can conclude that the bilayer kagome metal V₃Sb₂ is a paramagnetic metal and undergoes a CDW-like transition at T_dw ≈ 160 K, which is similar to the family of AV₃Sb₃. But no superconductivity was observed in V₃Sb₂ at ambient pressure down to 1.8 K. To explore whether superconductivity emerges after suppressing the CDW under pressure, we measured the ρ(T) of S1 under various hydrostatic pressures up to 1.8 GPa by using a piston-cylinder cell. The ρ(T) and its derivative dρ/dT at different pressures are shown in Fig. 7(a). The evolution of the CDW-like transition with pressure can be tracked clearly from the resistivity anomaly. With increasing pressure gradually, the anomaly in ρ(T) and the corresponding T_dw determined from the minimum of dρ/dT continuously move to lower temperatures. The pressure dependence of the determined T_dw is plotted in Fig. 7(b). As can be seen, T_dw is suppressed to about 60 K at 1.6 GPa, above which it cannot be clearly distinguished in both ρ(T) and dρ/dT, implying a complete suppression of CDW-like order above 1.6 GPa. However, no sign of superconductivity can be observed down to 1.5 K accompanying the complete suppression of CDW-like order. Whether superconductivity can be realized at much lower temperatures or on high-quality single-crystal samples deserves further studies. Although the above characterizations have revealed a first-order character for the CDW-like transition at ambient pressure, the resistivity anomaly around T_dw is weakened gradually by applying pressure, Fig. 7(a). If a crossover from first-order to second-order transition can take place, a putative quantum critical point can be realized under pressure. When the high-quality V₃Sb₂ single crystals become available, further high-pressure studies are desirable for in-depth investigations on the pressure-induced quantum critical phase transition.

Finally, we calculated the electronic structure of V₃Sb₂ by first-principles calculations. As shown in Fig. 8, the V₃Sb₂ shows a metallic nature and its Fermi surface is mainly composed by V’s d orbitals. In V₃Sb₂, there are two kinds of antimony, which are chemically inequivalent, forming different bands. The hybridization between Sb2 and V is relatively stronger than that between Sb1 and V, because Sb2 are intralayer with V atoms. Meanwhile, we calculated the topological indices of V₃Sb₂, which are \( z_{2w,1} = 0, z_{2w,2} = 0, z_{2w,3} = 0 \) and \( z_4 = 2 \), showing a non-trivial topological crystalline property.[61–63]
The present work is a preliminary study on the physical properties of V$_3$Sb$_2$ polycrystalline samples and leaves many open questions for the future experimental and theoretical studies. For example, electrical transport and magnetic properties at much lower temperatures should be measured to explore possible superconductivity or magnetic order.

Low-temperature synchrotron XRD, transmission electron microscope, optical spectroscopy, and scanning tunneling microscope measurements should be performed to elucidate the nature of the density-wave-like transition. Moreover, to acquire high-quality single crystal samples is mandatory for in-depth characterizations of the intrinsic electronic structure by using the angle-resolved photoemission spectroscopy.

4. Conclusion

In summary, we have synthesized the polycrystalline sample of V$_3$Sb$_2$ with bilayer kagome lattice of V atoms through a traditional solid state reaction method and characterized its structural, electrical transport, magnetic, and thermodynamic properties via x-ray powder diffraction, resistivity, magnetic susceptibility, and specific heat measurements. We observed no long-range magnetic order in V$_3$Sb$_2$ above 1.8 K, which is completely different from the isostructural Fe$_3$Sb$_2$ but similar to the kagome metal AV$_3$Sb$_5$ (A = K, Rb, Cs) family. In addition, a density-wave-like anomaly was evidenced around 160 K in V$_3$Sb$_2$, making it more similar to the AV$_3$Sb$_5$ (A = K, Rb, Cs) family. Moreover, we found that the density-wave-like transition can be gradually suppressed by pressure but no sign of superconductivity can be observed down to 1.5 K. We proposed that V$_3$Sb$_2$ is a novel candidate kagome metal to study the interplay between density-wave order, nontrivial band topology and possible superconductivity.

Note added

During the preparation of this manuscript, we noticed that Shi et al. reported the synthesis and characterizations of the “V$_6$Sb$_4$” single crystal in a recent preprint arXiv: 2110.09782. The V$_6$Sb$_4$ single crystal was grown at a high temperature of 1100 °C and does not exhibit any density-wave-like transition, different from what we observed in the low-temperature phase of V$_3$Sb$_2$ in the present work. We attributed the observed different behaviors to the different sintering temperatures.

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