




Anisotropic superconductivity and quantum oscillations in the layered dichalcogenide TaSnS₂

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TaSnS₂ single crystal and polycrystalline samples are investigated in detail by magnetization, electrical resistivity, and specific heat as well as Raman spectroscopy and nuclear magnetic resonance (NMR). Studies are focused on the temperature and magnetic field dependence of the superconducting state. We determine the critical fields for both directions $B \parallel c$ and $B \perp c$. Additionally, we investigate the dependence of the resistivity, the critical temperature, and the structure through Raman spectroscopy under high pressure up to 10 GPa. At a pressure of ≈ 3 GPa the superconductivity is suppressed below our minimum temperature. The Sn NMR powder spectrum shows a single line which is expected for the TaSnS₂ phase and confirms the high sample quality. Pronounced de Haas-van Alphen oscillations in the ac susceptibility of polycrystalline sample reveal two pairs of frequencies indicating coexisting small and large Fermi surfaces. The effective mass of the smaller Fermi surface is $\approx 0.5m_e$. We compare these results with the band structures from DFT calculations. Our findings on TaSnS₂ are discussed in terms of a quasi-two-dimensional BCS superconductivity.

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I. INTRODUCTION

Superconductors with layered crystal structures have attracted the interest of researchers since the earlier 1960's. This is mainly due to their anisotropic superconducting properties and the associated very high critical fields [1–4]. In the 1980s, this research got a strong impetus with the discovery of high- T_c superconductivity (SC) in cuprates [4–9]. In the last decade, the investigation of such quasi-two-dimensional (2D) materials invigorated after reports about anisotropic superconductivity in BiS₂-based compounds and Fe pnictides [10–16].

The layered crystal structure is also characteristic for transition-metal dichalcogenides (TMD). Therefore, their properties are frequently said to be reminiscent of those of high- T_c cuprates and iron-based pnictides [4,17]. The most common polymorphic modifications of TMDs are the trigonal 1 T - and hexagonal 2 H -polytypes. Interestingly, pristine TMDs with the 1 T -polytype structure were found to be mostly semiconducting or semimetallic, while SC is never observed for them at ambient pressure. The reason is a charge density wave (CDW) instability of these materials which is eventually

suppressed by application of high pressure. In contrast, some 2 H -TMDs do not show this instability and frequently become superconducting at ambient pressure and low temperatures, as, e.g., 2 H -NbS₂ ($T_c = 5.8$ K) [18], 2 H -TaS₂ ($T_c = 0.8$ K) [19,20], 2 H -NbSe₂ ($T_c = 7.0$ K) [21].

Interestingly, there are several routes to enhance T_c of TMDs: (i) by increasing the transition-metal content, as it is observed for TaSe₂ ($T_c = 0.14$ K) [22,23] and Ta_{1.06}Se₂ ($T_c = 3.2$ K) [24]; (ii) by third elements, e.g., by substitutions on the transition-metal site of pristine 2 H -TMD. One example, TaSe₂ doped with Nb (i.e., Ta_{0.8}Nb_{0.2}Se₂) reveals a T_c up to 2.01 K [25,26]; (iii) intercalation of some organic molecules into TMD crystals by soft chemistry methods. These species are located between the chalcogenide layers which are separated by a van der Waals gap [27]. The most prominent example is TaS₂(pyridine)_{1/2}, a very anisotropic superconductor with strongly enhanced $T_c = 3.5$ K [3,4,28].

(iv) Finally, there are various ‘intercalation’ compounds, where in the space between the layers metals as Hg, In, Pb, Sn, etc. but also transition metals are incorporated [17]. Several such TaM_xS₂ ($x = 1/4 - 1$) materials are based on 2 H -TaS₂. Concerning superconductivity TaS₂ intercalated with Pd reveals a T_c up to 4.2 K [29], whereas Cu [30] and Ni intercalation [31] lead to maximum $T_c = 4.5$ K and $T_c = 4.15$ K, respectively.

Among the numerous intercalated layered TMDs with the basic 2 H -TaS₂ structure [32,33], TaSnS₂ (SG: $P6_3/mmc$, $a \approx 3.3$ Å, $c \approx 17.4$ Å) attracted special attention due to its rare structural arrangement, which is characterized by the linear coordination of the intercalated Sn atoms (i.e., appearance of

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linear S-Sn-S units), which connects the hexagonal $2H$ -TaS₂ layers [34,35]. Magnetic susceptibility and transport measurements revealed TaSnS₂ to be a diamagnetic metal with a superconducting transition temperature $T_c = 2.95$ K and the normal state transport properties to be mainly determined by the Sn $5p_x p_y$ band [36–38]. The average valency Sn¹⁺, which arises from rapid valence fluctuations between Sn⁰ and Sn²⁺ [38,39], was deduced from photoelectron- [37–39], Mössbauer- [40–43], and NMR-spectroscopy [44] measurements. This unusual valence state was confirmed by band structure calculations [38,45,46] and is associated with electron donation of the intercalated Sn until the Ta d_{z^2} band is completely filled [38]. Powder neutron and x-ray diffraction [34] as well as single crystal x-ray diffraction [35] confirmed the presence of only one crystallographic Sn site in TaSnS₂. These studies revealed a rather long Sn – S distance of about 2.8 Å, which again could be explained by the low charge of Sn.

Superconductivity in TaSnS₂ was reported recently [47]. As expected, TaSnS₂ is an anisotropic superconductor, where the second critical magnetic field $B_{c2}^\perp \approx 300$ mT is much larger than that measured parallel to the c direction ($B_{c2}^\parallel \approx 20$ mT). The same study reports TaSnS₂ to be a SC with moderately strong electron-phonon coupling as well as a nodal line semimetal.

Recently, some TMDs gained attention as a possible realization of topological SC. Candidate materials are Weyl type II systems like MoTe₂ [48] and WSe₂ (SC is induced by applying pressure) [49]. The ternary compounds TaSnS₂ [47], TaPbS₂ [50], and TaPbSe₂ [51–54] are discussed in the same context as superconducting topological nodal line semimetals. The signatures of such a behavior are band structures (spin-orbit coupling is not considered) exhibiting several band crossings near the Fermi level (E_F), which form three nodal lines in the $k_z = 0$ plane, resulting in drumheadlike surface states. However, the crystal structure of TaPbSe₂ is noncentrosymmetric. With this structural difference, the question remains open if superconductivity observed in both systems has to be associated to the presence of topological line node states at the Fermi level or to residual trivial states forming a flat band near the E_F . Contrasting that, recent findings (SC at $T_c = 2.6$ K) on the related centrosymmetric nodal line semimetal TaPbS₂ [50] are reminiscent of our TaSnS₂ results.

These new and controversial findings triggered us to perform a comprehensive study on TaSnS₂ single crystals and polycrystalline material. Anisotropic SC is studied as a function of temperature and magnetic field via magnetization, specific heat, and electrical transport, and results obtained are in good agreement with findings from Ref. [47]. TaSnS₂ is identified as an anisotropic BCS-like superconductor. Investigations beyond bulk properties presented here are resistivity- and Raman spectroscopy measurements under pressure, Sn-nuclear magnetic resonance (NMR) as well as the evaluation of quantum oscillations in the dc field dependent ac magnetic susceptibility. Pronounced de Haas-van Alphen oscillations confirm the presence of light charge carriers in the semimetal TaSnS₂. Resistivity measurements and Raman studies under high pressure reveal the suppression of superconductivity with pressure and suggest a pressure-induced structural phase transition.

II. EXPERIMENTAL

To synthesize polycrystalline TaSnS₂ the elemental powders (Sn: Chempur, 99.995 wt.%, Ta: Chempur, 99.9 wt.%, S: Chempur, 99.5 wt.%) were mixed with iodine (40 mg per g TaSnS₂) under protective Ar-atmosphere (MBraun glove box system [$p(\text{H}_2\text{O}) < 1$ ppm; $p(\text{O}_2) < 1$ ppm]), pressed into a pellet and enclosed in an evacuated quartz ampoule. The heat treatment was performed in two steps: first heating up to 450 °C within 24 h (kept at this temperature for another 24 h) and second heating up to 800 °C within 12 h and annealing for 7 days. The obtained powder was compacted applying spark plasma sintering (SPS-15 ET setup, Dr. Sinter Lab, Japan). It was also used for single crystal growth by chemical vapor transport (CVT). For this purpose, TaSnS₂ was mixed with chlorine (4 mg cm⁻³ of NH₄Cl [AlfaAesar, 99.999 wt.%] calculated for total ampoule volume of ≈ 8 cm³) as transport agent and placed in an evacuated quartz ampoule (10 cm × 1.6 cm). The temperature gradient from 925 °C (source) to 800 °C (sink) in the ampoule was kept for 12 days. Further it was cooled (60 K h⁻¹) down to 300 °C and finally air cooled to room temperature. The obtained crystals were thin plates with dimensions of $\approx 1 \times 1 \times 0.1$ cm³.

The samples (i.e., polycrystalline powder, compacted polycrystalline SPS sample, and single crystals) were characterized by powder x-ray diffraction (XRD) on a Guinier camera G670, CuK α_1 radiation. High-resolution powder XRD data were collected at room temperature at BM20 beamline of the European Synchrotron Radiation Facility (ESRF) ($\lambda = 0.45923$ Å, $2\theta_{\text{max}} = 32^\circ$) on powder enclosed in a quartz capillary with an outer diameter of 0.3 mm. Phase analysis was performed with the WinXpov [55] software package. Single crystal x-ray diffraction was performed on a Bruker AXS D8Quest single crystal diffractometer [56] with MoK α -radiation $\lambda = 0.71076$ Å, a Photon100 detector and a TRIUMPH monochromator. Integration and correction was performed with the APEX software [57]. The lattice parameters by least-squares fitting and crystal structure were refined with WinCSD [58].

Magnetization measurements are performed on single crystals using a standard magnetometer (MPMS XL7, Quantum Design) and ac susceptibility measurements are conducted on the powder sample (ACMS option, PPMS14, Quantum Design). The electrical resistivity was measured on a SPS sample down to 1.9 K and the specific heat on a SPS sample down to 0.35 K as well as on a single crystal in two orientations (with the applied magnetic field parallel and perpendicular to the c axis) in a commercial system equipped with a ³He cooling stage (ACT and HC options, PPMS, Quantum Design).

Field swept ^{117,119}Sn NMR measurements on polycrystalline material were performed using a Tecmag spectrometer employing standard pulse techniques at a given temperature of 5 K and at 35 MHz. The spectral intensity was obtained by integrating the spin echo in the time domain. In order to determine the Larmor field (NMR shift zero) we measured SnO₂ powder as a nonmagnetic reference with ¹¹⁹K = 0.5% [59].

For high-pressure Raman spectroscopy and electrical resistivity measurements, a screw-clamped diamond anvil cell with

a 500 μm culet was used. The tungsten gasket was insulated with a cubic BN/epoxy mixture. A single crystal sample of suitable size ($\sim 120 \mu\text{m} \times 120 \mu\text{m} \times 30 \mu\text{m}$) was cut and placed into the central hole of the gasket filled with NaCl as a pressure-transmitting medium along with a ruby chip for pressure calibration. The electrical leads were fabricated from 5 μm thick Pt foil and attached to the sample in a van der Pauw configuration. Electrical resistivity was measured in the temperature range 1.8–300 K using a direct current source and nanovoltmeter. The inaccuracy in the T_c in high-pressure experiments is estimated from calibration of our high-pressure measurement setup by measurements of pressure dependence of T_c of lead.

Raman spectra were collected at room temperature in backscattering geometry using a customary confocal micro-Raman spectrometer equipped with $20\times$ long-working-distance objective, HeNe laser as the excitation source, and a single-grating spectrograph with 1 cm^{-1} resolution.

Full potential linear augmented plane wave (LAPW) calculations were performed using the WIEN2k package [60]. We used the generalized gradient approximation [61] in the form of PBEsol [62] for the exchange-correlation potential. It is furthermore essential to use a very fine mesh in k space; we employed a $39 \times 39 \times 21$ mesh, corresponding to 1617 nonequivalent k points. To get the areas of the orbits (given here in Tesla units) with sufficient accuracy we used an integration engine built in the SURFER program [63], which internally interpolates the integrand with splines. The results reported here include the effect of spin-orbit coupling.

III. RESULTS AND DISCUSSION

A. Crystal structure

To check the quality of the synthesized TaSnS₂ crystals single crystal XRD was performed. All peaks in the collected dataset were successfully indexed in hexagonal symmetry with unit cell parameters presented in Table I. The analysis of the extinction conditions indicated three possible space groups (SG): $P6_3mc$, $P\bar{6}2c$, and $P6_3/mmc$. The highest symmetrical SG $P6_3/mmc$ was chosen for the first attempt to find a structural model. The atomic coordinates obtained from direct methods (Table I) were consistent with those reported for TaSnS₂ in Ref. [35]. The crystallographic details of the further performed refinement, atomic coordinates, equivalent and anisotropic displacement parameters are collected in Table I.

The obtained crystal structure is considered in the literature [34,35] as an intercalation of Sn layers in $2H$ -TaS₂ (Fig. 1). It is also characterized by interatomic distances close to the sums of atomic radii ($r_{\text{Ta}} = 1.43 \text{ \AA}$, $r_{\text{Sn}} = 1.41 \text{ \AA}$, $r_{\text{S}} = 1.04 \text{ \AA}$). The elongated (by $\approx 14\%$) Sn – S contacts allow enlarged thermal displacements B_{eq} which are much larger in comparison with the displacements of other atoms (Table I).

To confirm the obtained structural model NMR powder spectra were measured. They revealed two lines (Fig. 2), which could be assigned to the two predominant NMR active (spin 1/2) Sn isotopes. The NMR shift of those lines is positive and small (about +0.4%, in reasonable agreement with Ref. [44]) which indicates a small residual density of states at the Fermi level as expected for a semimetal. The

TABLE I. Crystallographic data and shortest interatomic distances for TaSnS₂ {SG $P6_3/mmc$, $Z = 2$, Ta in $2c$ ($1/3$, $2/3$, $1/4$), Sn in $2a$ ($0, 0, 0$), S in $4e$ [$0, 0, 0.16036(8)$].

Lattice parameters ¹	
a (\AA)	3.30648(1)
c (\AA)	17.4416(1)
V (\AA^3)	165.14(1)
ρ (g cm^{-3})	7.31(1)
$\text{MoK}\alpha$, λ (\AA)	0.71076
$2\theta_{\text{max}}$ ($^\circ$)	81.74
Minimum h, k, l	$-6, -5, -31$
Maximum h, k, l	$6, 6, 31$
$N(hkl)_{\text{measured}}$	6140
$N(hkl)_{\text{unique}}$	254
$N(hkl)_{\text{observed}}(F_{hkl} \geq 2\sigma(F))$	5334
$R_{\text{int}}/R_{\sigma}$	0.082/0.069
Refined parameters	
Extinction coefficient	0.0101(6)
Goodness of fit, S	1.010
R_F/wR_{F^2} ²	0.039/0.040
Min. and max. residual electronic density ($e \text{ \AA}^{-3}$)	$-4.5; +6.1$
$B_{\text{eq}}^3, B_{11}, B_{33}$ for Ta ⁴	0.29(1), 0.28(1), 0.32(1)
$B_{\text{eq}}^3, B_{11}, B_{33}$ for Sn ⁴	1.45(1), 1.69(2), 0.96(2)
$B_{\text{eq}}^3, B_{11}, B_{33}$ for S ⁴	0.45(2), 0.48(3), 0.40(4)
$d(\text{Ta-6S}); d(\text{Ta-6Ta})$, (\AA)	2.4675(9), 3.3065(1)
$d(\text{Sn-2S}); d(\text{S-1S})$, (\AA)	2.797(1), 3.127(2)

¹Powder XRD data

² $R = [\sum(|F_o| - |F_c|)] / \sum|F_o|$; $w = 0.1176 \lg(F_o)^4$; $wR = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)]\}^{1/2}$

³ $B_{\text{eq}} = 1/3[B_{11}a^2a^2 + \dots 2B_{23}b^*c^*bc \cos\alpha]$

⁴ $B_{22} = B_{11}, B_{12} = 1/2B_{11}, B_{13} = B_{23} = 0$

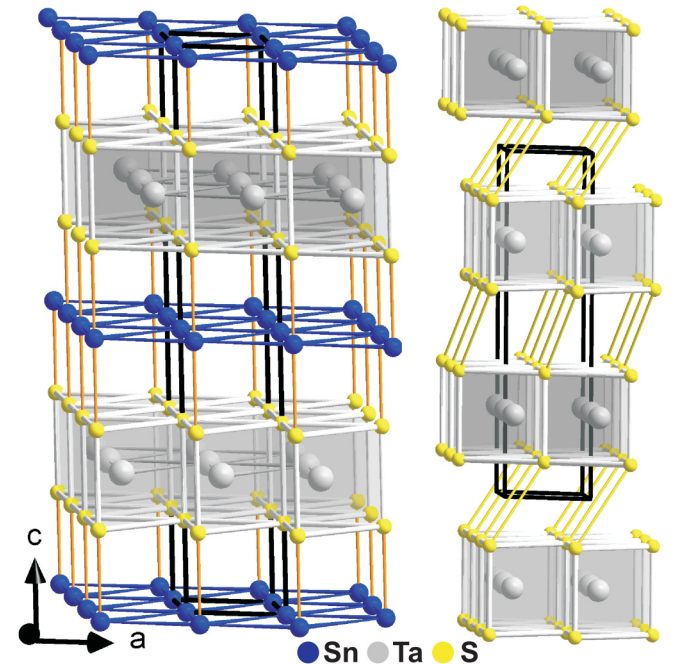


FIG. 1. The structural relationship between TaSnS₂ (left) and TaS₂ (right) illustrates the intercalation of Sn layers in $2H$ -TaS₂.

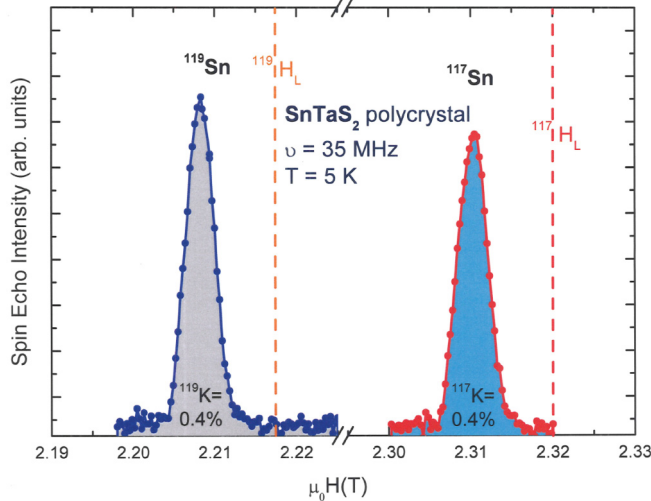


FIG. 2. Sn NMR field sweep spectra of the TaSnS₂ polycrystalline sample. The vertical dashed lines indicate the Larmor fields for the two Sn isotopes.

difference in the shift value to Ref. [44] (determined at about 0.5 T) might originate from dHvA oscillations in the shift itself. This is frequently found in semimetals [64]. There are no further NMR lines found which evidences that there is no additional line associated to other phases like Sn_{1/3}TaS₂ (with ¹¹⁹K ≈ 0.08%) [44]. The line positions (resonance fields) and the absolute intensities match with the prediction from the gyromagnetic ratios and the natural abundance of the respective Sn nuclei. So from our NMR study we have clear evidence for a well defined stoichiometry in the powder material and we could rule out other Sn containing foreign phases (like Sn_{1/3}TaS₂). This observation is in good agreement with the results of phase analysis performed on high-resolution powder XRD patterns (see Fig. S1 in Supplemental Material [65]).

B. Magnetic measurements

The temperature dependence of the critical fields $B_{c1}(T)$ and $B_{c2}(T)$ was determined from temperature- and field-dependent (ZFC-FC) isothermal magnetization measurements as well as ac susceptibility (for more details see Supplemental Material [65]). Figure 3 shows the transition curves at a nominal magnetic field $B = 0.5(2)$ mT for the orientation $B \perp c$ [Fig. 3(a)] and $B \parallel c$ [Fig. 3(b)], respectively. In the case of $B \perp c$, the resulting susceptibility leads to a maximum superconducting volume fraction of ≈82%. For $B \parallel c$ the measured magnetization is considerably enhanced due to the large demagnetization factor of the platelike sample. We define critical temperatures T_c by the onset of the diamagnetic transition as indicated by arrows in Fig. 3. For the lowest applied field the T_c is 3.0(1) K. Figure 4 shows further ZFC-FC transition curves for both field orientations. The resulting $B_{c2}(T)$ curves are plotted in Fig. 6. The transition temperature extrapolated to zero field is $T_c = 3.04$ K.

One branch of an isothermal magnetization curve at $T = 2$ K for the orientation $B \perp c$ is plotted in Fig. 5. It shows a nearly reversible behavior indicating weak flux pinning in the sample. A very similar behavior was found for TaPbS₂

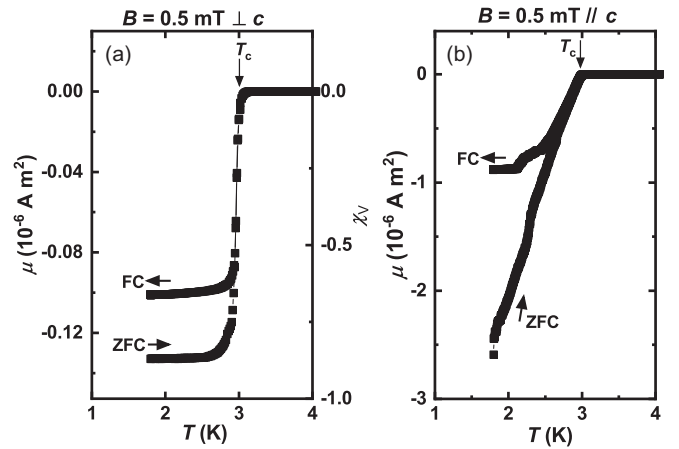


FIG. 3. Zero-field cooled (ZFC, shielding effect) and field cooled (FC, Meissner effect) susceptibility for TaSnS₂ single crystals with a nominal field of 0.5 mT applied in two directions: (a) $B \perp c$, (b) $B \parallel c$.

single crystals [50]. In the inset the respective ZFC and FC values are also plotted showing excellent agreement. The visible deviation from linearity with increasing field allows the estimation of the lower critical field at this temperature: $B_{c1}^{\perp}(2\text{K}) \approx 1.95$ mT.

The temperature evolution of the direction dependent upper critical fields B_{c2}^{\perp} and B_{c2}^{\parallel} estimated from the measurements of isothermal magnetization, electrical resistivity, and specific heat are depicted in Fig. 6. Interestingly, the results obtained from $c_p(T)$ and $\rho(T)$ measured on polycrystalline samples nicely coincide with those observed for $B \parallel c$ and $B \perp c$, respectively. Fitting $B \parallel c$ data to the Ginzburg-Landau (GL) relation: $B_{c2}(T) = B_{c2}(0)(1 - t^2)/(1 + t^2)$ with $t = T/T_c$ [66] the upper critical field is estimated as $B_{c2}^{\parallel}(0) = 27(2)$ mT (inset to Fig. 6).

The upward curvature of the $B_{c2}(T_c)$ dependence is known for both doped [67] and intercalated [68] tantalum dichalcogenides, including TaSnS₂ [47]. In the case of TaPbSe₂ [68] it

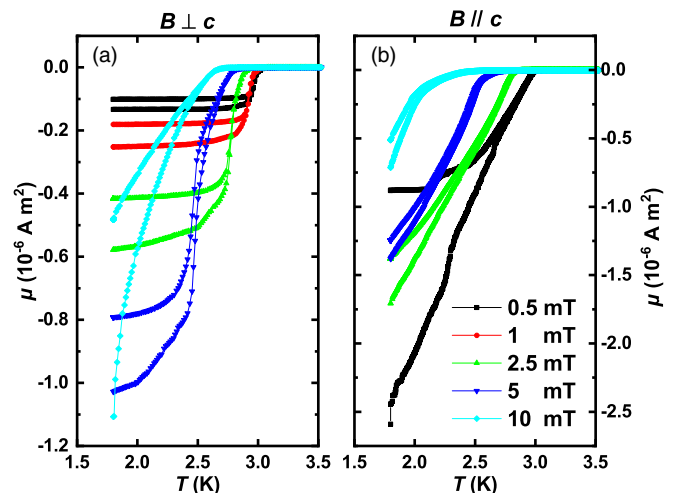


FIG. 4. Magnetic susceptibility of TaSnS₂ single crystals with higher applied magnetic fields: (a) $B \perp c$ and (b) $B \parallel c$.

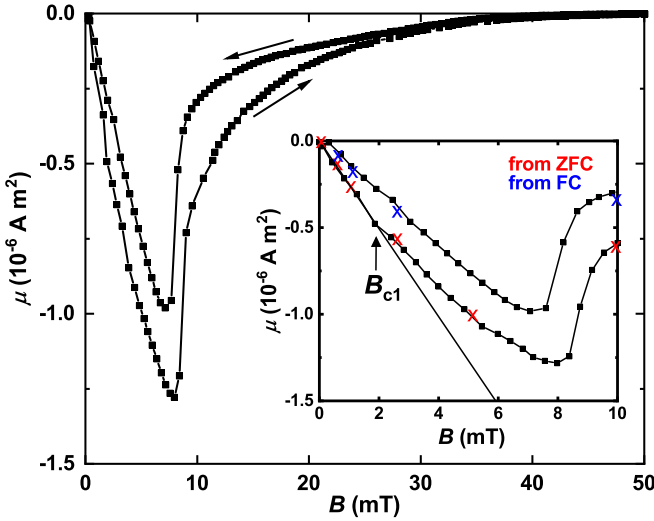


FIG. 5. Positive field branch of the magnetization curve of TaSnS₂ for the orientation $B \perp c$ and the temperature $T = 2$ K. The inset contains additionally the respective ZFC and FC values for comparison and the deviation from the first linear part to determine the lower critical field B_{c1} .

could be fitted with $B_{c2}(T) = B_{c2}(0)(1 - t^{3/2})^{3/2}$. However, this equation is reported to fail in the description of $B_{c2}^{\perp}(T_c)$ for TaSnS₂ [47]. As is seen from Fig. 6, this finding is also confirmed in our study. Interestingly, $B_{c2}(T) = B_{c2}(0)(1 - t^{5/2})^{5/2}$ with $B_{c2}^{\perp}(0) = 170(10)$ mT describes well the data deduced from the field dependent $\rho(T)$ measurements on the polycrystalline sample. Obviously, this critical field can be under/overestimated, taking into account the lack of the points for $T_c < 1.7$ K.

The anisotropy parameter of ≈ 6.3 is calculated from the relation of two upper critical fields. The GL coherence lengths

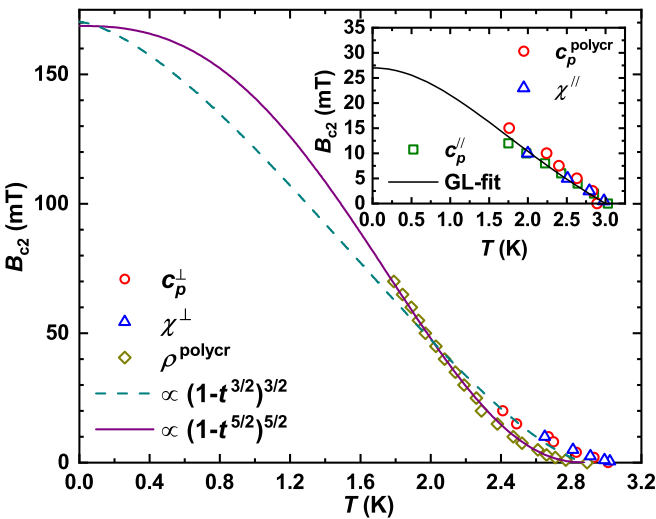


FIG. 6. Upper critical field B_{c2} of TaSnS₂ versus temperature from c_p , χ , and ρ measurements on polycrystalline (polycr) material as well as c_p and χ measurements on single crystals. Inset: Detailed view on the data in the temperature range 1.6–3.0 K. For the fits (lines) see the text.

$\xi_{GL}^{\parallel} = 17(2)$ nm and $\xi_{GL}^{\perp} = 110(6)$ nm were estimated using Eqs. (1) and (2), where Φ_0 is the magnetic flux quantum, respectively.

$$\xi_{GL}^{\perp} = \sqrt{\frac{\Phi_0}{2\pi B_{c2}^{\parallel}}} \quad (1)$$

$$\xi_{GL}^{\parallel} = \frac{\Phi_0}{2\pi B_{c2}^{\perp} \xi_{GL}^{\perp}} \quad (2)$$

Using $B_{c1}^{\perp}(2$ K) from the magnetization measurements, the London penetration depth $\lambda^{\perp} = 280(10)$ nm has been determined by a numerical solution of the equation $B_{c1}^{\perp} = (\Phi_0/4\pi(\lambda^{\perp})^2)\ln(\lambda^{\perp}/\xi_{GL}^{\perp})$. Thus, the GL parameter $\kappa_{GL}^{\perp} = \lambda^{\perp}/\xi_{GL}^{\perp} = 2.5(2)$ indicates TaSnS₂ to be a type-II superconductor.

Due to the positive curvature of the $B_{c2}^{\perp}(T_c)$ curve, the anisotropy decreases to a value of ≈ 3 . Similarly low values have been reported for other doped (e.g., with Nb [69]) or intercalated with Sn [70], Na [71], Pd [72] as well as with organic molecules [67,73] layer structured tantalum dichalcogenides. These observations are in agreement with the prediction by the dimensionality crossover model of Klemm *et al.* [74] developed for superconductor/insulator superlattices. It was also found in metal intercalated dichalcogenides [72,26] and was explained by special Fermi surface properties. Also for other layered superconductors like graphite intercalation compounds (GICs) [75] and especially for the high- T_c -cuprates [6,7,16] positive curvatures were reported. It was speculated that such a behavior is a common feature for two-dimensional superconducting systems. However, there also exist distinct deviations from this rule, especially for GICs, where extended linearity of $B_{c2}(T)$ was reported [76]. The positive curvatures near T_c occasionally found in isotropic systems like superconducting fullerenes [77,78] might originate from the presence of different phases with variations in the local T_c . In view of such a variety of results further investigations are desired to find an appropriate model for the positive curvature analysis for TaSnS₂.

C. Electrical resistivity and specific heat

The electrical resistivity $\rho(T)$ in different magnetic fields is measured on the SPS-compacted TaSnS₂ sample (Fig. 7). In zero-field $\rho(T)$ decreases with decreasing temperature down to ≈ 3 K indicating TaSnS₂ to be a metallic system. The residual resistivity ratio $\text{RRR} = \rho^{300\text{K}}/\rho_0 = 10.6$ indicates a fair quality of this SPS-compacted polycrystalline sample. The onset of the rounded superconducting transition occurs at $T_c = 2.9(1)$ K, slightly lower than the value of 3.04 K deduced for single crystalline material.

The specific heat was measured on single crystals applying different magnetic fields $B \parallel c$ and $B \perp c$ (inset Fig. 8) as well as on the polycrystalline SPS sample. Further analysis of the $c_p(T, B)$ data is performed on the base of bulk specimen, since they reproduce the $B \parallel c$ results of single crystal (Fig. 8) and reveal a better statistic due to higher sample mass.

The overcritical specific heat is fitted in the temperature range 0.35–1.7 K to the ansatz $c_p = \gamma_{\text{tot}}T + \beta T^3$ (not

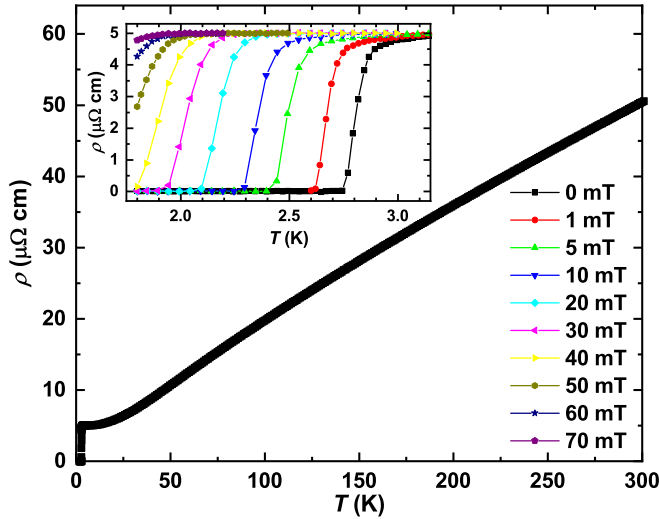


FIG. 7. Electrical resistivity $\rho(T)$ for SPS-compacted polycrystalline TaSnS₂. Inset: $\rho(T)$ in different magnetic fields.

shown in Fig. 8) with $\gamma_{\text{tot}} = 5.4(1) \text{ mJ mol}^{-1} \text{ K}^{-2}$ and $\beta = 0.64(2) \text{ mJ mol}^{-1} \text{ K}^{-4}$ [corresponds to an initial Debye temperature $\theta_D = 229(2) \text{ K}$].

The transition temperature midpoint $T_c = 2.88(2) \text{ K}$ (i.e., the middle of the falling flank of the anomaly) observed in c_p measurements is in agreement with the T_c derived from the other properties. The steplike anomaly corresponding to the superconducting transition is rounded (Fig. 8), which is due to chemical inhomogeneities appearing in the specimen after SPS. The estimated specific heat jump for the sintered sample and single crystal is $\Delta c_p/\gamma T_c \approx 1.2$ (obtained by a graphical equal-areas construction in a c_p/T vs T plot, i.e., entropy conserving) and is in fair agreement with the BCS model (1.43).

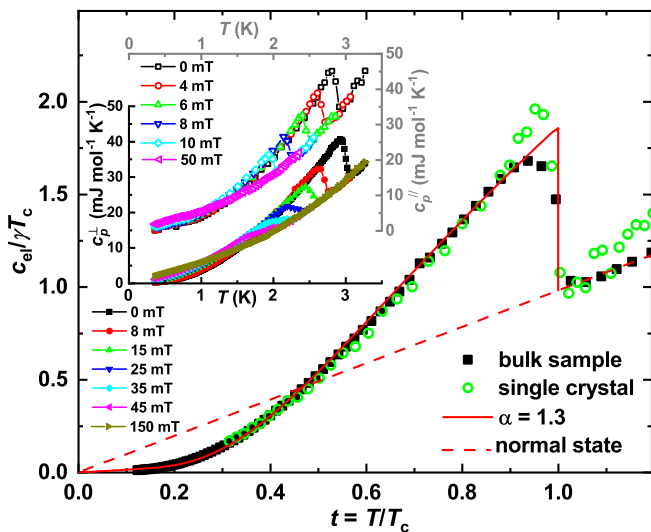


FIG. 8. Electronic specific heat $c_{\text{el}}/\gamma T_c$ versus $t = T/T_c$ for TaSnS₂ [midpoint $T_c = 2.88(2) \text{ K}$] and comparison with the α model [79]. Inset: Specific heat in various magnetic fields for TaSnS₂ single crystals with the magnetic field applied $\parallel c$ (right scale) and $\perp c$ (left scale).

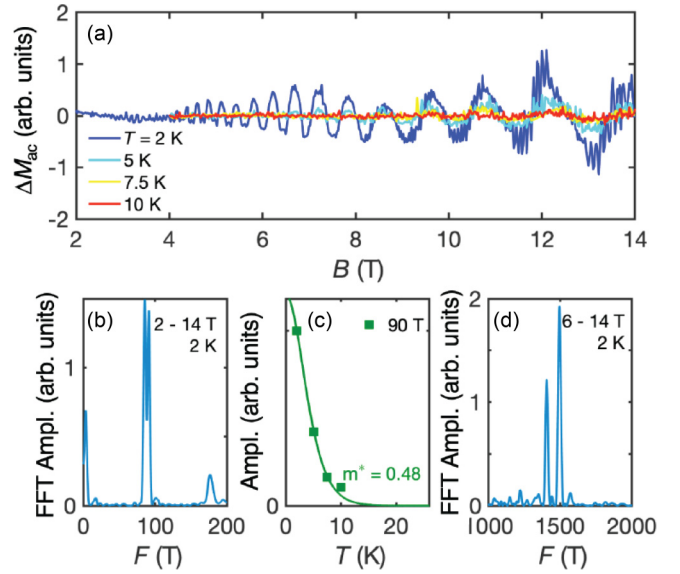


FIG. 9. Quantum oscillations in polycrystalline TaSnS₂ (a) oscillatory component of the ac susceptibility (b) Fourier transform over 2–14 T window (c) decay of the oscillatory amplitude with increasing temperature at the field value $B_{\text{osc}} = 13.1 \text{ T}$ (dominated by the 90 T oscillation at this field value) and (d) Fourier transform over the field window 6–14 T.

After subtracting the phononic part (βT^3), we obtain the electronic specific heat for polycrystalline sample and single crystal (Fig. 8). Both curves excellently match for $T < 0.8T_c$ and are well described by the α model for $\alpha \equiv \Delta(0)/k_B T_c \approx 1.3$. Although the value of α is below that for the weak-coupling limit of the BCS theory ($\alpha_{\text{BCS}} = 1.76$ [79]), there are no visible indications for possible multigap superconductivity in our data. We thus conclude that TaSnS₂ is a weak-coupling s -wave superconductor.

D. Quantum oscillations and electronic structure

The small effective masses of semimetals tend to result in a pronounced de Haas-van Alphen (dHvA) effect [80]. Here, the frequency F of the oscillation is related with the extremal Fermi surface (FS) cross section S_{ext} perpendicular to the applied magnetic field by the Onsager relation $F = \hbar S_{\text{ext}}/2\pi e$. The temperature damping of the oscillation amplitude $A(T)$ at a fixed magnetic field B_{osc} is given by the Lifshitz-Kosevitch formular $A(T) = \chi/\sinh(\chi)$ with $\chi = 2\pi^2 m^* k_B T/e\hbar B_{\text{osc}}$ [80]. This behavior allows us to extract the effective cyclotron mass m^* of the charge carriers. Figure 9(a) shows well-resolved quantum oscillations (QO) in the ac magnetization as a function of applied dc field of the polycrystalline sample. Since the dHvA signal is periodic in $1/B$, the field axis is inverted and a Fourier transform (FFT) performed over a window of 2–14 T [Fig. 9(b)] and 6–14 T [Fig. 9(d)]. The FFT reveals two sets of QO frequencies, each one split into two: One at 90/100 T and one at 1400 and 1500 T. The beating patterns observable in Fig. 9(a) are a result of the splitting of the lower frequencies. The fact that we found pronounced QOs even in polycrystalline powder certifies the high sample quality.

Given the quick decay of the amplitude with temperature, we can get a rough estimate of the effective mass of the orbit corresponding to the dominant 90 T frequency. The temperature dependence of the amplitude at 13.1 T is shown in Fig. 9(c). With this, we estimate the effective mass to be $\approx 0.48m_e$.

We can also compare the QO frequencies we found with the ones observed in the related material TaPbS₂ and pristine 2H-TaS₂, in order to get an idea which pockets or orbits are responsible for the observed QOs. In TaPbS₂ a rather large FS was found by density-functional theory (DFT) and confirmed by angle-resolved photoemission spectroscopy (ARPES), consisting of a hexagonal center connected to another, almost cylindrical surface along the H-K line at the corner of the Brillouin zone (BZ) [81,51]. Within this there are also a number of cylindrical nested FS pockets. Around the Γ point, two nested pillow-shaped FS pockets are found. Experimentally, QO frequencies between 6 and 1200 T with an angular dependence in agreement with the predicted almost 2D nature (i.e., cylindrical shape of the FS) were observed.

In the pristine compound 2H-TaS₂, two large 2D FS both located at the center and the corner of the BZ are found by electronic structure calculations [82]. These common quasi-2D structures of the two closely related materials lead us to search for similar FS pockets in TaSnS₂. As the calculations below show, the small, almost cylindrical FS sheets at the corner of the BZ in TaSnS₂ (similar to those observed in TaPbS₂) could appear if the Fermi energy is slightly shifted to the electron-doped region. This could explain the lower pair of QO frequencies.

Since the QOs are observed in the polycrystalline sample it is difficult to assign FS pockets with observed frequencies, because of the expected angular dependence of the frequencies and arbitrary field directions in the polycrystal. A full angular-dependent study on single crystals would give further insight if the observed FS pockets have quasi 2D or 3D character. We observed dHvA oscillations in fields of several Tesla on the largest presently available single crystal ($m \approx 30$ mg). They were more or less consistent with the slow ones observed on the much heavier polycrystalline sample. However, the obtained data were noisy, indicating the sample mass to be too low. Therefore, to perform such a study syntheses of large enough crystals should be further optimized.

The band structure of TaSnS₂ has been reported before in the context of ARPES results [38] and very recently upon the discussion of TaSnS₂ as a nodal line semimetal [47]. In order to estimate the extreme orbits observed in the dHvA experiments we performed highly accurate and well converged LAPW calculations. Figure 10 shows the FS of TaSnS₂ which consist of an ellipsoid sheet (holelike) and—due to symmetry—doubly degenerated open hexagonal sheet (electronlike), which nearly shows no k_z dispersion.

The extremal cross section of the hole sheet in the Γ -K-A plane (field perpendicular to that plane) is about 1700 T. Shifting the Fermi level up by 4 mRy (54 meV) would bring this value to 1500 T. In contrast, shifting the E_F down would increase the extremal area and at some point even create an open orbit where no QO would be observable. Similar discrepancies between calculation and experiment have been observed before [83]. One possible explanation could be the

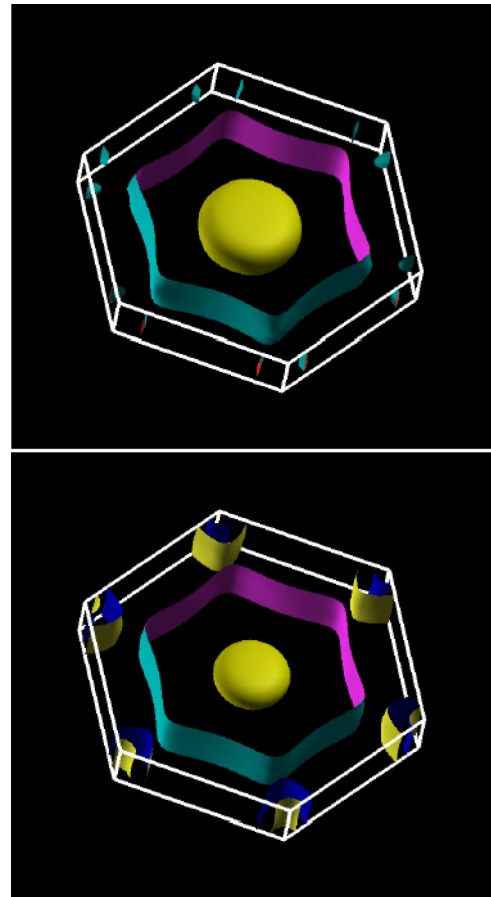


FIG. 10. Fermi surface of TaSnS₂ (a) and the same with shift of the Fermi level by 20 mRy (= 0.27 eV) (b). The hole sheet in the Γ -K-A plane is given in yellow color.

well known limitation of DFT caused by the error introduced by the self interaction. This will lead to the overestimation of the delocalization of atomic orbitals and thus should overestimate the interplane interactions.

However, the small orbits of about 100 T would not be consistent with this FS without shifting the Fermi level E_F . As one can see in Fig. 10(b), small pockets close to the K point of the Brillouin zone will open and the size of these orbits depends on the shift of E_F . As discussed in Ref. [47] for TaSnS₂ this could lead to the line nodes under some conditions. For TaPbS₂ the band structure and the observed dHvA oscillations are discussed in great detail [81]. The studies confirm that the position of E_F is crucial in the formation of line nodes around K and Γ . A relatively large shift of about 20 mRy (0.27 eV) would be required for TaSnS₂ to get a match with some of the dHvA oscillations observed. While the disagreement could be at least partially due to failures of DFT, this appears to be somewhat large and inconsistent. Eventually it may also be a hint towards a small deviation from stoichiometry, because electron doping could have a similar effect to E_F . Another possibility could be a small deviation of the c/a ratio of the polycrystalline samples compared to the single crystal due to slightly different compositions, which could produce relative shifts of the bands to each other.

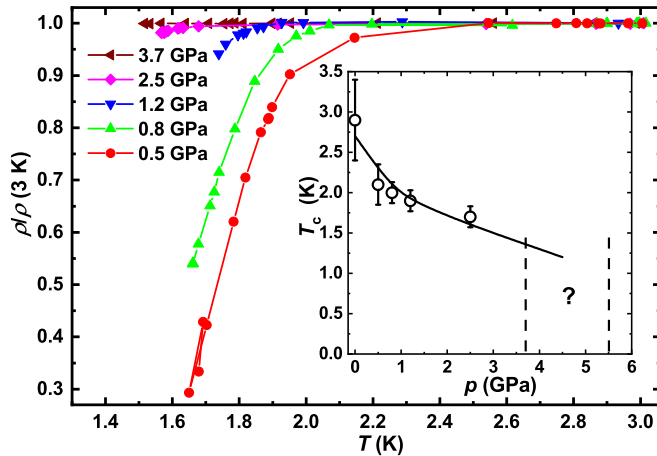


FIG. 11. The *in situ* resistivity measurements at high pressures reveal the pressure dependence of T_c (inset). No superconducting transition was observed down to 1.5 K for pressures of 3.7 and 5.5 GPa (not shown), so that we assume T_c to be in the temperature range 0–1.5 K. The solid line is a guide to the eye.

E. Pressure effect on superconductivity and structure of TaSnS₂

Electrical resistivity measurements under application of high pressure reveal a continuous decrease of the superconducting T_c with pressure increase (inset to Fig. 11). This behavior is contrary to the related misfit layered (SnS)_{1.15}(TaS₂) compound [70]. The decrease of T_c in TaSnS₂ results primarily from a weakening of electron-phonon coupling due to the stiffening of the crystalline lattice (shift of phonon spectrum to higher frequencies) upon compression [84]. The onset of SC can be observed as small resistivity drop at the temperature below 1.8 K as pressure increases up to the 2.5 GPa while no indication for SC is observed by cooling down to 1.5 K at further pressure increase above 3 GPa (Fig. 11).

The suppression of superconducting state at pressures above 3 GPa might be associated with onset of structural phase transition indicated by emergent asymmetry (low-frequency shoulder) of the Raman peak located at ~ 400 cm⁻¹ as pressure increases above 3 GPa and its split with further pressure increase (Fig. 12). To clarify the structure of the TaSnS₂ high-pressure phase, high resolution synchrotron x-ray diffraction studies are required.

IV. CONCLUSIONS

The fully-intercalated TMD compound TaSnS₂ was synthesized by powder metallurgical methods and further compacted by SPS. Single crystals of a size up to $1 \times 1 \times 0.1$ cm were grown by chemical vapor transport. Single crystal x-ray diffraction confirmed the earlier reported [34], [35] space group $P6_3/mmc$ with the lattice parameters $a = 3.30648(1)$ Å and $c = 17.4416(1)$ Å. No indications for a possible structural phase transition were observed below 300 K.

Measurements of the magnetization, specific heat, and resistivity show superconductivity at $T_c = 3.0(1)$ K. The upper critical fields in both directions (i.e., $B \perp c$ and $B \parallel c$) evidence a moderate anisotropy in TaSnS₂. The observed specific heat

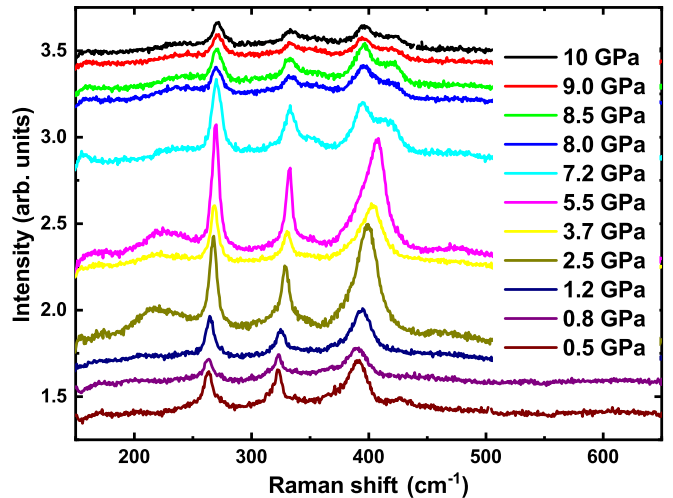


FIG. 12. Raman spectra in the pressure range 0.5–10 GPa showing a peak splitting at 400 cm⁻¹.

jump $\Delta c_p/\gamma T_c \approx 1.2$ and energy gap ratio $\Delta(0)T/k_B T_c \approx 1.3$ agree fairly well with the values (i.e., 1.43 and 1.76, respectively) predicted by weak coupling BCS theory. Together with the Ginzburg-Landau parameter $\kappa_{GL,ab} \approx 3 > 1/\sqrt{2}$, we conclude TaSnS₂ to be a weakly coupled type-II BCS *s*-wave superconductor.

De Haas-van Alphen quantum oscillations, revealing an effective mass of about $0.5m_e$, have been observed in TaSnS₂ polycrystalline sample. These oscillations originate probably from a small Fermi-surface pocket at the corner of the Brillouin zone and an ellipsoid in the center as comparisons with the band-structure calculations show.

In contrast to other nodal line semimetals the application of pressure leads to a strong suppression of the superconductivity in TaSnS₂. A pressure of $p_c = 3.7$ GPa is sufficient to shift the superconducting transition temperature below $T = 1.5$ K. Such a comparatively strong pressure dependence could originate from a pressure-induced structural phase transition, which is seemingly visible in the pressure dependent Raman study.

Our results demonstrate that TaSnS₂ is an interesting superconductor with a moderate anisotropy. So far the impact of the topological line nodes present in the band structure on the physical properties and especially on the superconductivity has not been fully clarified which certainly triggers further studies on TaSnS₂.

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- [1] N. B. Hannay, T. H. Geballe, B. T. Matthias, K. Andres, P. Schmidt, and D. MacNair, *Phys. Rev. Lett.* **14**, 225 (1965).
- [2] E. A. Antonova, S. A. Medvedev, and I. Y. Shebalin, *J. Exp. Theor. Phys. (Rus)* **30**, 181 (1970).
- [3] F. R. Gamble, F. J. DiSalvo, R. A. Klemm, and T. H. Geballe, *Science* **168**, 568 (1970).
- [4] R. A. Klemm, *Layered Superconductors* (Oxford Science Publications, Oxford, 2012).
- [5] J. G. Bednorz and K. A. Müller, *Z. Phys. B* **64**, 189 (1986).
- [6] Y. Hidaka, Y. Enomoto, M. Suzuki, M. Oda, A. Katsui, and T. Murakami, *Jpn. J. Appl. Phys.* **26**, 1133 (1987).
- [7] Y. Iye, T. Tamegai, H. Takeya, and H. Takei, *Jpn. J. Appl. Phys.* **26**, L1057 (1987).
- [8] T. K. Worthington, W. J. Gallagher, and T. R. Dinger, *Phys. Rev. Lett.* **59**, 1160 (1987).
- [9] T. R. Dinger, T. K. Worthington, W. J. Gallagher, and R. L. Sandstrom, *Phys. Rev. Lett.* **58**, 2687 (1987).
- [10] Z.-S. Wang, H.-Q. Luo, C. Ren, and H.-H. Wen, *Phys. Rev. B* **78**, 140501 (2008).
- [11] M. Fang, J. Yang, F. F. Balakirev, Y. Kohama, J. Singleton, B. Qian, Z. Q. Mao, H. Wang, and H. Q. Yuan, *Phys. Rev. B* **81**, 020509(R) (2010).
- [12] P. C. Canfield and S. L. Bud'ko, *Annu. Rev. Condens. Matter Phys.* **1**, 27 (2010).
- [13] M. Nagao, A. Miura, S. Demura, K. Deguchi, S. Watauchi, T. Takei, Y. Takano, N. Kumada, and I. Tanaka, *Solid State Commun.* **178**, 33 (2014).
- [14] T. Yoshida, S. Ideta, T. Shimojima, W. Malaeb, K. Shinada, H. Suzuki, I. Nishi, A. Fujimori, K. Ishizaka, S. Shin *et al.*, *Sci. Rep.* **4**, 7292 (2014).
- [15] Y. Mizuguchi, A. Miyake, K. Akiba, M. Tokunaga, J. Kajitani, and O. Miura, *Phys. Rev. B* **89**, 174515 (2014).
- [16] Y. C. Chan, K. Y. Yip, Y. W. Cheung, Y. T. Chan, Q. Niu, J. Kajitani, R. Higashinaka, T. D. Matsuda, Y. Yanase, Y. Aoki *et al.*, *Phys. Rev. B* **97**, 104509 (2018).
- [17] R. A. Klemm, *Physica C* **514**, 86 (2015).
- [18] K. Onabe, M. Naito, and S. Tanaka, *J. Phys. Soc. Jpn.* **45**, 50 (1978).
- [19] J. Wilson, F. D. Salvo, and S. Mahajan, *Adv. Phys.* **24**, 117 (1975).
- [20] J. M. E. Harper, T. H. Geballe, and F. J. DiSalvo, *Phys. Rev. B* **15**, 2943 (1977).
- [21] E. Revolinsky, G. Spiering, and D. Beerntsen, *J. Phys. Chem. Solids* **26**, 1029 (1965).
- [22] M. van Maaren and H. Harland, *Phys. Lett. A* **29**, 571 (1969).
- [23] K. Yokota, G. Kurata, T. Matsui, and H. Fukuyama, *Phys. B: Condens. Matter* **284-288**, 551 (2000).
- [24] X. Li, M. Zhou, and C. Dong, *Supercond. Sci. Technol.* **32**, 035001 (2018).
- [25] M. Ikebe, N. Kobayashi, K. Katagiri, and Y. Muto, *Physica B+C* **105**, 435 (1981).
- [26] B. Dalrymple and D. Prober, *J. Low Temp. Phys.* **56**, 545 (1984).
- [27] M. S. Whittingham, *Prog. Solid State Chem.* **12**, 41 (1978).
- [28] F. R. Gamble, J. H. Osiecki, and F. J. DiSalvo, *J. Chem. Phys.* **55**, 3525 (1971).
- [29] M. H. Zhou, X. C. Li, and C. Dong, *Supercond. Sci. Technol.* **31**, 065001 (2018).
- [30] K. E. Wagner, E. Morosan, Y. S. Hor, J. Tao, Y. Zhu, T. Sanders, T. M. McQueen, H. W. Zandbergen, A. J. Williams, D. V. West *et al.*, *Phys. Rev. B* **78**, 104520 (2008).
- [31] L. Li, X. Zhu, Y. Sun, H. Lei, B. Wang, S. Zhang, X. Zhu, Z. Yang, and W. Song, *Physica C: Supercond.* **470**, 313 (2010).
- [32] R. Eppinga and G. Wieggers, *Physica B+C* **99**, 121 (1980).
- [33] E. A. Marseglia, *Int. Rev. Phys. Chem.* **3**, 177 (1983).
- [34] R. Eppinga and G. Wieggers, *Mater. Res. Bull.* **12**, 1057 (1977).
- [35] A. van der Lee and G. Wieggers, *Mater. Res. Bull.* **25**, 1011 (1990).
- [36] F. J. Di Salvo, G. W. Hull, L. H. Schwartz, J. M. Voorhoeve, and J. V. Waszczak, *J. Chem. Phys.* **59**, 1922 (1973).
- [37] R. Eppinga, G. Wieggers, and C. Haas, *Physica B+C* **105**, 174 (1981).
- [38] J. Dijkstra, E. A. Broekhuizen, C. F. van Bruggen, C. Haas, R. A. de Groot, and H. P. van der Meulen, *Phys. Rev. B* **40**, 12111 (1989).
- [39] R. Eppinga, G. A. Sawatzky, C. Haas, and C. F. van Bruggen, *J. Phys. C: Solid State Phys.* **9**, 3371 (1976).
- [40] R. H. Herber and R. F. Davis, *J. Chem. Phys.* **63**, 3668 (1975).
- [41] R. H. Herber and R. F. Davis, *J. Chem. Phys.* **65**, 3773 (1976).
- [42] P. Gentile, D. Driscoll, and A. Hockman, *Inorg. Chim. Acta* **35**, 249 (1979).
- [43] R. H. Herber, F. J. DiSalvo, and R. B. Frankel, *Inorg. Chem.* **19**, 3135 (1980).
- [44] A. C. Gossard, F. J. d. Salvo, and H. Yasuoka, *Phys. Rev. B* **9**, 3965 (1974).
- [45] G. Y. Guo and W. Y. Liang, *J. Phys. C: Solid State Phys.* **20**, 4315 (1987).
- [46] P. Blaha, *J. Phys.: Condens. Matter* **3**, 9381 (1991).
- [47] D.-Y. Chen, Y. Wu, L. Jin, Y. Li, X. Wang, J. X. Duan, J. Han, X. Li, Y.-Z. Long, X. Zhang, D. Chen, and B. Teng, *Phys. Rev. B* **100**, 064516 (2019).
- [48] Y. Qi, P. G. Naumov, M. N. Ali, C. R. Rajamathi, W. Schnelle, O. Barkalov, M. Hanfland, S.-C. Wu, C. Shekhar, Y. Sun *et al.*, *Nat. Commun.* **7**, 11038 (2016).
- [49] Y. Fang, Q. Dong, J. Pan, H. Liu, P. Liu, Y. Sun, Q. Li, W. Zhao, B. Liu, and F. Huang, *J. Mater. Chem. C* **7**, 8551 (2019).
- [50] J. J. Gao, J. G. Si, X. Luo, J. Yan, Z. Z. Jiang, W. Wang, C. Q. Xu, X. F. Xu, P. Tong, W. H. Song *et al.*, *J. Phys. Chem. C* **124**, 6349 (2020).
- [51] G. Bian, T.-R. Chang, R. Sankar, S.-Y. Xu, H. Zheng, T. Neupert, C.-K. Chiu, S.-M. Huang, G. Chang, I. Belopolski *et al.*, *Nat. Commun.* **7**, 10556 (2016).
- [52] S.-Y. Guan, P.-J. Chen, M.-W. Chu, R. Sankar, F. Chou, H.-T. Jeng, C.-S. Chang, and T.-M. Chuang, *Sci. Adv.* **2**, e1600894 (2016).
- [53] B.-T. Wang, P.-F. Liu, J.-J. Zheng, W. Yin, and F. Wang, *Phys. Rev. B* **98**, 014514 (2018).
- [54] P.-J. Chen, T.-R. Chang, and H.-T. Jeng, *Phys. Rev. B* **94**, 165148 (2016).
- [55] STOE Powder Software, WinXPow (version 2), Darmstadt, STOE and Cie GmbH, 2001.
- [56] Bruker AXS Inc., DOC-M86-EXX190 D8 QUEST User Manual (2012).
- [57] Bruker AXS Inc., DOC-M86-EXX229 APEX3 Software User Manual (2016).
- [58] L. Akselrud and Y. Grin, *J. Appl. Crystallogr.* **47**, 803 (2014).

- [59] G. Carter, L. Bennett, and D. Kahan, in *Progress in Materials Science*, edited by B. Chalmers, J. Christian, and T. Massalski (Pergamon Press, Oxford, 1977), Vol. 81, pp. 779–780.
- [60] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. H. Madsen, and L. D. Marks, *J. Chem. Phys.* **152**, 074101 (2020).
- [61] J. P. Perdew and Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).
- [62] J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, *Phys. Rev. Lett.* **100**, 136406 (2008).
- [63] <http://www.goldensoftware.com/products/surfer/surfer.shtml>.
- [64] S. A. Khan, J. M. Reynolds, and R. G. Goodrich, *Phys. Rev.* **163**, 579 (1967).
- [65] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.102.214501> for results of powder XRD phase analysis and magnetic ac susceptibility measurement.
- [66] R. Gross and A. Marx, *Festkörperphysik* (Oldenbourg Verlag, München, 2012).
- [67] D. E. Prober, R. E. Schwall, and M. R. Beasley, *Phys. Rev. B* **21**, 2717 (1980).
- [68] M. N. Ali, Q. D. Gibson, T. Klimczuk, and R. J. Cava, *Phys. Rev. B* **89**, 020505(R) (2014).
- [69] M. Ikebe, K. Katagiri, K. Noto, and Y. Muto, *Physica B+C* **99**, 209 (1980).
- [70] R. Sankar, G. Peramaiyan, I. Panneer Muthuselvam, C.-Y. Wen, X. Xu, and F. C. Chou, *Chem. Mater.* **30**, 1373 (2018).
- [71] L. Fang, Y. Wang, P. Y. Zou, L. Tang, Z. Xu, H. Chen, C. Dong, L. Shan, and H. H. Wen, *Phys. Rev. B* **72**, 014534 (2005).
- [72] D. Bhoi, S. Khim, W. Nam, B. S Lee, C. Kim, B.-G. Jeon, B. H. Min, S. Park, and K. Kim, *Sci. Rep.* **6**, 24068 (2016).
- [73] R. Coleman and S. Hillenius, *Physica B+C* **105**, 428 (1981).
- [74] R. A. Klemm, A. Luther, and M. R. Beasley, *Phys. Rev. B* **12**, 877 (1975).
- [75] Y. Iye and S. I. Tanuma, *Phys. Rev. B* **25**, 4583 (1982).
- [76] A. Chaiken, M. S. Dresselhaus, T. P. Orlando, G. Dresselhaus, P. M. Tedrow, D. A. Neumann, and W. A. Kamitakahara, *Phys. Rev. B* **41**, 71 (1990).
- [77] K. Holczer, O. Klein, G. Grüner, J. D. Thompson, F. Diederich, and R. L. Whetten, *Phys. Rev. Lett.* **67**, 271 (1991).
- [78] M. Baenitz, M. Kraus, S. Gärtner, H. M. Vieth, H. Werner, R. Schlögl, W. Krätschmer, M. Kanowski, and K. Lüders, in *Electronic Properties of High-Tc Superconductors*, edited by H. Kuzmany, M. Mehring, and J. Fink (Springer Berlin Heidelberg, Berlin, Heidelberg, 1993), pp. 475–481.
- [79] D. C. Johnston, *Supercond. Sci. Technol.* **26**, 115011 (2013).
- [80] D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge University Press, Cambridge, UK, 1984).
- [81] X. Xu, Z. Kang, T.-R. Chang, H. Lin, G. Bian, Z. Yuan, Z. Qu, J. Zhang, and S. Jia, *Phys. Rev. B* **99**, 104516 (2019).
- [82] G. Wexler and A. M. Woolley, *J. Physics C: Solid State Phys.* **9**, 1185 (1976).
- [83] I. I. Mazin and J. Kortus, *Phys. Rev. B* **65**, 180510(R) (2002).
- [84] J. Schilling, in *Handbook of High-Temperature Superconductivity*, edited by J. R. Schrieffer (Springer, Berlin, 2007), pp. 427–462.