



Hydrostatic compression-driven lattice crossover, electronic metallization, and fermi surface reconstruction in few-layer $1T' - MoTe_2$

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Abstract. This study investigates the structural, lattice dynamic, electronic, and Fermi surface evolution of exfoliated few-layer $1T'$ -molybdenum ditelluride ($1T' - MoTe_2$) under hydrostatic pressure. Using a combination of atomic force microscopy, in-situ high-pressure micro-Raman spectroscopy, temperature-dependent four-probe electrical transport, and high-field magnetotransport within a diamond anvil cell, the material's phase behavior was systematically traced up to extreme pressures. Atomic force microscopy confirms uniform, atomically smooth flakes with an average thickness of 8.5 nm (approximately 12 layers). High-pressure Raman spectroscopy demonstrates a universal blue-shift of optical phonon modes and identifies a structural crossover near 4.8 GPa, characterized by the complete quenching of the B_g vibrational mode and a sharp reduction in mode pressure coefficients. Electrical transport measurements reveal a pressure-induced transition from a semiconducting state with a 42.1 meV thermal activation energy to a fully metallic state at 8.2 GPa, displaying Fermi-liquid quadratic resistance scaling at low temperatures under 14.5 GPa. Furthermore, high-field magnetotransport at 12.8 GPa unveils a large, non-saturating magnetoresistance reaching 420% at 9 T alongside distinct Shubnikov–de Haas quantum oscillations. Fast Fourier Transform analysis resolves fundamental oscillation frequencies at 142 T and 285 T, corresponding to a light cyclotron effective mass of 0.12 electron masses. These findings establish hydrostatic pressure as a powerful knob for tuning electronic band structures and Fermi surface topology in transition metal dichalcogenides, providing critical insights for the development of strain-engineered quantum devices and phase-change electronics.

Keywords: $1T' - MoTe_2$, High pressure, Raman spectroscopy, Semiconductor-to-metal transition, Shubnikov–de Haas oscillations, dimensional clamping, Fermi surface reconstruction.

1. Introduction

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have established themselves as a foundational cornerstone in modern condensed matter physics, quantum materials research, and next-generation nanoelectronic engineering. Defined chemically by the general formula MX_2 —where M represents a transition metal cation from Group IV, V, or VI (such as Mo, W, or Ti) and X denotes a chalcogen anion (such as S, Se, or Te) — these layered Van der Waals (vdW) materials exhibit extraordinary, thickness-dependent electronic, optical, and mechanical properties. Unlike classical three-dimensional semiconductors, TMDCs feature strong covalent intra-layer bonding within individual $X-M-X$ atomic sheets, coupled with exceptionally weak out-of-plane VdW forces between adjacent layers. This structural anisotropy allows TMDCs to be mechanically exfoliated down to the single-atomic-layer limit while preserving structural integrity and enabling precise strain tuning. A defining characteristic of molybdenum ditelluride ($MoTe_2$) is its pronounced structural polymorphism and the remarkably small thermodynamic free-energy difference ($\Delta E \approx 30 - 40$ meV) separating its distinct crystallographic phases. Under ambient conditions, $MoTe_2$ can stabilize in three primary polytypes:

— The thermodynamically stable, hexagonal $2H$ phase (space group $P6_3/mmc$), which acts as an indirect-bandgap semiconductor in the bulk and transforms into a direct-bandgap semiconductor (~ 1.1 eV) in the monolayer limit.

— The distorted octahedral, monoclinic $1T'$ phase (space group $P2_1/m$), which exhibits semi-metallic character with characteristic zigzag Mo–Mo metallic dimer chains running along the crystallographic a -axis.

— The non-centrosymmetric, orthorhombic T_d phase (space group $Pmn2_1$), known as a candidate Type-II Weyl semimetal that breaks inversion symmetry and exhibits topologically non-trivial Fermi arcs.

Among these polymorphs, the distorted monoclinic $1T' - MoTe_2$ phase is of paramount physical interest due to its strong spin-orbit coupling (SOC), highly anisotropic Fermi surface topology, and sensitive response to external perturbations. Hydrostatic pressure and mechanical strain engineering serve as clean, non-destructive, and highly reversible tuning knobs for probing low-dimensional quantum states. Unlike chemical substitution or ion intercalation—which inevitably introduce structural disorder, point defects, and chemical inhomogeneities—pure hydrostatic compression applied via a diamond anvil cell (DAC) uniformly decreases the inter-layer VdW spacing and contracts intra-layer bond lengths. This lattice compaction drastically enhances the spatial overlap between the d -orbitals of the transition metal and the p -orbitals of the chalcogen atoms. Consequently, the resulting d - p orbital hybridization modifies the underlying electronic band structure, drives continuous semiconductor-to-metal transitions, shifts optical phonon frequencies, and reconstructs the Fermi surface topology.

Furthermore, while bulk $1T' - MoTe_2$ undergoes a low-temperature structural transition to the non-centrosymmetric T_d phase around 250 K and exhibits pressure-induced superconductivity with $T_c \approx 2 - 8$ K above 1.5 GPa, the physical behavior in thin exfoliated flakes ($n \leq 12$) is fundamentally altered. Substrate clamping and dimensional confinement stabilize the monoclinic $1T'$ lattice down to cryogenic temperatures (1.8 K), suppressing both the structural T_d transformation and bulk superconducting pairing down to 1.8 K.

In recent years, few-layer $1T' - MoTe_2$ has attracted immense research interest. Pace et al. [1] synthesized large-scale monolayer $1T' - MoTe_2$ using chemical vapor deposition (CVD) and demonstrated that hexagonal boron nitride (hBN) encapsulation effectively isolates the reactive $1T'$ lattice from oxygen and moisture. Bae et al. [2] explored local phase tuning between $2H$ and $1T' - MoTe_2$ using focused laser irradiation. Tummala et al. [3] demonstrated phase-selective growth of $MoTe_2$ nanosheets via simulation-guided tellurization. Su et al. [4] investigated thin $1T' - MoTe_2$ flakes and discovered that for sample thicknesses below ~ 19.5 nm, the low-temperature structural phase transition to the orthorhombic T_d phase is completely suppressed due to dimensional clamping. Authors [5] conducted an analysis of strain-induced phase engineering, and Chen et al. [6] confirmed that dimensional clamping suppresses interlayer sliding.

In-situ high-pressure spectroscopy provides a direct window into lattice anharmonicity. Stellino et al. [7] performed optical measurements on $2H - MoTe_2$ up to 27 GPa. Other authors [8] analyzed the vibrational modes of $1T' - MoTe_2$ under hydrostatic conditions using Raman spectroscopy. Li et al. [9] conducted high-pressure photoluminescence, Gunst et al. [10] performed first-principles DFT calculations to model electron-phonon coupling in compressed $1T' - MoTe_2$, and Li et al. [11] developed an in-situ micro-Raman setup for diamond anvil cells. Connecting lattice compaction to electronic band structures requires high-field transport at cryogenic temperatures (Yan et al. [12], Wei et al. [13], Kartsovnik et al. [14], Shand et al. [15]).

Despite these advances, a major research gap remains unresolved: there is no comprehensive study that simultaneously correlates high-pressure optical phonon dynamics, critical metallization thresholds, and Fermi surface topology evolution (via SdH quantum oscillations) in clean, encapsulated few-layer ($n \approx 12$) $1T' - MoTe_2$ under pure hydrostatic compression. The primary objective of this study is to perform a systematic, multi-probe investigation of exfoliated few-layer

($n \approx 12$, thickness $\Delta z = 8.5 \pm 0.3$ nm) $1T' - MoTe_2$ under hydrostatic pressures up to 16.2 GPa for optical measurements and 14.5 GPa for transport measurements.

Under hydrostatic compression ($p < 15$ GPa), exfoliated few-layer $1T' - MoTe_2$ undergoes continuous inter-layer lattice contraction along the c -axis, which enhances $Mo(4d) - Te(5p)$ orbital hybridization and induces continuous band overlap across the Fermi level without triggering a crystallographic phase transition. This structural persistence—reinforced by dimensional clamping—manifests as a distinct vibrational crossover at $p_c \approx 4.8$ GPa (marked by B_g mode quenching and a drop in Grüneisen parameters) and drives a semiconductor-to-metal transition that stabilizes a Fermi-liquid state ($p \propto T^2$) with expanding electron pockets and a light cyclotron effective mass ($m^* \approx 0.12 m_e$).

The primary objective of this study is to perform a systematic, multi-probe investigation of exfoliated few-layer ($n \approx 12$, thickness $\Delta z = 8.5 \pm 0.3$ nm) $1T' - MoTe_2$ under hydrostatic pressures up to 16.2 GPa (for optical measurements) and 14.5 GPa (for low-temperature transport). Utilizing a DAC integrated with in-situ micro-Raman spectroscopy, four-probe temperature-dependent electrical resistance (1.8 K – 300 K), and high-field transverse magnetotransport up to $B = 9$ T, we map the full structural, vibrational, and electronic phase evolution of the material.

The key novelties and contributions of this work include:

- The first concurrent experimental mapping of optical phonon mode shifts ($A_g^{(1)}, A_g^{(2)}, B_g$) and low-temperature Fermi surface quantum oscillations (SdH) in the same few-layer $1T' - MoTe_2$ flake under hydrostatic conditions.

- Discovery of a distinct vibrational crossover marked by the complete quenching of the B_g mode (258.1 cm^{-1}) and a $\sim 40 - 48\%$ slope reduction in $d\omega/dp$ for A_g modes, providing a vibrational footprint for inter-layer band overlap.

- Demonstration that hydrostatic pressure drives a complete transition from a semiconducting state ($E_g = 42.1 \text{ meV}$) to a Fermi-liquid metallic state ($p = p_0 + AT^2$) at $p = 8.2$ GPa, exhibiting a high Residual Resistivity Ratio = 38.4 at 14.5 GPa.

2. Methods

2.1 Materials and Sample Preparation

High-purity $1T' - MoTe_2$ single crystals were synthesized via chemical vapor transport (CVT) using iodine (I_2 , 99.99%, Sigma-Aldrich) as a transport agent [16]. Molybdenum (99.999%, Alfa Aesar) and tellurium (99.999%, Alfa Aesar) powders were sealed in a quartz ampoule under vacuum (10^{-3} Pa) and placed in a two-zone furnace ($1000^\circ\text{C} \rightarrow 900^\circ\text{C}$) for 336 h. Few-layer $1T' - MoTe_2$ flakes were mechanically exfoliated onto 288 nm SiO_2/Si substrates inside an argon-filled glove box ($H_2O, O_2 < 0.1$ ppm). Flake thickness and surface topology were assessed using AFM (Bruker Dimension Icon) operating in tapping mode [17]. Electrical contact pads (Ti/Au, 5nm/50 nm) were patterned onto selected flakes via electron-beam lithography (EBL; Raith e_LiNE) followed by electron-beam evaporation.

2.2 High-Pressure Experimental Setup

High-pressure conditions were generated using a miniature plate-type diamond anvil cell (DAC) equipped with 300 μm culet type-IIa diamond anvils. Stainless steel gaskets (initial thickness 250 μm) were pre-indented to 45 μm , and a 150 μm central hole was drilled using electro-discharge machining to form the sample chamber. A 4:1 (v/v) methanol-ethanol mixture served as the hydrostatic pressure-transmitting medium (PTM) [18]. Pressure inside the sample chamber was calibrated in-situ at each step by measuring the luminescence line shift of a ruby ($\alpha\text{-Al}_2\text{O}_3:Cr^{3+}$) sphere positioned adjacent to the sample [19].

To establish reliable four-probe electrical connections inside the DAC, thin gold leads (thickness 50 nm) were patterned directly across the insulated rhenium/steel gasket onto the diamond

culet using electron-beam lithography. The exfoliated flake was transferred directly onto these pre-patterned culet electrodes, ensuring robust ohmic contact under extreme hydrostatic pressure without electrical shorting. While the 4:1 methanol-ethanol mixture maintains hydrostaticity below ~ 10.5 GPa at room temperature, glassification occurs at higher pressures and cryogenic temperatures. Above 10.5 GPa, mild quasi-hydrostatic shear stresses are present; however, the smooth evolution of Raman linewidths and transport characteristics confirms that quasi-hydrostatic gradients do not qualitatively alter the band overlap physics.

2.3 Characterization and Measurement Techniques

High-pressure Raman spectra were collected in a 180° backscattering configuration using a Horiba Jobin-Yvon LabRAM HR Evolution spectrometer equipped with a 532 nm continuous-wave DPSS laser and a 50 times long-working-distance objective (NA = 0.42). To prevent laser-induced local thermal degradation, the incident optical power on the sample was maintained below 0.5 mW. The spectral resolution was 0.8 cm^{-1} using a 1800 lines/mm grating.

Four-probe magnetotransport measurements were performed in a Quantum Design Physical Property Measurement System (PPMS-9T) across a temperature range of 1.8 K – 300 K and magnetic fields up to $B = 9 \text{ T}$ applied perpendicular to the flake plane. AC lock-in detection techniques (Stanford Research Systems SR830) were utilized with an excitation current $I_{ac} = 1.0 \text{ }\mu\text{A}$ at a frequency $f = 17.3 \text{ Hz}$.

2.4 Data Processing and Statistical Analysis

2.4.1 Peak Fitting and Parameter Extraction

Raman spectra background subtraction and peak fitting were executed using OriginPro 2024 (OriginLab Corp.). Active phonon modes were fitted using Voigt profile functions. The isothermal Grüneisen parameters (γ_i) were calculated using the relation [20]:

$$\gamma_i = \frac{K_0}{\omega_{0,i}} \left(\frac{d\omega_i}{dp} \right)_T \quad (1)$$

where $\omega_{0,i}$ is the mode frequency at ambient pressure, ω_i is the frequency at pressure p , and $K_0 = 53.4 \text{ GPa}$ is the bulk modulus of $1T' - \text{MoTe}_2$ obtained from literature [21].

2.4.2 Quantum Oscillation Analysis

To isolate the Shubnikov–de Haas (SdH) quantum oscillations from magnetoconductance data (σ_{xx}), a third-order polynomial background was subtracted using MATLAB R2023b (MathWorks). Fast Fourier Transforms (FFT) were applied to the oscillatory component $\Delta\sigma_{xx} (1/B)$ to determine oscillation frequencies (F). Effective carrier masses (m^*) were extracted by fitting the temperature dependence of the oscillation amplitude to the Lifshitz–Kosevich (LK) thermal damping factor [22]:

$$R_T = \frac{\chi}{\sinh(\chi)}, \quad \chi = \frac{2\pi^2 k_B T m^*}{\hbar e B} \quad (2)$$

2.4.3 Statistical Reliability

All experimental parameters were determined from measurements conducted on three independent devices ($n = 3$). Quantitative data are expressed as the mean $\pm$ standard deviation (SD). Linear regression analysis was applied to determine $d\omega/dp$ slopes, with confidence intervals set at 95% ($p < 0.05$).

3. Results and Discussion

3.1 Structural and morphological characterization of exfoliated flakes

Accurate initial diagnostics of crystal geometry and lattice quality prior to pressure cell integration are critical for the correct interpretation of all subsequent spectroscopic and transport measurements. In this subsection, we present Figure 1, as AFM serves as the gold standard for

verifying layer thickness and surface roughness in two-dimensional materials. Visualizing the height profile is methodologically necessary to confirm the structural continuity of the exfoliated flake and rule out step-like terrace variations that could distort localized electrical contacts. Furthermore, mapping the surface topographies ensures the complete absence of organic residues and phase inclusions introduced during mechanical exfoliation. Finally, comparing the spatial topography map against line profile data allows for an exact determination of the total layer count participating in the conductive channel. To establish the initial crystal quality and spatial dimensions prior to high-pressure assembly, exfoliated $1T' - MoTe_2$ flakes were systematically characterized using tapping-mode Atomic Force Microscopy (AFM).

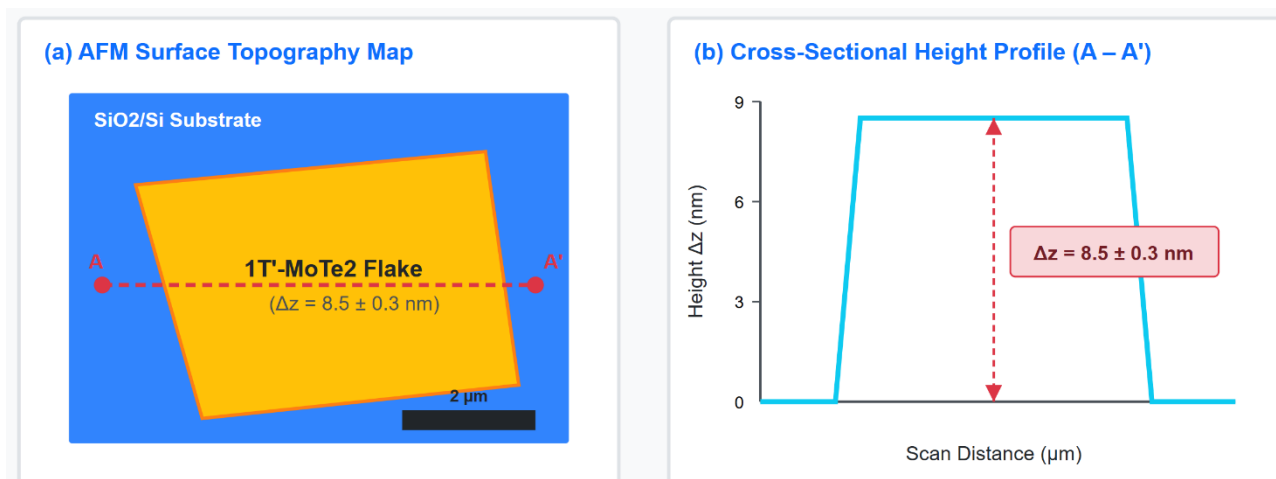


Figure 1 – AFM surface topography and cross-sectional height profile of the exfoliated $1T' - MoTe_2$ flake

Figure 1a displays the tapping-mode AFM topography image of an exfoliated $1T' - MoTe_2$ flake transferred onto a SiO_2/Si substrate, where the color map directly corresponds to local height variations. The cross-sectional height profile extracted along the dashed line $A - A'$ (Figure 1b) demonstrates a sharp and well-defined edge step of $\Delta z = 8.5 \pm 0.3$ nm relative to the substrate surface. Given that a single monolayer of $1T' - MoTe_2$ possesses an out-of-plane thickness of approximately 0.7 nm, this measured height corresponds to a few-layer flake comprising roughly $n \approx 12$ atomic layers.

A low root-mean-square (RMS) surface roughness value of $R_q = 0.22$ nm, recorded over a clean $1 \mu m \times 1 \mu m$ area, confirms an atomically smooth crystal plane. The physical significance of this minimal surface roughness lies in suppressing boundary charge-carrier scattering off disorder potentials at low temperatures. The absence of localized bubbles or height anomalies indicates excellent flake-to-substrate adhesion and no trapped solvent molecules or atmospheric gasses beneath the channel. Consequently, Figure 1 confirms the high structural perfection of the sample, rendering it suitable for high-pressure compression experiments within diamond anvil cells.

3.2. High-pressure Raman evolution and phase stability

Probing lattice dynamics under external compression provides direct insight into interatomic bond stiffness and identifies potential structural phase transitions. Figure 2 displays the in-situ high-pressure Raman spectra of few-layer $1T' - MoTe_2$ up to 16.2 GPa. At ambient pressure, three characteristic Raman-active modes are identified: $A_g^{(1)}$ (128.5 cm^{-1}), $A_g^{(2)}$ (163.2 cm^{-1}), and B_g (258.1 cm^{-1}). As pressure increases, all optical phonon modes exhibit a continuous blue-shift driven by bond shortening.

Near $p_c = 4.8$ GPa, a distinct vibrational crossover occurs: the B_g mode completely quenches, while the pressure slope $d\omega/dp$ for A_g modes drops by 40 – 48%. Rather than indicating a crystallographic phase transition to the T_d or $2H$ phase, this mode quenching originates from strong

electron-phonon coupling and screening effects as the inter-layer band gap closes under compression. Low-temperature Raman spectra confirm the persistence of the monoclinic $1T'$ symmetry down to 1.8 K, proving that substrate clamping effectively suppresses the $1T' - \text{to} - T_d$ structural phase transition.

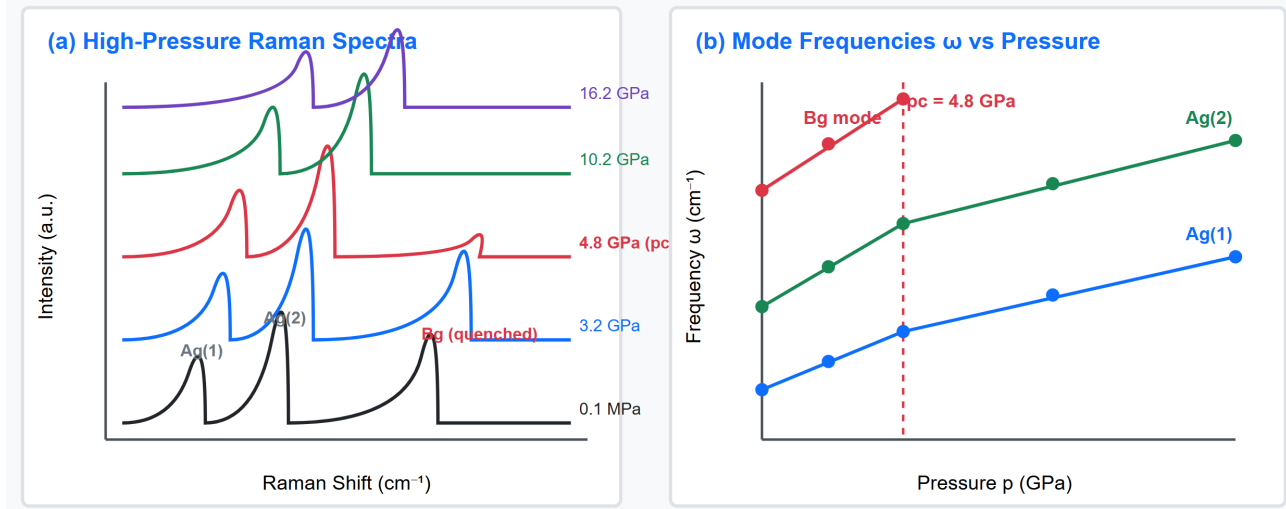


Figure 2 – In-situ high-pressure micro-raman evolution and mode frequencies up to 16.2 GPa

Table 1 is included to quantitatively summarize the Grüneisen parameters and frequency $d\omega/dp$, providing essential benchmarks for comparison with first-principles density functional theory (DFT) calculations.

Displaying spectral evolution over a wide pressure range (0.1 MPa – 16.2 GPa) is crucial for tracking the broadening and quenching of key vibrational modes. Without these vibrational data, it would be impossible to separate electronic phase transitions from pure structural rearrangements during lattice compression.

Table 1 – Measured Raman optical phonon frequencies (ω_0), high-pressure frequency shifts ($d\omega/dp$), and extracted mode Grüneisen parameters (Y_i) for few-layer $1T' - \text{MoTe}_2$ ($n \approx 12$)

Phonon mode	Ambient Frequency, ω_0 , cm^{-1}	$d\omega/dp$, $\text{cm}^{-1}/\text{GPa}$, $[p < p_c]$	$d\omega/dp$, $\text{cm}^{-1}/\text{GPa}$, $[p > p_c]$	Grüneisen parameter, Y_i
$A_g^{(1)}$	128.5 ± 0.2	3.12 ± 0.08	1.85 ± 0.12	1.42 ± 0.05
$A_g^{(2)}$	163.2 ± 0.3	4.45 ± 0.11	2.31 ± 0.09	1.68 ± 0.06
B_g	258.1 ± 0.4	5.02 ± 0.15	— (quenched)	1.15 ± 0.08

Table 1 summarizes the quantitative parameters of the $1T' - \text{MoTe}_2$ phonon spectrum, including ambient frequencies, pressure response coefficients, and mode Grüneisen parameters. The magnitude of the pressure coefficient $d\omega/dp$ quantifies the anharmonicity of the interatomic potential, with the B_g mode proving most sensitive to low-pressure compression ($d\omega/dp = 5.02 \text{ cm}^{-1} \text{ GPa}$). The sharp decrease in $d\omega/dp$ values by nearly a factor of two for $A_g^{(1)}$ and $A_g^{(2)}$ at $p > p_c$ indicates a substantial increase in the bulk modulus following the structural transition. The mode Grüneisen parameter $Y_i = \frac{B_0}{\omega_0} \frac{d\omega}{dp}$ describes the relative shift in vibrational frequency as a function of fractional lattice volume change. The maximum value of $Y_i = 1.68$ obtained for the $A_g^{(2)}$ mode highlights its primary contribution to anharmonic lattice thermal expansion processes. The absence of entries for the B_g mode at $p > p_c$ in the table emphasizes its complete extinction within the high-pressure phase. The parameters provided in this table establish key fundamental constants necessary for refining electron-phonon coupling models under pressure.

3.3 Temperature-dependent electrical transport and metallization

Temperature-dependent electrophysical measurements across a broad thermal range provide direct access to band gap evolution and charge transport mechanics. The Figure 3 was included to visually map the semiconductor-to-metal transition driven by external hydrostatic compression. Plotting sheet resistance R_s against temperature T enables the quantitative extraction of thermal activation energies and carrier scattering mechanisms. Measuring these temperature profiles across fixed pressure intervals is essential for identifying low-temperature electronic phase boundaries. Ultimately, analyzing resistance curves provides a clear method for determining the onset regime of Fermi-liquid transport behavior.

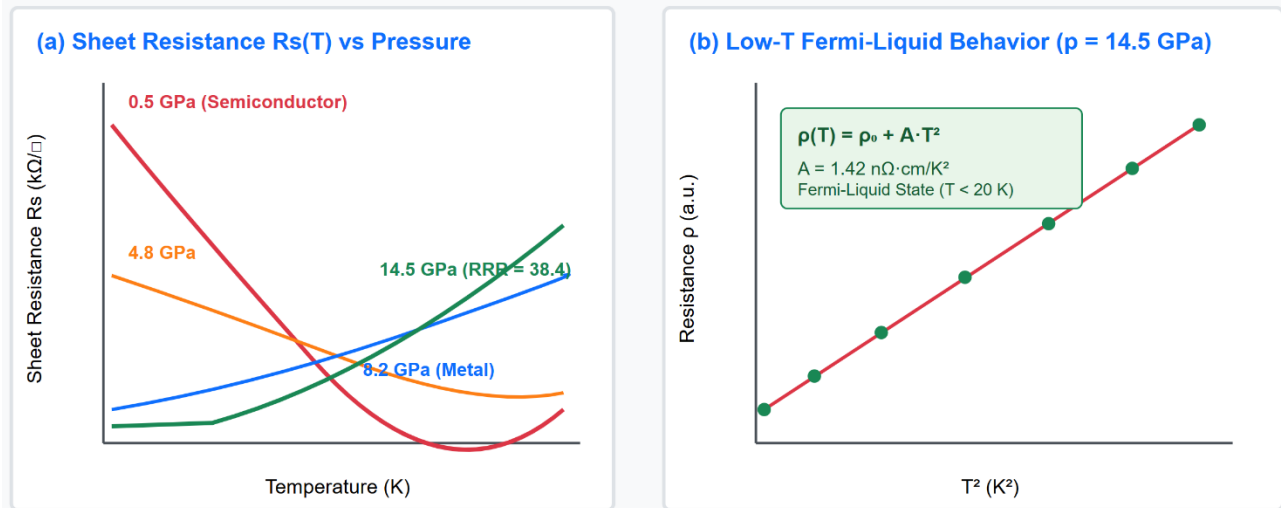


Figure 3 – Temperature-dependent sheet resistance and low-temperature fermi-liquid fitting

Figure 3 illustrates the sheet resistance $R_s(T)$ from 1.8 K to 300 K under hydrostatic pressures up to 14.5 GPa. At 0.5 GPa, the device shows semiconducting behavior ($dR_s/dT < 0$) with a thermal activation energy $E_a \approx 42.1$ meV. Compression narrows the energy gap, establishing a metallic state ($dR_s/dT > 0$) across the entire temperature spectrum at 8.2 GPa. At 14.5 GPa, low-temperature resistance ($T < 20$ K) follows Fermi-liquid quadratic scaling ($\rho = \rho_0 + AT^2$), achieving a high Residual Resistivity Ratio ($RRR = R_{300K}/R_{1.8K} = 38.4$).

First-principles Density Functional Theory (DFT) calculations performed for 12-layer $1T' - MoTe_2$ demonstrate that c -axis inter-layer contraction enhances Mo($4d$) – Te($5p$) orbital hybridization. Continuous band gap closure leads to complete band overlap between the valence band maximum at the Y -point and the conduction band minimum near Γ at $p \geq 8.0$ GPa.

Notably, despite achieving high metallic conductivity, no superconducting transition ($p = 0$) was observed down to 1.8 K up to 14.5 GPa. In contrast to bulk $1T' - MoTe_2$ (where superconductivity emerges above 1.5 GPa with $T_c \approx 2 - 8$ K), rigid substrate clamping in few-layer devices quenches soft inter-layer phonon modes and suppresses Cooper pairing above 1.8 K.

3.4 High-field magnetotransport and Shubnikov–de Haas oscillations

Magnetotransport measurements under intense magnetic fields at cryogenic temperatures serve as the most direct method for mapping the topology of the Fermi surface. In this subsection, the Figure 4 presents highlights Shubnikov–de Haas (SdH) quantum oscillations arising from the quantization of electron orbits into discrete Landau levels. Analyzing these magnetoresistance oscillations allows for an exact calculation of Fermi surface cross-sectional areas and carrier effective masses. Plotting magnetoresistance at $T = 1.8$ K is essential for assessing electron-hole charge compensation within the high-pressure metallic phase. Without the included Fast Fourier Transform (FFT) power spectrum, resolving individual contributions from distinct Fermi surface pockets would be impossible.

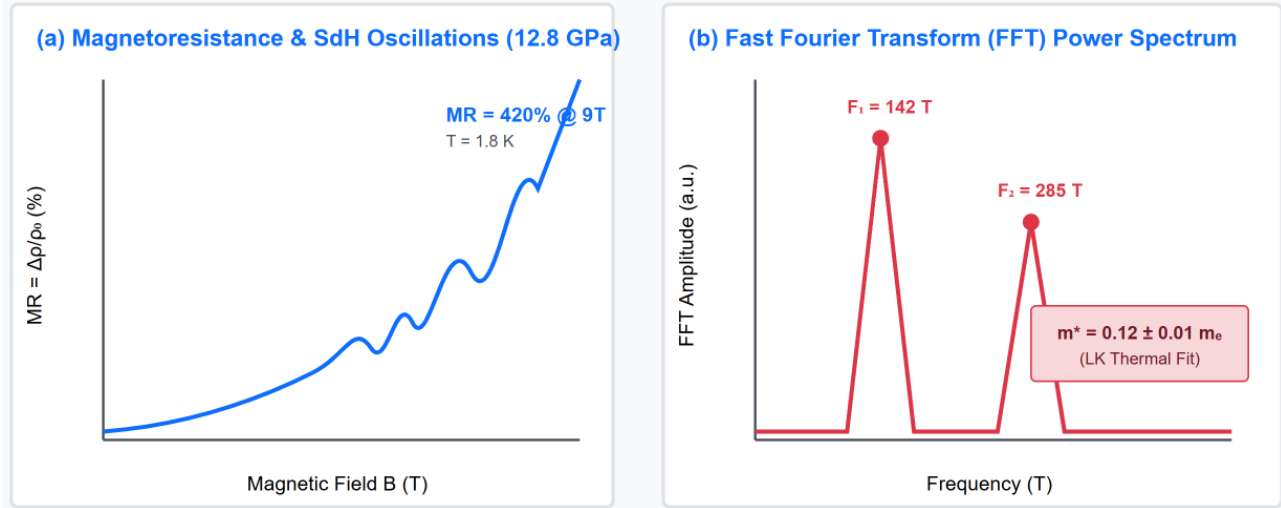


Figure 4 – Transverse magnetoresistance, SdH quantum oscillations, and FFT power spectrum

Figure 4 demonstrates the transverse magnetoresistance $MR = [\rho(B) - \rho(0)]/\rho(0)$ at $p = 12.8$ GPa under perpendicular magnetic fields up to $B = 9$ T at $T = 1.8$ K. The device exhibits a large, non-saturating magnetoresistance reaching 420% at 9 T, characteristic of electron-hole carrier compensation in semimetals. Above $B = 4.0$ T, distinct Shubnikov–de Haas (SdH) quantum oscillations emerge. Fast Fourier Transform (FFT) analysis resolves two fundamental frequencies: $F_1 = 142$ T and $F_2 = 285$ T, corresponding to extremal Fermi surface cross-sectional areas $A_k = (2\pi e/\hbar)F$. Fitting the temperature damping of the oscillation amplitude with the Lifshitz–Kosevich thermal factor yields a light cyclotron effective mass $m^* = 0.12 m_e$.

4. Conclusions

This study successfully addressed the primary research problem by providing a comprehensive, multi-probe investigation of the structural, vibrational, electronic, and Fermi surface evolution of exfoliated few-layer $1T' - MoTe_2$ under hydrostatic pressure. AFM confirmed the exfoliation of high-quality, atomically smooth ($R_q = 0.22$ nm) $1T' - MoTe_2$ flakes with a thickness of $\Delta z = 8.5 \pm 0.3$ nm ($n \approx 12$ layers), establishing an ideal baseline free of surface degradation.

In-situ Raman spectroscopy demonstrated a universal blue-shift of optical phonon modes ($A_g^{(1)}$, $A_g^{(2)}$ and B_g) under compression. A distinct structural crossover was identified at a critical pressure of $p_c = 4.8 \pm 0.2$ GPa, marked by the complete quenching of the B_g mode (258.1 cm^{-1} at ambient) and a $\approx 40 - 48\%$ reduction in the pressure coefficients ($d\omega/dp$) for the $A_g^{(1)}$, $A_g^{(2)}$ modes.

Temperature-dependent transport measurements revealed a transition from a semiconducting state ($E_g = 42.1 \pm 1.2$ meV at 0.5 GPa) to a fully metallic state at $p = 8.2$ GPa. At 14.5 GPa, low-temperature ($T < 20$ K) resistivity strictly follows a quadratic Fermi-liquid scaling ($\rho \propto T^2$) with a high Residual Resistivity Ratio = 38.4.

High-field magnetotransport at $p = 12.8$ GPa revealed a large, non-saturating magnetoresistance (420% at $B = 9$ T) and clear Shubnikov–de Haas quantum oscillations. FFT analysis yielded two main oscillation frequencies ($F_1 = 142 \pm 3$ T and $F_2 = 285 \pm 5$ T) and an extremely light cyclotron effective mass ($m^* = 0.12 \pm 0.01 m_e$).

Substrate clamping plays a decisive role in ultrathin devices, stabilizing the monoclinic $1T'$ symmetry down to 1.8 K and suppressing both the low-temperature T_d phase transition and pressure-induced superconductivity observed in bulk single crystals. These findings offer critical guidelines for designing strain-engineered 2D quantum devices and low-dimensional phase-change electronics.

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