Crystal growth, low temperature electron transport and ARPES study of $TaAs_2$

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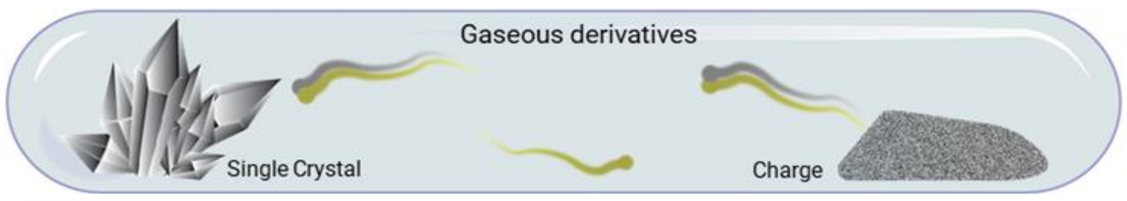
Abstract:

Conducting materials with extremely large magnetoresistance are interesting from the point of view of applications in various magneto-electronic devices. we report **crystal growth, electron-transport and angle-resolved photoemission spectroscopy studies which in conjunction with theoretical calculations allowed us to obtain a coherent picture of the electronic properties of the $TaAs_2$ topological semi-metal exhibiting extremely large magnetoresistance.**

ARPES enabled us to map the electronic band structure of $TaAs_2$. The constant energy cuts parallel to the $(\bar{2}\ 0\ 1)$ plane were compared with the corresponding Fermi surface diagrams obtained by the first-principle calculations. In the experimental contours, seven Fermi surface pockets can be discerned, in agreement with the bulk pockets of the theoretical Fermi surface. The bulk states pockets at the constant energy surfaces are elliptical, in an agreement with the first-principle calculation results, and that can be correlated with the outcome of the transport angle dependent studies.

Single crystal growth:



- symmorphic space group 12 (C 2/m1)
- centrosymmetric base-centered monoclinic crystal structure

a= 7.758 Å, b= 3.392 Å, c=8.705 Å, $\beta = 111.18^{o}$

Low-temperature electron transport:

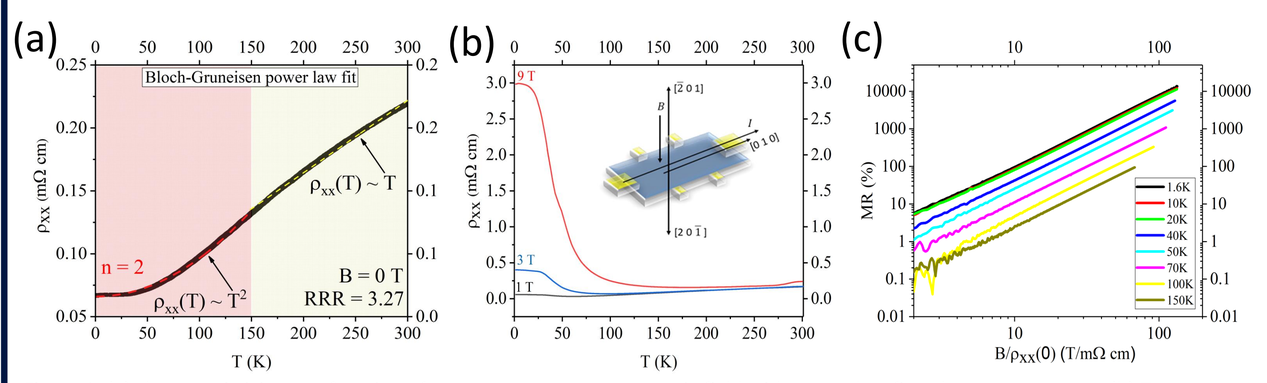


Figure 1. (a) shows resistivity as a function of temperature at zero magnetic field with power law fit at low temperatures, (b) Temperature dependence of resistivity at magnetic fields 1, 3 and 9 T, (inset) shows sample configuration in which B⊥ $(\bar{2}\ 0\ 1)$ and I ∥ b axis, (c) shows the violation of Kohler's law which is a sign of topological semimetal.

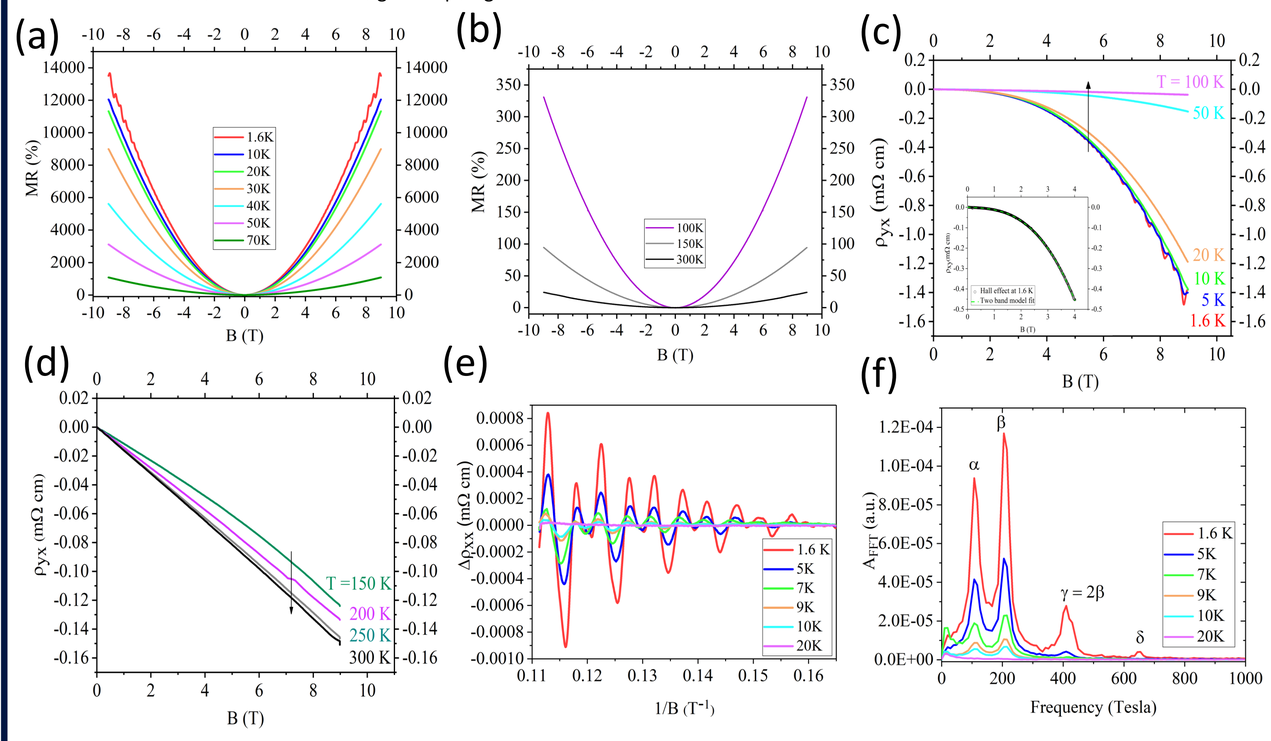


Figure 2. (a, b) shows percent magnetoresistance at low and high temperatures showing the existence of quantum oscillations at low temperature and high magnetic field, (c) Hall resistivity as a function of magnetic field, B with an inset showing the two band model fitting at 1.6 K (d) Hall effect at higher temperatures showing the sign change from 150 K to 300 K, (e) Pronounced quantum oscillations from 1.6 K to 20 K, extracted by subtracting background signal, (f) a fast Fourier transform of SdH oscillation with four different frequencies.

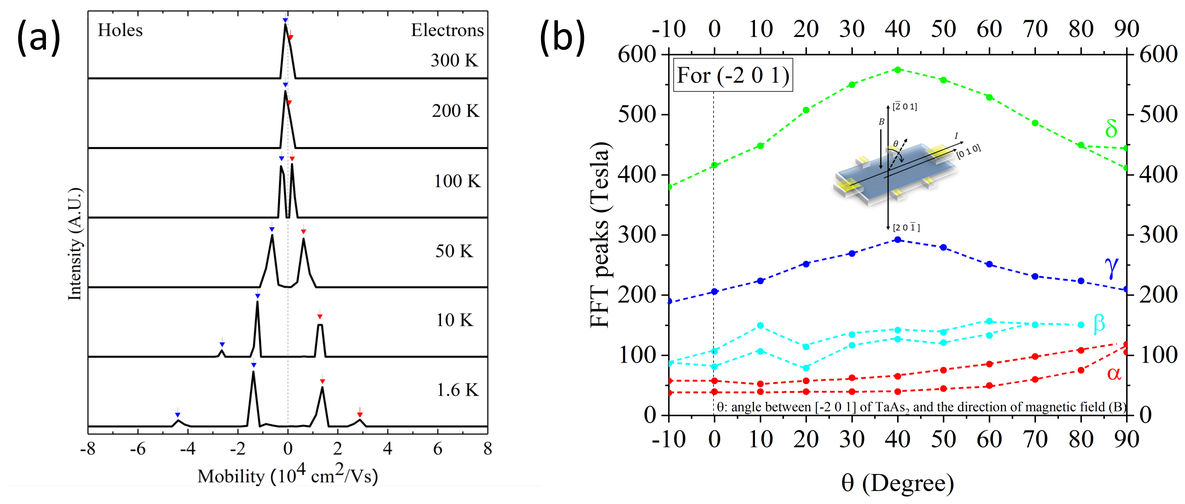


Figure 3. (a) shows mobility spectrum analysis to show the multicarrier nature of the $TaAs_2$, (b) angle dependent measurements indicating the elliptical trajectories of Fermi surface cross section. (inset) shows the sample configuration in where the sample was rotated with the reference of magnetic field (B).

Two band model fit to ρ_{xx} and ρ_{yx} gives concentrations as $\mathbf{n_e = 1.4 \times 10^{19}\ cm^{-3}}$ and $\mathbf{n_h = 1.0 \times 10^{19}\ cm^{-3}}$ by substituting the values of mobilities $\mathbf{\mu_e = 1.3{\times}10^4\ cm^2/Vs}$ *and* $\mathbf{\mu_h = 1.4{\times}10^4\ cm^2/Vs}$ obtained from Mobility spectrum analysis.

ARPES study with DFT calculations

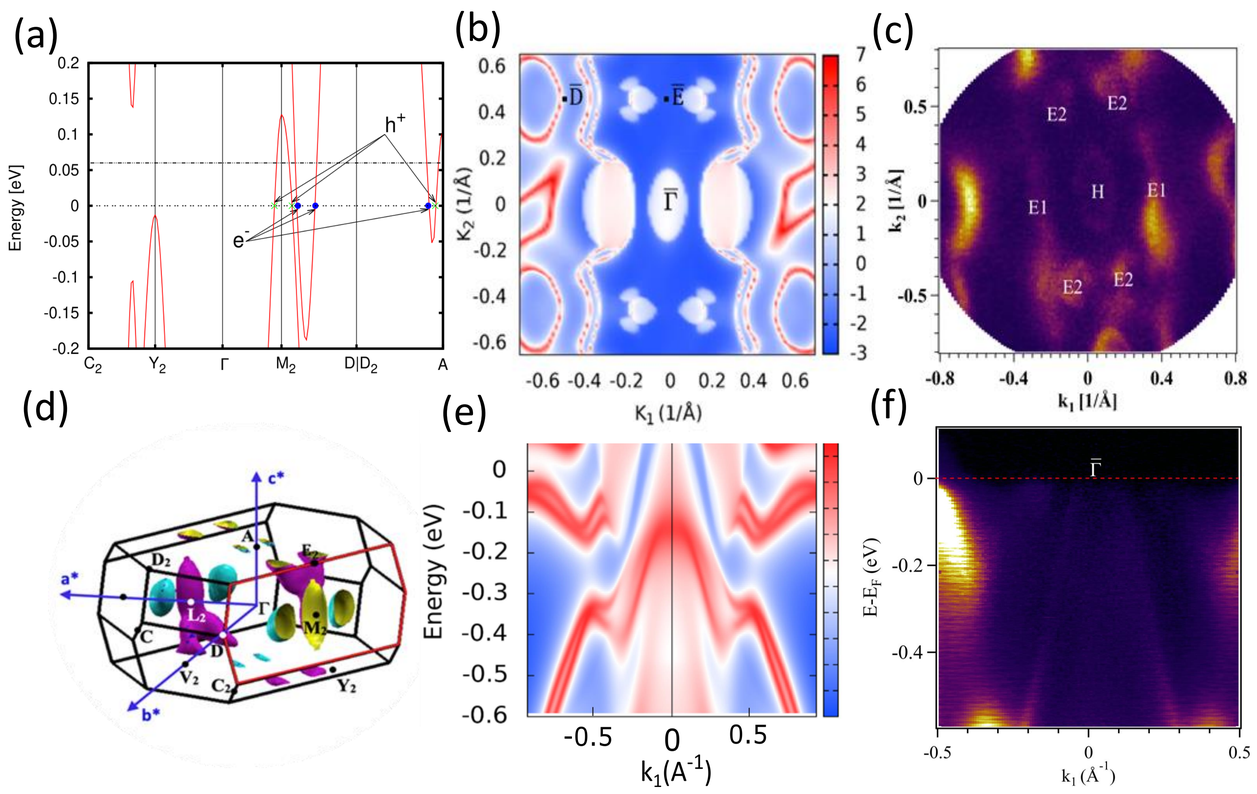


Figure 4. (a) Magnification of band structure with electron and hole effective masses indicated by blue and green markers, respectively, (b, c) theoretically calculated constant energy contour compared with experimental ARPES results showing electron and elliptical hole pockets, (d) 3D Brillouine zone of $TaAs_2$ indicating electron and hole pockets, (e, f) comparison of theoretical and experimental electronic structure at $k_2 = 0$.

Summary:

- **Single crystals of $TaAs_2$** were prepared by using **chemical vapor transport** route
- At zero magnetic field, longitudinal resistivity as a function of temperature shows **semi-metallic nature**
- Bloch-Grüneisen power law gives n=2, showing **electron-electron interaction** at low temperatures
- It shows the violation of Kohler's law which is proportional to $B/\rho_{xx}(0)$
- Our crystal shows Shubnikov de Haas oscillations at helium temperatures, allowing us to analyze details of the band structure of the material.
- Mobility spectrum analysis shows evidence that two kinds of electrons and two kinds of holes participate in the total conductance
- $TaAs_2$, **$(\bar{2}\ 0\ 1)$** plane has **the lowest cleavage energy**
- The constant energy cuts parallel to the $(\bar{2}\ 0\ 1)$ plane were compared with the corresponding Fermi surface diagrams obtained by the first-principle calculations
- In the experimental diagrams, **seven Fermi surface pockets** can be discerned, in agreement with the bulk pockets of the theoretical Fermi surface. The bulk states pockets at the constant energy surfaces are **elliptical**, in agreement with the first-principles calculation results. These results are also consistent with the outcome of the transport angle dependent studies

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