Magnetotransport properties of Dirac semimetal ZrSiS

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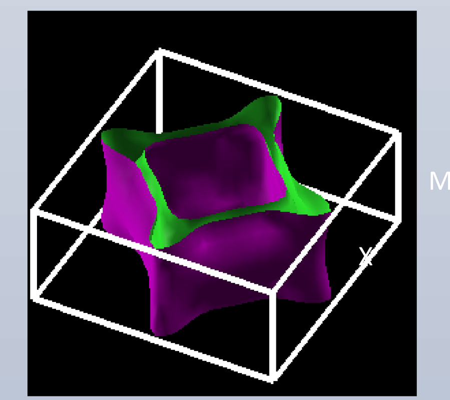
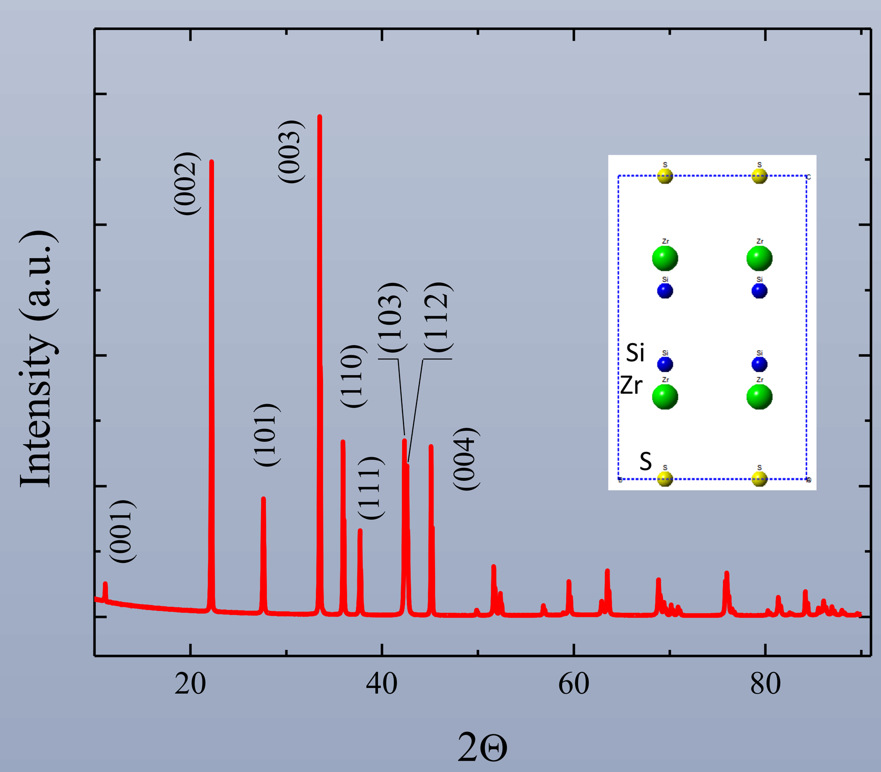
- *ZrSiS is a 3D Dirac semimetal with a Q2D Fermi surface*
- *Crystal structure TETRAGONAL with P4/nmm (No. 129) symmetry*
- *Material possess interesting Non-Symmorphic Symmetry protected 3D Dirac states – deep in the valence and conduction bands, thus not seen in the transport measurements!*
- *Fermi surface is Q2D with diamond shaped touching edge of the Brillouin zone*



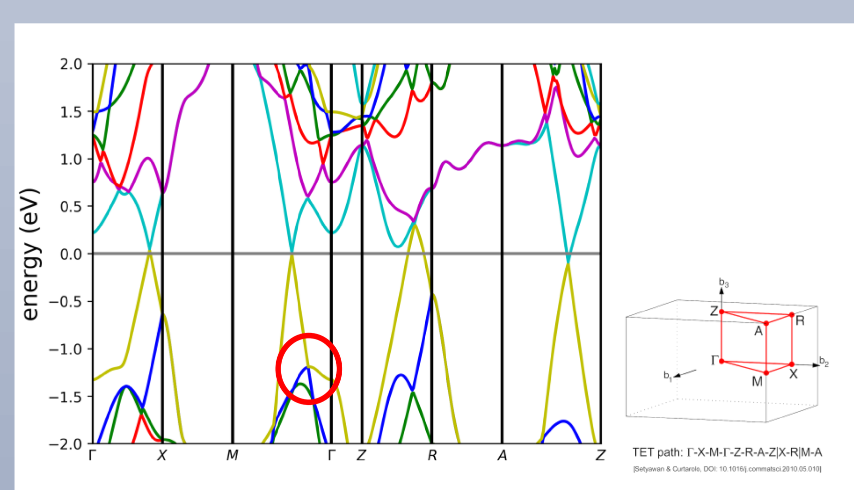
Fermi surface for -200 meV below the theoretical Fermi level. This Fremi surface resembles ARPES mapped fermi surface. Not showed at the present. ARPES indicates Q2D nature of the Fermi surface.

- Structural analysis

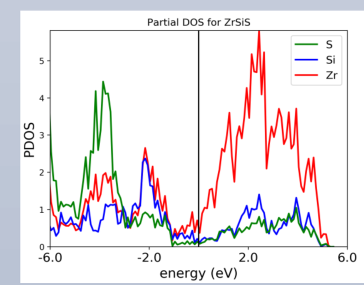


XRD confirmed single phase structure of material with P4/nmm symmetry.
No traces of elemental Zr or Si, crystal were grown by CVT method

- DFT calculations

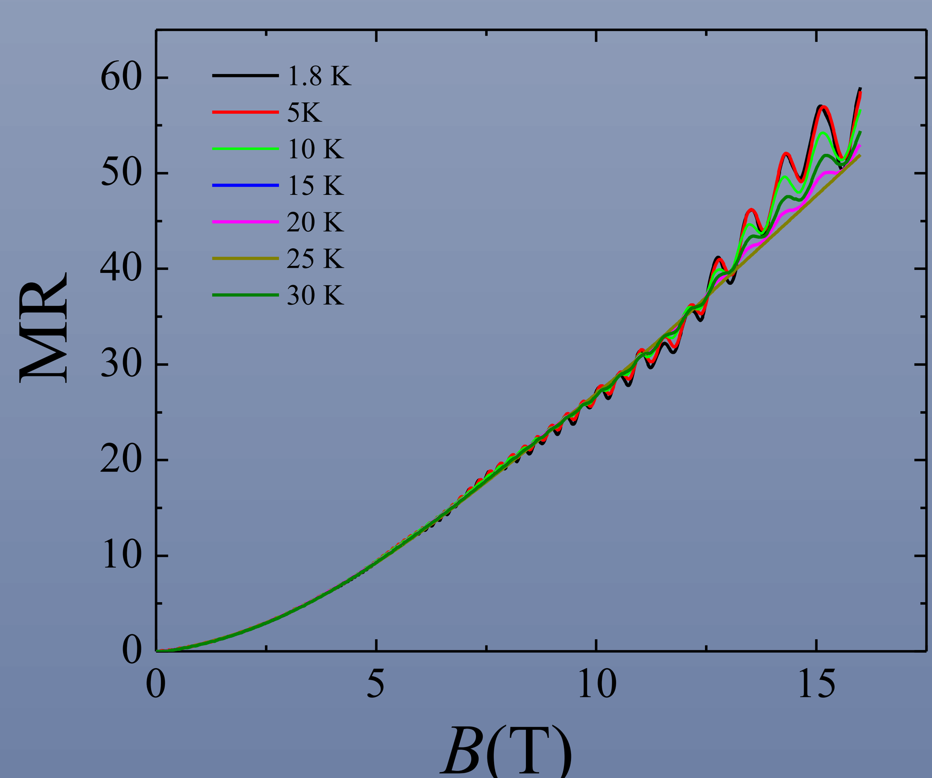


Band structure of ZrSiS without SO interaction. Non-Symmorphic Symmetry protected 3D Dirac states are deep in the valence band.

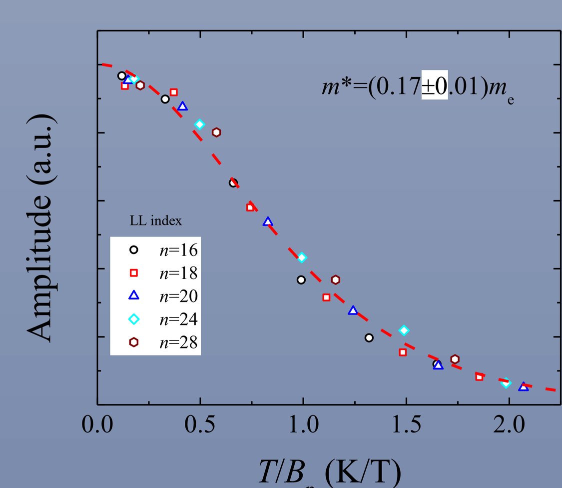


Zr 4d stared acts as dominate states at the Fermi level. Sulphur atoms have little contribution to the total density of states.

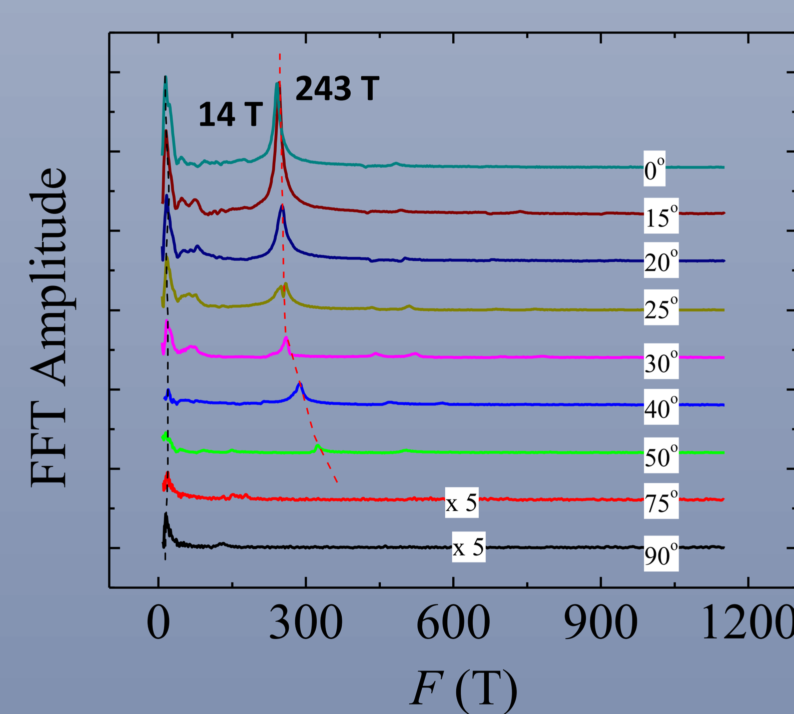
Measurement of magnetoresistance and SdH oscillations



MR shows strong dependence on magnetic field due to several types of charge carriers. Two frequencies can be distinguished form the MR data. **The first one at around 7 T and second done at round 243 T.**



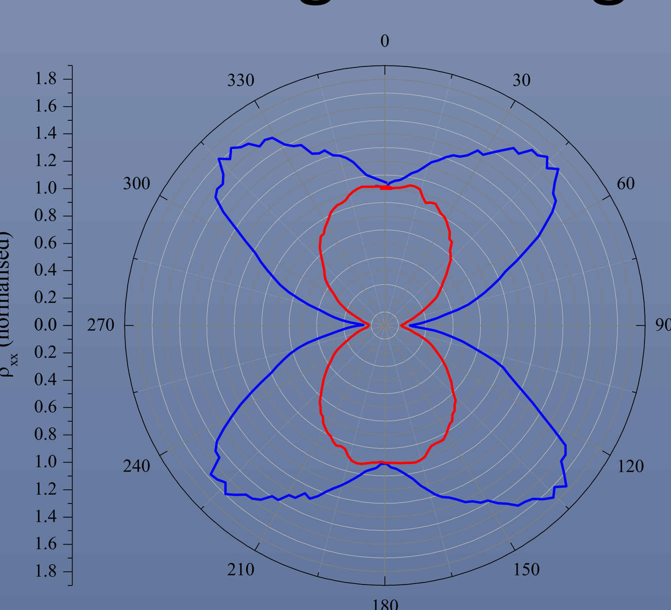
Effective mass for the high frequency channel F=243 T. For the low frequency channel SQUID measurement will be applied to extract the effective mass.

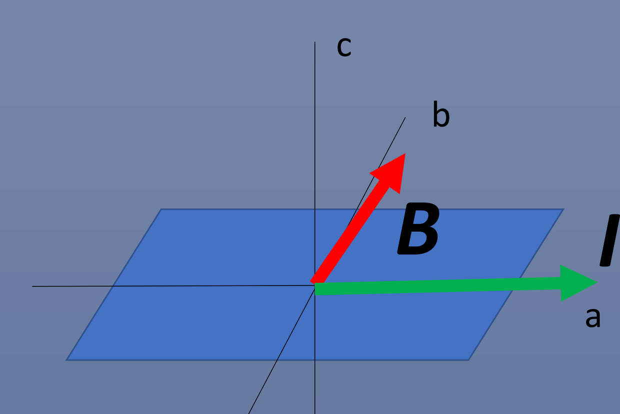


Angular dependence of the SdH oscillations.
The low frequency channel F=7 T (2F=14 T) does not show dispersion with rotation of the magnetic field.

The high frequency channel shows shifting to higher frequencies with rotation of the magnetic field and disappears above 50 deg. This indicates possible Q2D nature of this channel.

Angular magnetoresistance



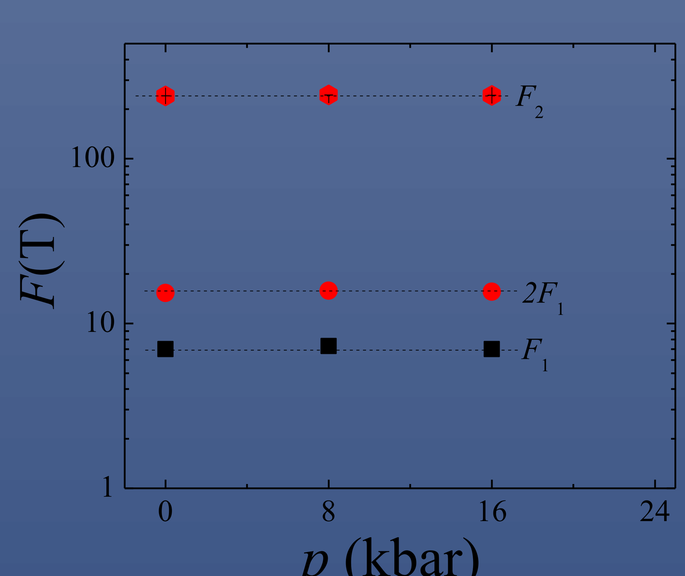


AMR was measured in two directions.
I. Magnetic field is rotated in c-a plane
II. Magnetic field is rotated in c-b plane
Current is caped in a-direction

AMR shows 2-fold symmetry reflecting the crystal symmetry. There are ripples on the AMR which have to be studied in more detail. This ripples could reflect the topology of the Fermi surface.

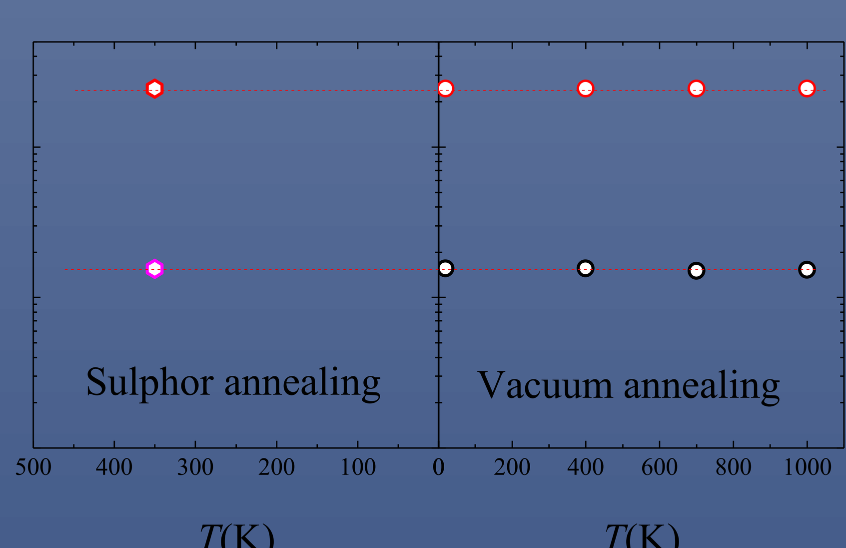
Tuning the Fermi level

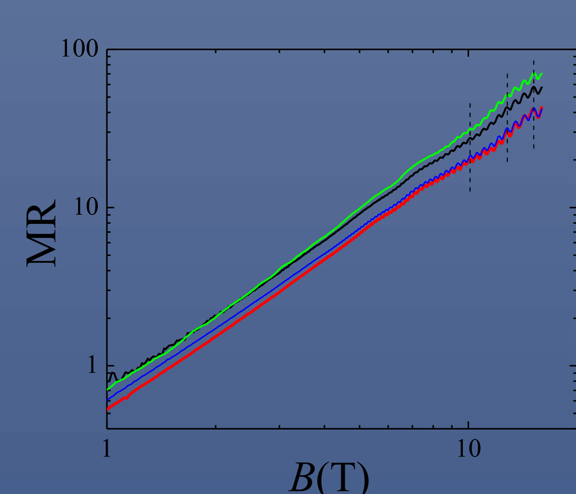
- External pressure



Applyng external hydrostatic pressure did not result in any change of the Fermi surface. The high and the low component of the SdH oscillations did not shift which indicated rigidity of the Fermi surface.

- Annealing





Vacuum annealing and S-vapour annealing also surprisingly did not move the Fermi energy. Naively one would expect that changing a Sulphur concentration Fermi energy can be easily tuned. DFT calculations give the answer, Zr states mostly contribute to the charge carriers on the Fermi energy.

Summary and outlook

- Crystals of ZrSiS show Q2D nature of its Fermi surface (seen by ARPES)
- Transport measurements give robust and strong SdH oscillations
- Applying hydrostatic pressure did not induce observable changes in the Fermi surface, SdH oscillation have not been changed.
- Vacuum and S-vapour annealing did not move position of the Fermi energy
- AMR gives interesting behaviour reflecting the crystal symmetry with unusual features
- Future extensive measurements are needed in the field of AMR to understand the unusual angular behaviour, which could be even richer due to Q2D nature of Fermi surface.