Irreversible Effect of Pressure-Driven Phase Transitions in Cd_3As_2

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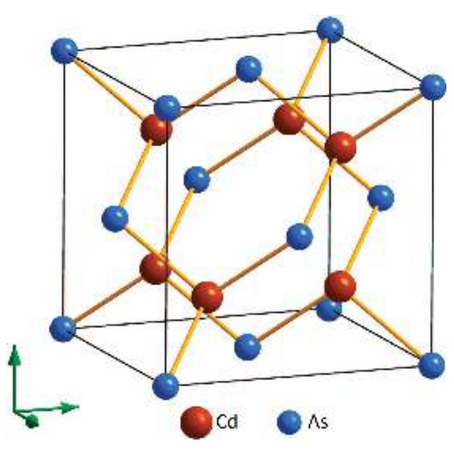
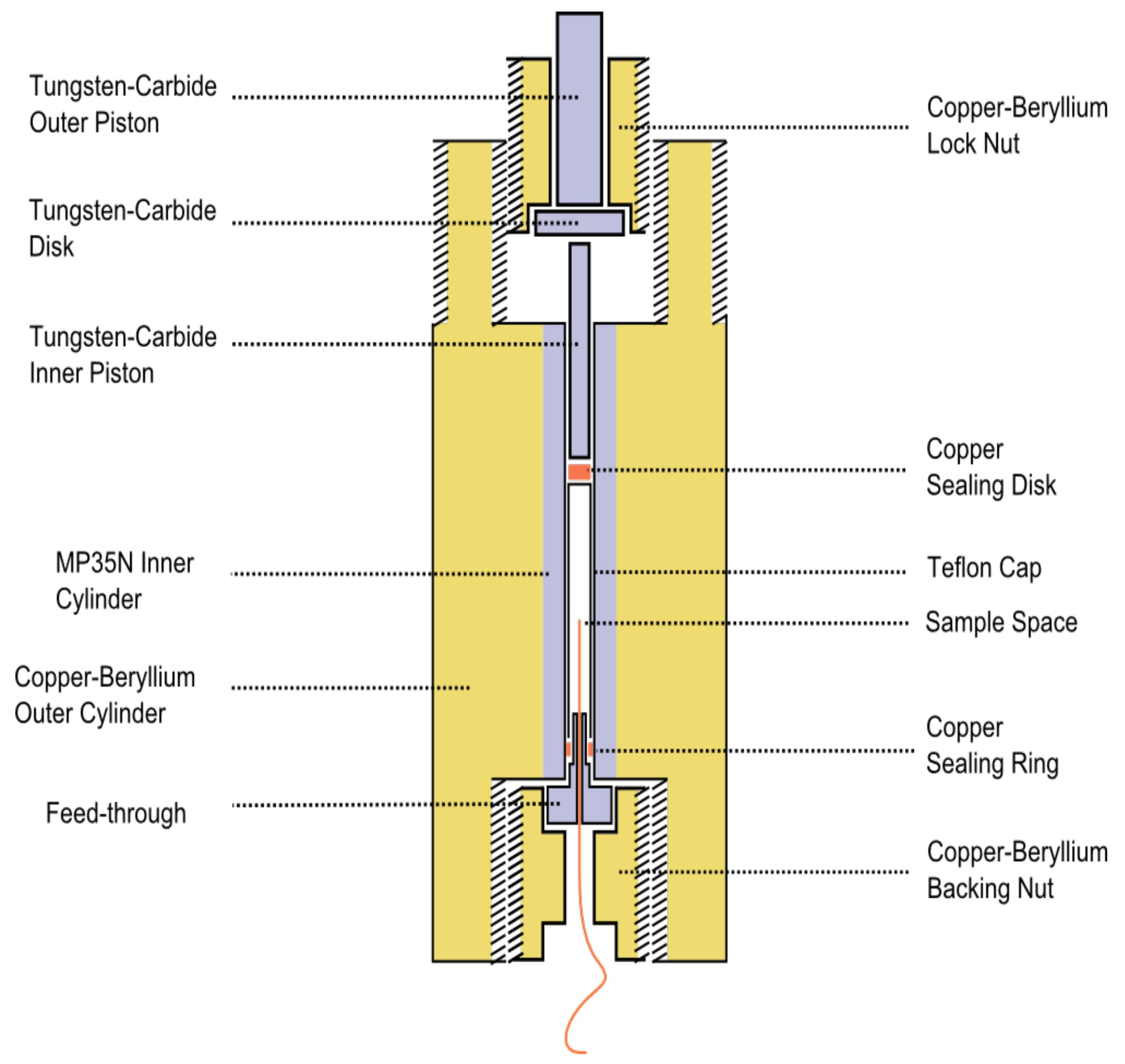
Cadmium Arsenide

Cd_3As_2 is a 3D Dirac semi-metal (DSM) [1]. It has been shown to be superconductive (possible topological superconductivity) under pressure [2], and the breakdown of the 3D-DSM has been shown to occur when pressure is applied [3]. A pressure induced phase transition from tetragonal (spacegroup $I4_1/acd$) to monoclinic (spacegroup $P2_1/c$) has been reported to occur at 2.57 GPa [3].

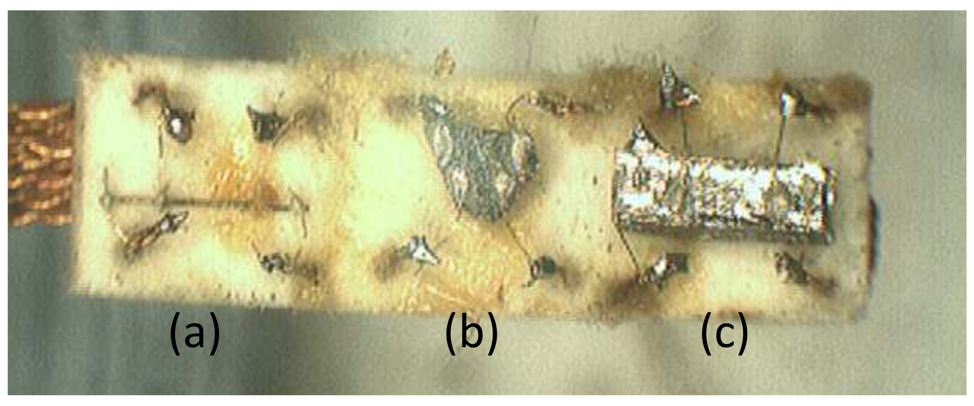


High Pressure Techniques

Samples mounted within a piston cylinder pressure cell were subject to pressures up to 2.9 GPa. To apply pressure in a controlled manner a digital controller was used in conjunction with an hydraulic ram.



Four-point electrical transport measurements of Manganin (a), Cd_3As_2 (b) and bismuth (c) samples were made via an electrical feedthrough. The samples were contained within a Teflon cap filled with glycerin; the pressure transmitting medium.



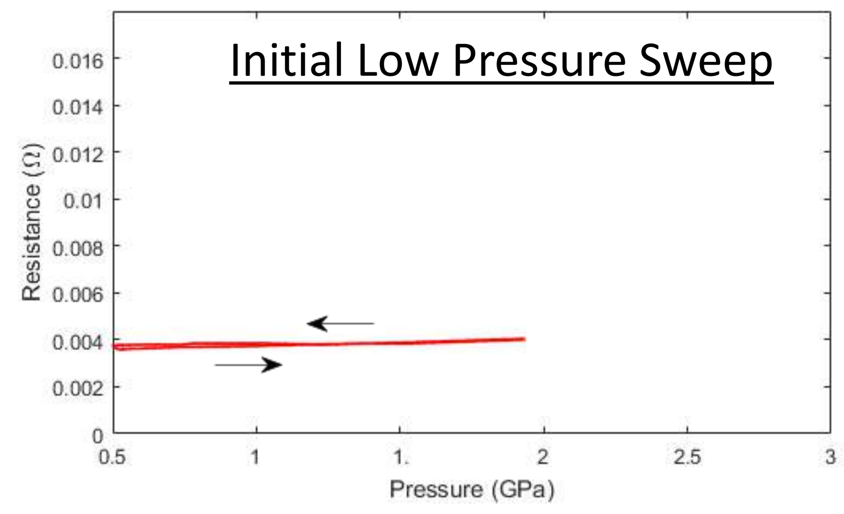
The pressure dependent resistance of Manganin is approximately linear for pressures up to 3.7 GPa [4], as described by the following equation:

$$P = A\frac{\Delta R}{R_0},$$

where P is pressure (in GPa), A is a constant, R_0 is the resistance at ambient pressure and ΔR is the change in resistance due to a change in pressure. Measuring the resistance of Manganin and bismuth throughout the experiment allowed the sample pressure to be measured and calibrated. Abrupt changes in the resistance of bismuth at 2.5380(2) GPa and 2.69(2) GPa [4] allowed the constant A to be calculated. It was found that A = 3.90(4) GPa.

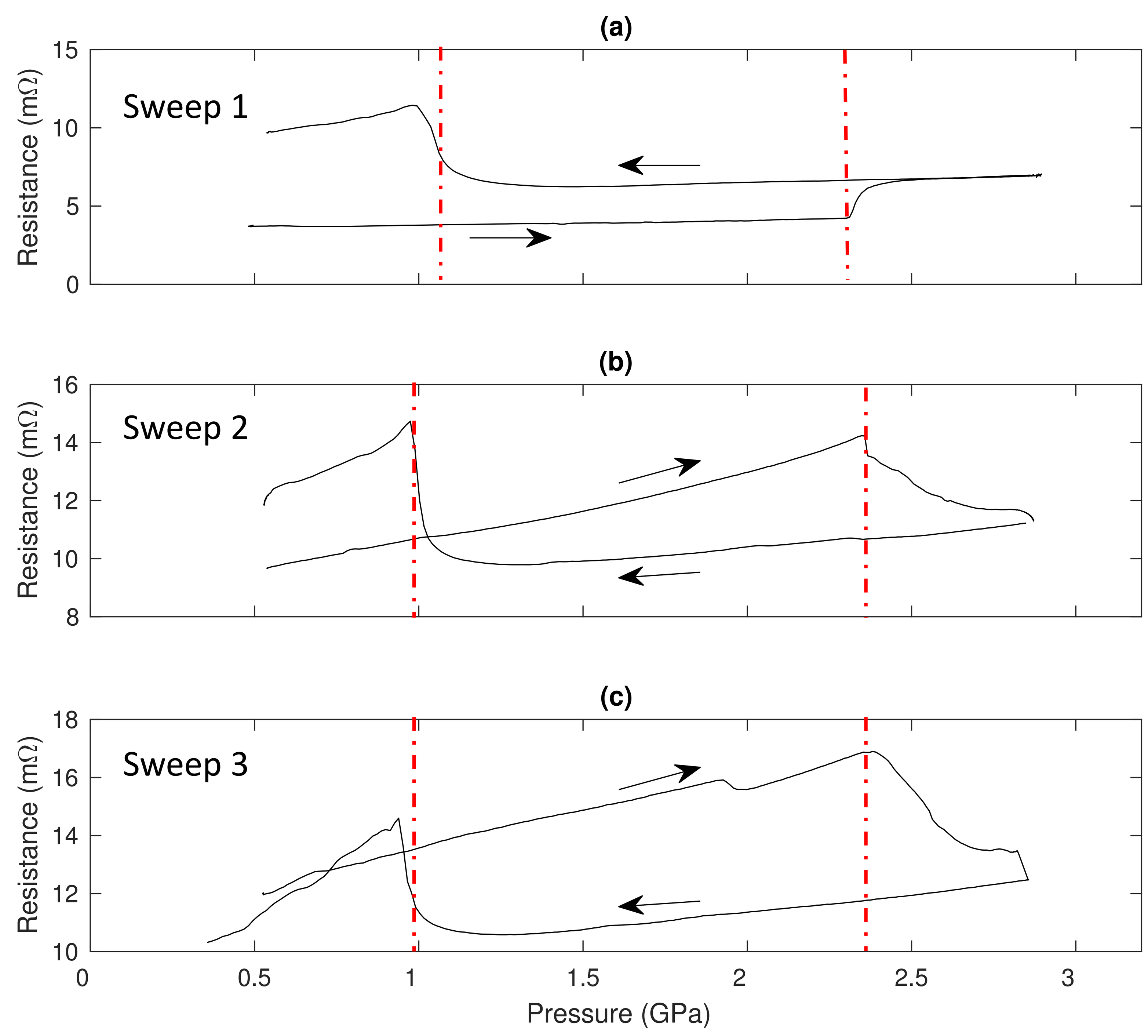
Results

The graphs show the pressure dependent resistance of Cd_3As_2. An initial low pressure sweep to 2 GPa shows no irreversible effects.



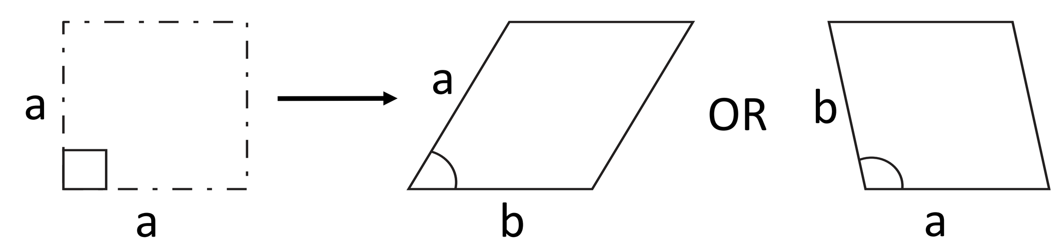
The first high pressure sweep (sweep 1) to 2.9 GPa shows an increase in the resistance of Cd_3As_2 at ≃2.3 GPa, indicating a structural phase transition, as expected. Upon decreasing pressure, the resistance shows an interesting feature. It does not show reversibility, but instead shows another increase at ≃1 GPa. Subsequent high pressure sweeps (sweep 2,3) again show unexpected behaviour. The resistance decreases at ≃2.3 GPa where previously it had increased.

High Pressure Sweeps



Microscopic Theory

The structural phase transition from tetragonal to monoclinic is shown by the 2D representation below. Each outcome can have angle ab = 90˚ ± δ, giving four possible transformations.



All transformations are equally likely, therefore different regions of the Cd_3As_2 crystal may transform into different monoclinic structures. This behaviour will lead to domains with walls between them. Upon transition back to a sample wide tetragonal structure, domain walls will leave dislocations/defects in the crystal. Applying this simple idea allows the observed behaviour to be explained by the Drude model, from which we have

$$\rho = \frac{m_e}{ne^2\tau},$$

where ρ is the resistivity, m_e is the mass of an electron, n is the electron number density, e is the electronic charge and τ is the relaxation time.

References

[1] Z. Wang et al., "*Dirac semimetal and topological phase transitions in A3Bi (A=Na, K, Rb)*", Phys. Rev. B **85** (2012)
[2] He, L. *et al*, "*Pressure-Induced Superconductivity in the Three-Dimensional Topological Dirac Semimetal Cd3As2*", npj Quant. Mat., **1** (2016)
[3] Zhang, S. *et al*, "*Breakdown of Three-Dimensional Dirac Semimetal State in Pressurized Cd_3As_2*", Phys. Rev. B, **91** (2015)
[4] Zeto, R. J., Vanfleet, H. B. "*Pressure Calibration to 60 kbar Based on the Resistance Change of a Manganin Coil under Hydrostatic Pressure*", J. App. Phys., **40** (1969)

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