

Quantum Oscillations in the High Pressure Metallized Mott Insulator NiS₂

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Introduction

The electronic structure in the correlated state near a Mott metal-insulator transition can be examined in the nickel pyrite NiS₂, which metallises at moderate applied pressures. We have grown single crystals of NiS₂ with residual resistivities of less than 1 $\mu\Omega$ cm in the metallic state above 3GPa. To enable quantum oscillation measurements high pressure anvil cells, we have combined a microcoil in the sample space with a tank circuit oscillator circuit. Quantum oscillations can be observed by tracking the tank circuit resonance frequency, and in high-pressure NiS₂ we have previously resolved oscillations at a frequency of about 6kT [1]. DFT calculations attribute this frequency to a large, cubic hole pocket in the center of the Brillouin zone, with significantly renormalised carrier mass. The objective of the April 2018 experiments was to extend these measurements to pressures beyond the previous maximum pressure of 115 kbar, in order to explore the limits of this technique and to follow the evolution of the Fermi surface and of the effective carrier mass as the sample is tuned further away from Mott localization.

Experimental

A microcoil with a diameter of <0.3 mm is located in the gasket hole of a miniature diamond anvil pressure cell. A Van Degrift-type tunnel diode oscillator was mounted near the pressure cell on a low temperature insert. Wiring the microcoil as the tank circuit inductance, we have obtained stable oscillations in the range 450-550 MHz. Measurements were performed at NHMFL in a ³He system in cell 9 for three days in 4/2018, to compensate for measurement time lost because of technical problems during the previous visit in 2017.

Results and Discussion

Quantum oscillations at a frequency near 6.5 kT were observed clearly at a pressure of 122 kbar (Fig. 1), and a rotation study was carried out. A second run at 130 kbar showed weak quantum oscillations. These data supplement the longrunning study of Fermi surface geometry and carrier mass as a function of pressure in NiS₂, which now extends over a wide pressure range from 33 kbar to 130 kbar. Our data suggest that the carrier mass is strongly renormalized on approaching Mott localization, whereas the Fermi surface volume remains almost unchanged.

Conclusions

Quantum oscillations have been detected in pressure metallised NiS_2 up to pressures of 130 kbar.



Frequency (T) the tunnel-diode oscillator technique at a pressure of 122 kbar and a temperature of 590 mK, after background subtraction (top panel). Fourier analysis (bottom left panel) brings out the main frequency near 6.4 kT, which can be attributed to a large cube-shaped hole sheet at the center of the Brillouin zone (bottom right panel). While this frequency dominated the spectra in previous runs at lower pressures, it is becoming harder to resolve at this elevated pressure, possibly because of increasing pressure inhomogeneity.

This demonstrates that detailed electronic structure measurements can be extended into pressure regimes which were previously considered out of reach. Our study helps resolve the nature of the correlated electronic state on the threshold of Mott localisation in high pressure NiS₂, and it motivates similar studies in other materials in which the electronic excitation spectrum under high pressure is of interest.

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References

[1] S. Friedemann *et al.* Large Fermi Surface of Heavy Electrons at the Border of Mott Insulating State in NiS₂ Scientific Reports **6**, 25335 (2016).