Tuning the Fermi Level through the Dirac Point of Giant Rashba Semiconductor Bitei with Pressure

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Introduction

First-principles calculations have predicted that, under pressure, BiTeI undergoes a band inversion and becomes a rare instance of a non-centrosymmetric topological insulator.[1] Infrared reflectance and transmission measurements under pressure found signatures of the predicted topological quantum phase transition.[2] In an effort to detect transport signatures of the topological phase transition, we carried out series of high pressure measurements of Shubnikov-de Haas oscillations in BiTeI.

Experimental

Resistivity and Hall measurements were performed on single crystals of BiTeI at temperatures between 1.5-300 K, magnetic fields up to 18 T, and several pressures up to 2.4 GPa. The samples were loaded in a piston-cylinder pressure cell constructed from MP35N alloy with Daphne 7474 oil as the pressure transmitting medium. Pressure was measured at low temperature using the fluorescence a small ruby chip. The sample resistance was measured in the crystalline ab-plane, while the magnetic field was applied parallel to the c-axis.

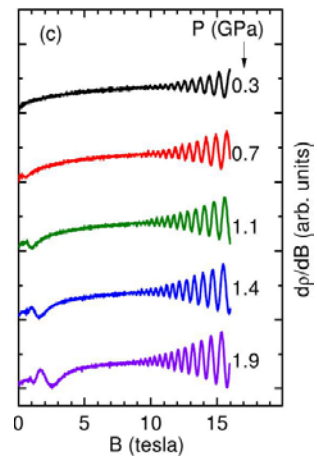

Figure 1: Derivative of the electrical resistivity with respect to field for BiTeI at several pressures.

Results and Discussion

Figure 1 presents on overview of our results.[3] For all pressures, oscillations of the resistivity are visible both in the raw data and in the field derivative of the resistivity. At low pressures, only one set of oscillations is apparent, while for pressures above ~1 GPa a second, lower frequency oscillation appears at low fields.

An analysis of the results in terms of a simple model Hamiltonian allows an estimate of the pressure dependence of various band structure parameters such as the band mass, the chemical potential, and the Rashba parameter. BiTeI has a conduction band bottom that is split into two sub-bands due to the strong Rashba coupling, resulting in a "Dirac point". Our data suggests a clear increase in the chemical potential from below the Dirac point to above it as pressure is increased. This analysis suggests a lowering of the conduction band minimum with pressure. The sign of this trend (although not the magnitude) is consistent with the approach to a pressure induced band inversion as predicted in Reference [1].

Conclusions

The parameters extracted from the data via our model support the notion that pressure brings the system closer to the predicted topological quantum phase. We are currently pursuing further studies at higher pressures and in lower carrier density samples, which will be necessary to explore the possible appearance of novel surface states in the high-pressure non-centrosymmetric topological insulator phase.

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