Probing the metal-insulator transition of $BaCo_{1-x}Ni_xS_2$ by optical conductivity

David Santos-Cottin[1, 2], Yannick Klein[1], Andrea Gauzzi[1], R.P.S.M. Lobo[2]

[1]*Université Pierre et Marie Curie, Institut de Minéralogie de Physique des Matériaux et de Cosmologie, Paris, France*
[2]*Laboratoire de Physique et d'Étude des Matériaux, ESPCI, CNRS, UPMC Paris, France*

Understanding the metal-insulator transition (MIT) driven by electronic correlations (Mott transition) remains a challenge in many-body physics because, in most real systems, such as V_2O_3 or VO_2, the electronic degrees of freedom are coupled to those of the lattice or to disorder.

In this respect, the 2D MIT system $BaCo_{1-x}Ni_xS_2$ offers a unique playground, for x-ray [2] and neutron diffraction [3] measurements carried on powders indicate a small orthorhombic structural modulation near 200 K, however no structural changes are detected at the MIT for x=0.2. In addition, this system shares with superconducting cuprates and heavy fermions a similar electronic phase diagram (Fig 1) where the MIT is controlled by pressure or chemical substitution, x, and is concomitant to an antiferromagnetic (AFM) to paramagnetic (PM) transition [1].

Previous optical studies on $BaCo_{1-x}Ni_xS_2$ in the x=0-0.28 range suggest that the undoped system (x=0) is a charge transfer-type Mott insulator with more pronounced 2D electronic character than expected from electronic structure calculations [4]. On the other hand, recent ARPES measurements on high-quality single crystals and band structure calculations suggest that $BaNiS_2$ is a Fermi liquid with moderate band renormalization [5]. However, no Drude-like peak has been detected in the metallic phase near the MIT for x= 0.28.

In order to elucidate this issue, we measured the optical conductivity in the *ab* plane of insulating ($BaCoS_2$) and metallic ($BaNiS_2$) single crystals as a function of temperature. Surprisingly, we find that the optical response of $BaCoS_2$ is typical of a bad conductor showing an overall negative slope in the reflectivty and no indication of Drude peak. This suggests that $BaCoS_2$ is a lightly doped insulator with characterized by an incoherent conductivity and a weak temperature dependence. The splitting of various phonon modes reveals a structural phase transition near room temperature. On the other hand, metallic $BaNiS_2$ displays a large temperature dependence of the optical conductivity and a strong redistributed of spectral weight possibly attributed to spin-orbit coupling effects. An estimate of the scattering rate and of the mass enhancement factor from the Drude peak suggests a picture of Fermi liquid at low temperature with m^*/m~2. These results point at a picture of a transition from a Fermi liquid to a non Fermi liquid driven by electron-electron correlations that differs substantially from the conventional Mott picture.

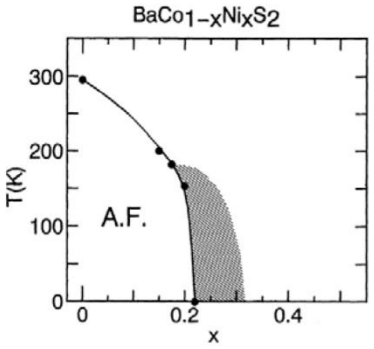

Figure 1 Electronic phase diagram T Vs x of $BaCo_{1-x}Ni_xS_2$.

[1] S. Shamoto et al., J. Phys. Soc. Jpn, **66**, 1138 (1997).
[2] M. C. Gelabert et al., . Solid State Chem. **127**, 211 (1996).
[3] D. Mandrus et al., J. Appl. Phys. **81**, 4620 (1997).
[4] K. Takenaka et al., PRB, **63**, 115113 (2001).
[5] D Santos-Cottin et al., Nat. Commun **7**, 11258. (2016).