

## Optical Properties of Barium Vanadium Sulfide

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Abstract No. miha1409

Beamline(s): U10A, U2A

**Introduction:** The crystal structure of  $\text{BaVS}_3$  suggests one-dimensional electronic structure: the  $\text{V}^{4+}$  ions form a chain where the distance between the atoms is almost the same as in the vanadium metal. In spite of this, from electronic point of view, the  $\text{BaVS}_3$  is almost isotropic. The small conduction anisotropy ( $\sigma_c/\sigma_a=3$ ) is believed to be the result of the octahedral S environment around each V atom, which determines the orientation of the  $d$ -orbitals, and tilts them out from the chain direction.  $\text{BaVS}_3$  has a metal-insulator transition at  $T_{\text{MI}}=69$  K, accompanied by a sharp spike in the magnetic susceptibility<sup>1,2</sup>. The high-temperature phase is a strongly correlated metal with mean free path in the order of the lattice constant. It appears that the 69K transition is not symmetry breaking: it is a pure Mott transition which does not involve either magnetic order or any static displacement of atoms. Susceptibility<sup>3</sup>, NMR and NQR measurements<sup>4</sup> indicate another, symmetry breaking, phase transition around 30K. Single crystal resistivity measurements under hydrostatic pressure<sup>5</sup> indicate the possibility of a quantum critical point at about 20kbar.

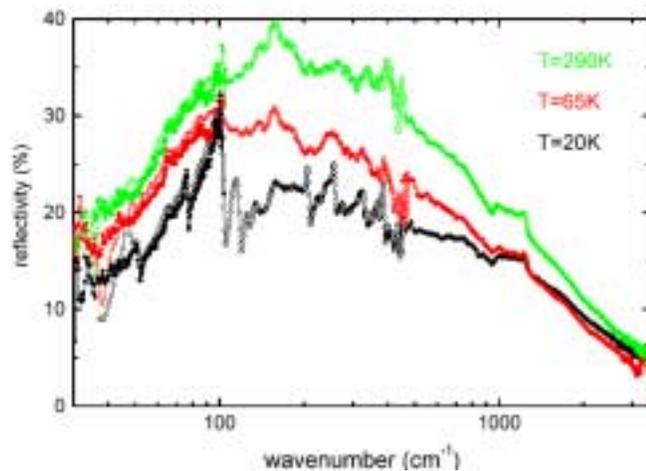
**Methods and Materials:** We performed an IR reflectivity study on three well-characterized single crystal  $\text{BaVS}_3$  samples at U10A. We also attempted to study the IR and Raman properties in a diamond anvil cell at the U2B beamline.

**Results:** Representative reflectivity results at ambient pressure are shown in Fig. 1. These spectra were obtained on the largest of the three samples. Notice the lower cut-off frequency of about  $20\text{cm}^{-1}$ . The brightness of the synchrotron source was critical in performing the low frequency measurements. The results on the smaller crystals were similar, but of lesser quality. Crystals of about  $300\mu\text{m}$  width and  $10\mu\text{m}$  thickness were successfully mounted in the diamond anvil cell, and measurements were performed at several pressures and temperatures, but the results do not lend themselves to a quantitative analysis.

**Conclusions:** The reflectivity of a metal should approach 100% in the low frequency limit. The most striking feature of the results is the non-metallic character over the whole temperature range. This indicates the presence of a pseudo-gap even at room temperature, where the dc conductivity is metallic. The phase transition at 70K is accompanied by a slight drop of the reflectivity and a re-arrangement of the low frequency spectral weight. The transition at 30K leads to the appearance of pronounced phonon lines in the spectrum. The presence of sharp phonon lines and the further reduction of the reflectivity points to a low electronic background absorption, i.e. the opening of a true energy gap in the electronic excitation spectrum. A more detailed analysis of the results, including the calculation of the optical conductivity, is in progress.

**Acknowledgments:** This work was supported by US DOE contract no. DE-ACo2-98CH10886. The travel expenses of the Hungarian participants have been paid by Research Funds AKP 98-66 and FKFP 0355.

**References:** <sup>1</sup> O. Massenet et al., J. Phys. Chem. Solids **40**, 573 (1979); <sup>2</sup> T. Graf et al., Phys. Rev. B **51**, 2037 (1995); <sup>3</sup> G. Mihaly, I. Kezsmarki, F. Zamborszky, M. Miljak, K. Penc, P. Fazekas, H. Berger and L. Forro, Phys. Rev. B **61**, R7831 (2000); <sup>4</sup> H. Nakamura, H. Imai, and M. Shiga, Phys. Rev. Lett. **79**, 3779 (1997); <sup>5</sup> L. Forro, R. Gaal, H. Berger, P. Fazekas, K. Penc, I. Kezsmarki, G. Mihaly, Phys. Rev. Lett. **85**, 1938 (2000)



**Figure 1.** Reflectivity of a  $\text{BaVS}_3$  single crystal at three representative temperatures