Experimental report

09/02/2022

Proposal: 5-31-2772 **Council:** 4/2020

Title: Search for long-range order in murunskite (K2Cu3FeS4)

Research area: Physics

This proposal is a new proposal

Main proposer: Davor TOLJ

Experimental team: Clemens RITTER

Local contacts: Clemens RITTER

Samples: K2Cu3FeS4

Instrument	Requested days	Allocated days	From	To
D20	2	1	11/02/2021	12/02/2021

Abstract:

Over the past three decades, most extensively studied ionic metals were the high-temperature superconductors: oxides and pnictides, where the coordinating anions are oxygen and arsenic/phosphorus, respectively. Murunskite (K2FeCu3S4) interpolates between the best known High-Tc superconductors with the same tetragonal ThCr2Si2-type structure as 122 pnictides and sharing chalcogen anions as cuprates. Resistivity measurements on as-synthesized single crystal murunskite show insulating behavior, same as undoped cuprates and pnictides, while measurements of magnetization and specific heat indicate a transition into a long range ordered state below ~90K. We propose a neutron diffraction experiment to elucidate the magnetic structure within the ordered state.

ILL report 5-31-2772 (D20), neutron powder diffraction

Powder neutron diffraction was performed from 11.02-12.02.2021 on D20 beamline at ILL, Grenoble, France. Approximately 1.1g of murunskite ($K_2FeCu_3S_4$) powder was sent beforehand to a local contact scientist Clemens Ritter. Because of the restrictions imposed by COVID-19 I was unable to attend the measurement. Powder was loaded in vanadium container by Clemens Ritter for experiment and measured with a wavelength range of 2.4 Å.

Murunskite powder was prepared at EPFL, CH by thorough grinding of multiple single crystals grown from the melt. Purity of the sample was confirmed by powder XRD and SEM-EDX measurements. Following magnetization and heat capacity measurement we have planned the experiment to closely observe interesting temperature range. Measurements were done in 1.7 – 300 K temperature range in 2theta angles 0-150^o. Long acquisitions (2h each) were done at 1.7, 70, 110, 150, 200, 250, 300 K. Additionally, Data was measured during heating in temperature range 1.7-110K to obtain temperature dependence in the most interesting temperature range.

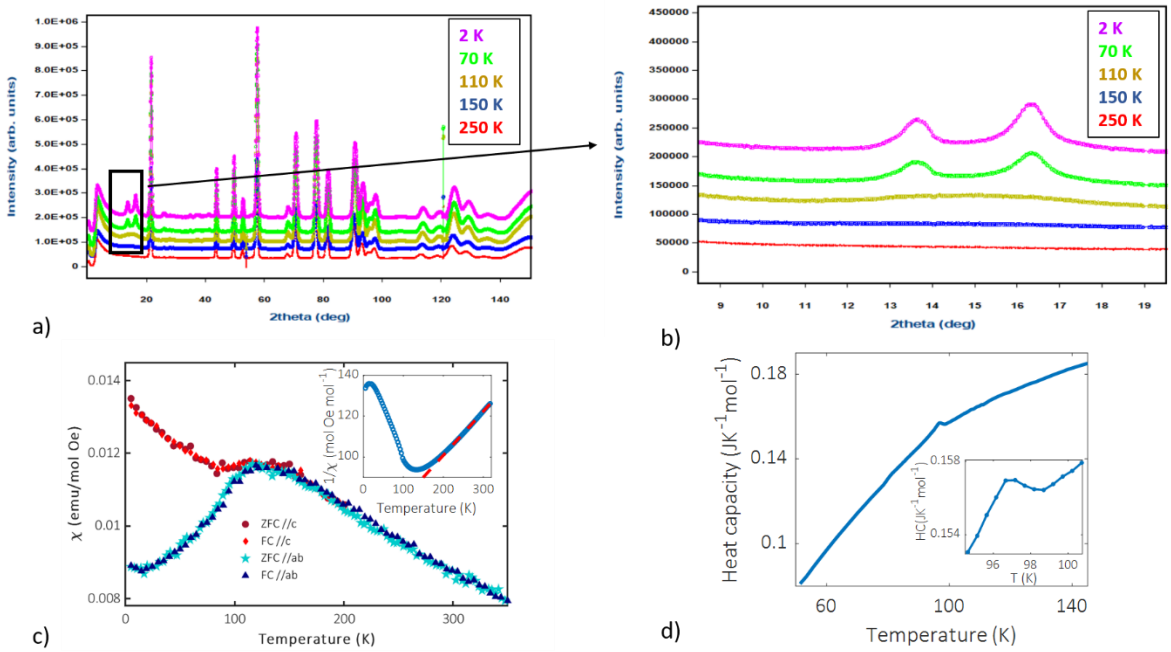

Figure 1 a) Neutron powder diffraction diffraction at different temperatures, b) Zoomed area of the two most pronounced magnetic peaks at different tempreature, c) H II ab and H I Ic magnetization curves of single crystal of nominal composition murunskite $K_2FeCu_3S_4$ at 1T field, d) Heat capacity curves

The powder neutron diffraction data agrees well with magnetization and heat capacity measurements. Under 200 K broad peak develops which can be observed on most pronounced magnetic area (magnetic susceptibility measurement starts to deviate from Curie-Weiss law in same range) evolving to well defined double peak under 100 K (magnetic transition observed in heat capacity). Additionally, 3 low intensity peaks develop at the same temperatures in 2theta range of 20-40^o. In the conclusion, data fits well with the other measurements but the small number of observable magnetic peaks makes it difficult to determine the reliable magnetic propagation k-vector. To solve this problem, we have applied for a single crystal neutron Laue at Cyclops at ILL. Combing Laue and powder neutron data should give us exact solution which we will use in combination with further measurement to reliable determine magnetic structure of murunskite.