

Structural analyses and properties of complex sulphides with very low thermal conductivities in the Cr-Sn-S System

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The design and optimization of thermoelectric (TE) materials rely on the intricate balance between thermopower (S), electrical resistivity (ρ) and thermal conductivity (κ). Perfecting such a balance is the key to reach high TE performances - determined by the dimensionless figure of merit $ZT = S^2T/\rho\kappa$ - necessary to improve energy recovery systems and thermoelectric cooling devices [1]. Among the most promising TE materials at medium temperature, complex copper-based sulphides are of double interests as they are usually made of eco-friendly and low-cost elements [2] and exhibit intrinsically low thermal conductivity [3]. However, the use of copper-based sulphides in TE devices is limited by the performances of the n -type materials compared to those of the p -types [4]. Consequently, it appears now necessary to develop more performant n -type sulphide materials. In this context, my Ph.D. work consists to synthesize and characterize the structural and physical properties of potential new n -type TE sulphide materials.

In this seminar, I will present our recent results obtained from several complementary techniques (X-ray and electron diffraction, scanning and transmission electron microscopies, magnetic measurements, spectroscopies, transport measurements) on two phases with complex crystal structure, leading to very low thermal conductivity, in the Cr-Sn-S ternary system: n -type $\text{Cr}_2\text{Sn}_3\text{S}_7$ [5] and p -type Cr_2SnS_4 . With the help of theoretical calculations, I will discuss also on the relationships between their properties and crystal and electronic structures.

Keywords: Crystal structure, X-ray diffraction, Electron microscopy and diffraction, Mössbauer spectroscopy, Thermoelectricity, Magnetism, Theoretical calculations

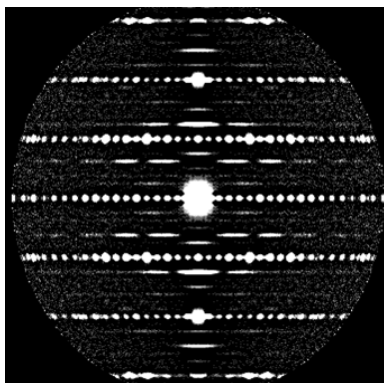


Fig.1: Reconstructed reciprocal space from electron diffraction pattern ([101] zone axis) of $\text{Cr}_2\text{Sn}_3\text{S}_7$ revealing its complex crystal structure highlighted by diffuse scattering.

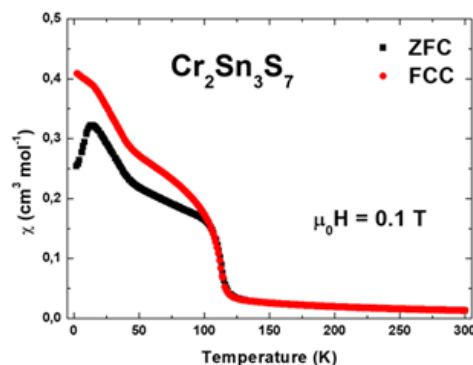


Fig.2: Magnetic measurement of the $\text{Cr}_2\text{Sn}_3\text{S}_7$ sample revealing its magnetic ordering at low temperature.

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