ESRF	**Experiment title:** Thermodynamic quantities in a metal-insulator transition determined by Compton scattering	**Experiment number:** HE-3800
Beamline: ID15B	**Date of experiment:** from: 16. 5. 2012 to: 22. 5. 2012	**Date of report:** 6. 9. 2013
Shifts: 18	**Local contact(s):** Thomas Buslaps	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
Kari Ruotsalainen*, Mikko Hakala, Szabolcs Galambosi, Keijo Hamalainen, Simo Huotari, Iina Juurinen, University of Helsinki, Finland

Report:

The purpose of the experiment was to investigate the metal insulator transitions (MIT) of pristine and Cr doped VO_2 with x-ray Compton scattering (CS) and diffraction (XRD), and to extract configurational enthapies of the transitions.

Pelletized powder samples were used. The samples were heated with a gas flow and the temperature was monitored by a thermocouple placed close to the sample. Incident photon energy of 90 keV was used. The CS spectra were recorded with a 13 element solid state detector positioned at a mean scattering angle of 151 degrees. XRD patterns were recorded in transmission geometry with a CCD placed downstream of the samples.

For pristine VO_2 the CS and XRD results confirm the phase transition taking place at roughly 70 degrees Celsius, which is in agreement with literature. The difference Compton profile between the metallic R phase and the rutile M1 phase has two major features: 1) depression at $p_z = \pm$ 2 a.u. and 2) a peak at $p_z = 0$ a.u. The analysis of the features is still underway. Part of the signal must originate from the V 3d electron delocalization, but quantification of the effect requires theoretical calculations beyond typical density functional theory approaches, which are in progress at the moment. Disentangling lattice effects from electronic effects in the transition also requires these calculations for the determination of the electronic latent associated with the transition.

We did not observe clear phase transition signatures in the Compton difference profiles within our statistical accuracy for the Cr doped samples. The XRD patterns demostrated that the samples did change phase, but were of poor crystalline quality compared to the prisine sample.

It is possible that the Cr distribution was inhomogenous, which contributed additional noise and broadened the momentum density features associated with the transition. Jointly these effects could explain the lack of features is the difference profiles, in comparison with the clear changes we observed for the pristine sample.