ESRF	**Experiment title:** Lattice dynamics of WO3 as a function of temperature	**Experiment number**: HC-3119
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Shifts:	**Local contact(s)**: Thanh Tra Nguyen	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Michal Stekiel*, Thanh Tra Nguyen*, Bjoern Winkler

Dept,. Kristallographie, Goethe-Universitaet, 60438 Frankfurt am Main, Germany

Report:

Summary

The aim of the measurements was to determine whether the phase transitions in WO3 that occur with lowering the temperature are driven by soft modes, that is, they are connected to instabilities in the atomic arrangement and their displacement of the atoms.

Results

First, we conducted measurements at the side station, TDS diffractometer, of the ID28. We obtained maps of the reciprocal space, which indicate regions with potentially low-energy phonons. We measured at 350 290 165 K, which correspond to three distinct phases of WO3. The results of TDS on a selected plane are presented in Figure 1.

The strongest diffusive signal is observed in the high-temperature phase, in form of diffusive rods along the (00L) direction. One can also observe a cloud of thermal diffuse scattering around Bragg reflections. Both signals decrease in intensity with lowering the temperature, suggesting that it has origin in lattice dynamics.

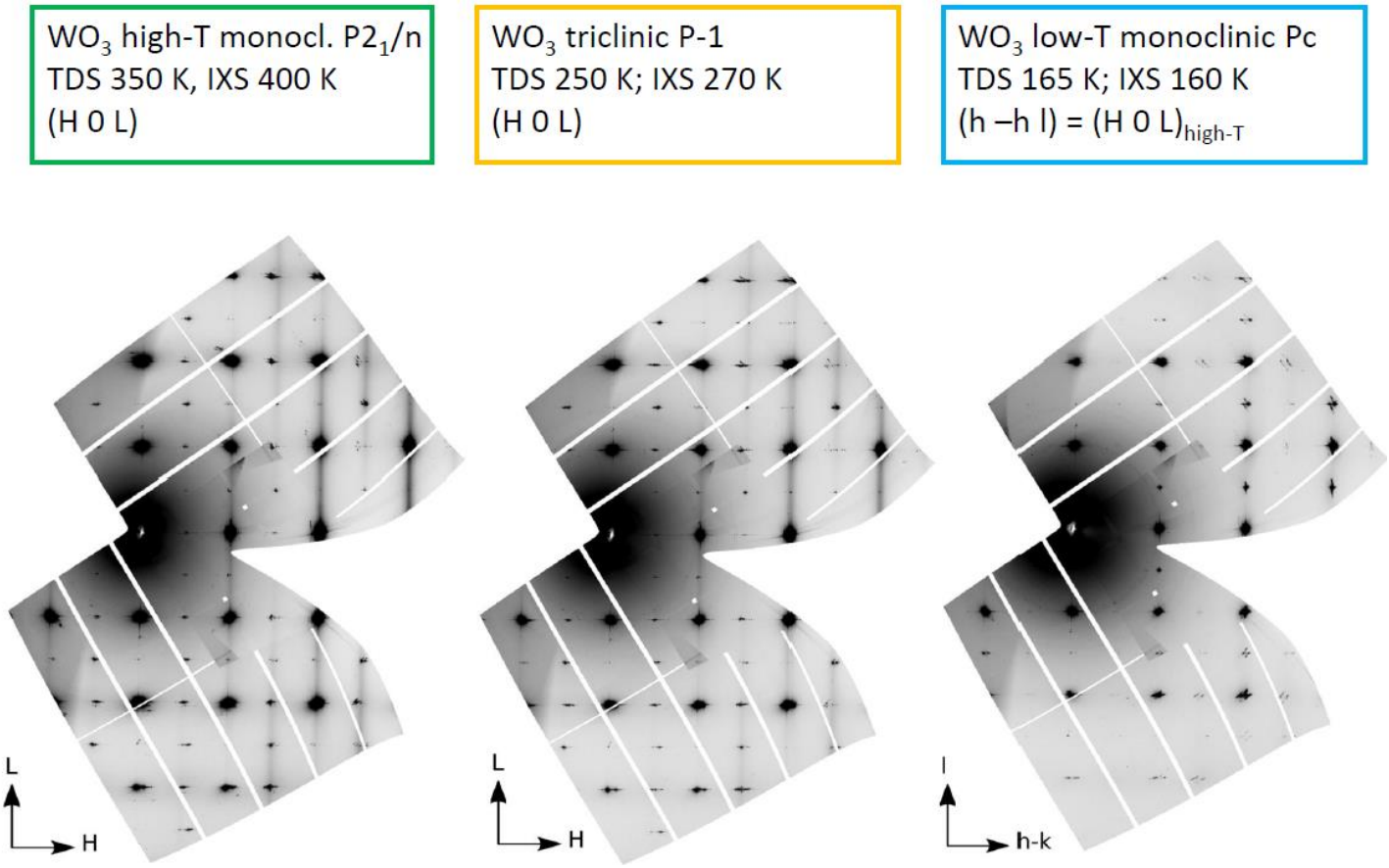

Figure 1. Reconstruction of intensity on the (H0L) plane in three different phases of WO_3.

In the next step we measured the same sample at the main station spectrometer, which allowed us to determine phonon dispersion curves. We measured at various temperatures, trying to compare the data directly to the intensity maps obtained at the diffractometer. We have observed a softening of some phonon modes at the edge of the Brillouin zone upon approaching the high-T to triclinic transition and then consequent hardening of the same mode.

Outlook

We are in a process of interpreting the result and cross checking with theoretical predictions of Kawaminami and Hirose [1], as well as our own DFT calculations, and our recently obtained high-pressure single-crystal X-ray diffraction measurements.

Bibliography:

[1] M. Kawaminami and T. Hirose, *J. Phys. Soc. Jpn.*, vol. 46, pp. 864-870, (1979).