Structure of UO_2 at low temperatures

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We studied the crystalline structure of UO_2 from ambient conditions down to 20 K. The structure of UO_2 at ambient conditions is a fluorite type structure, although the local symmetry might be distorted [1]. At 30.8 K UO_2 undergoes a magnetic phase transition from paramagnetic to antiferromagnetic, which is believed to involve a shift of the oxygen atoms in [111] leading to a lowering in symmetry from $Fm\bar{3}m$ to $Pa\bar{3}$ [2]. This low temperature structure was inferred from the intensities of neutron diffraction experiments, but has not been refined against a high resolution X-ray dataset yet.

Here, we present results of synchrotron diffraction experiments using 18 keV (ID28@ESRF) and 100 keV (P21.1@PETRA III) photons, which allowed a structure refinement with a precise determination of the oxygen positions as a function of temperature.

Samples were UO_2 single crystals grown at FZJ or provided by Los Alamos National Laboratory. Crystals employed for the experiments have dimensions of about 25 x 25 x 25 μm^3. Raman spectra show only one peak at 445 cm^{-1} corresponding to the T_{2g} mode of the fluorite type structure. The absence of additional broad peaks implies that our samples are nearly stoichiometric [3]. A preliminary data analysis (Fig. 1) shows no anomaly in the thermal expansion down to ~50 K. Further results will be presented at the meeting.

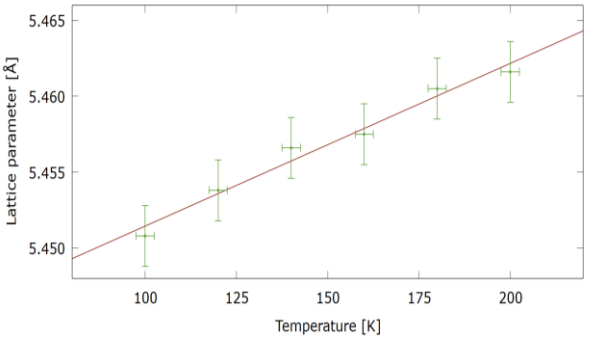

Figure 1 Lattice parameter vs. temperature plot of UO_2

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