ESRF	**Experiment title:** *Low Temperature Structural Distortions of $SrCrO_3$*	**Experiment number**: *HE 2334*
Beamline: ID31	**Date of experiment**: from: 10-Nov-2006 to: 13-Nov-2006	**Date of report**: 26-Feb-2007
Shifts: 6	**Local contact(s)**: *Andy FITCH*	*Received at ESRF:*

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Report:

Transition metal oxide perovskites are of great interest because of the properties that result from highly correlated d-band electrons and strong electron-lattice couplings. $SrCrO_3$ is fundamentally important as an intrinsic metallic conductor, but little is know about this compound due to the high pressure required for its synthesis. The original study [1] reported that $SrCrO_3$ is an undistorted cubic perovskite (a_p = 3.818 Å) and is Pauli paramagnetic and metallic down to 4 K, with a low residual resistivity of 10^{-5} Ωcm. In the present case a 20mg $SrCrO_3$ sample was prepared under 1100°C and 105kbar pressure in a 'Walker' type multianvil cell as part of a study of the series $SrCr_xRu_{1-x}O_3$ [2].

Neutron powder diffraction measurements recorded at 10 and 100 K on ILL diffractometer D20 showed the presence of prominent peak splittings in the 10 K profile compared to the 100K and motivated the present study by high resolution Synchrotron X-ray diffraction study. To elucidate the origin of the splitings and to clarify the ground state properties of $SrCrO_3$, highly resolved powder X-ray diffraction patterns on ID31 at 10-100 K were collected.

The sample was first cooled down to 10K and patterns were collected every 5K up to 50K and then at 100K during one hour at each temperature. Data were collected in the range $3 \leq 2\theta \leq 60$, with a wavelenght of 0.41274 Å using a capillary stage and a 0.7mm capillar. The sample was cooled back to 10K and data were collected following the same process but two hour scans were measured. A Rietveld fit to the powder diffraction data at 100K (cubic phase) is shown in Figure 1.

Below 35 K, extra diffraction peaks are seen in addition to those from the high temperature, cubic $Pm\bar{3}m$ phase of $SrCrO_3$, see Figure 2. These peaks can be indexed on a tetragonally compressed perovskite cell with the unit cell parameters $a \sim a_p$ and $c \sim a_p$ (space group *P4/mmm*). The two structures coexist below 35 K and down to the lowest temperature measured. A Rietveld fit at 10K is shown in Figure 3.

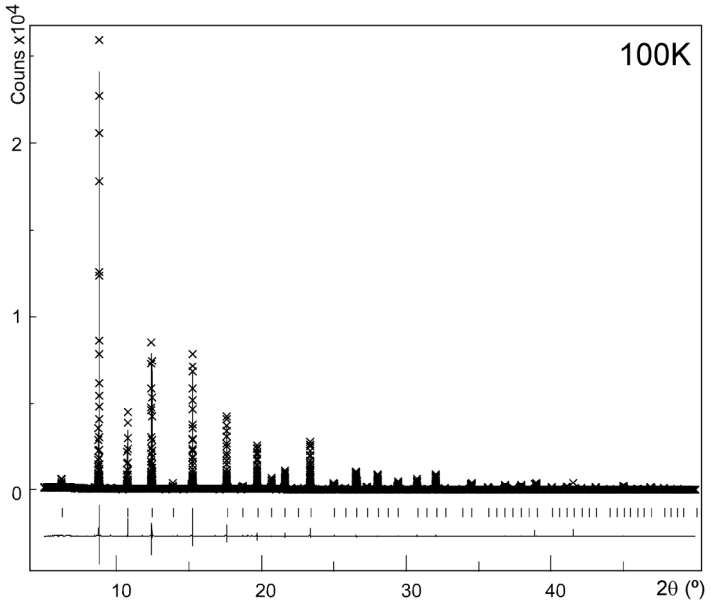

Figure 1. *Rietveld fit of the Cubic $SrCrO_3$ phase measured at 100K.*

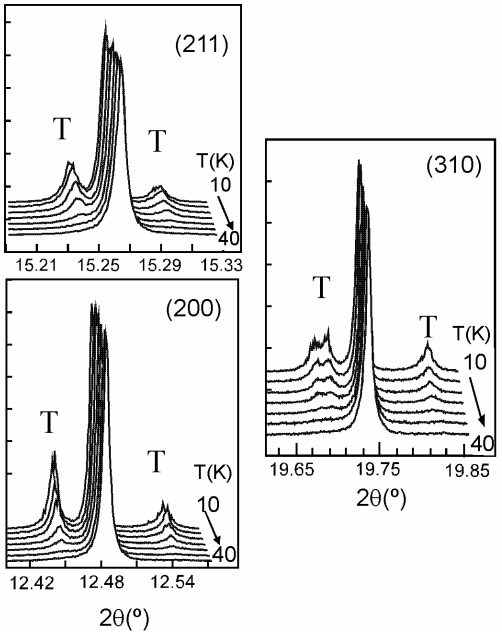

Figure 2. *Diffraction peaks of $SrCrO_3$, showing the growth of additional reflections from the tetragonal phase below 40 K. Capital "T"s denote the presence of the tetragonal reflections.*

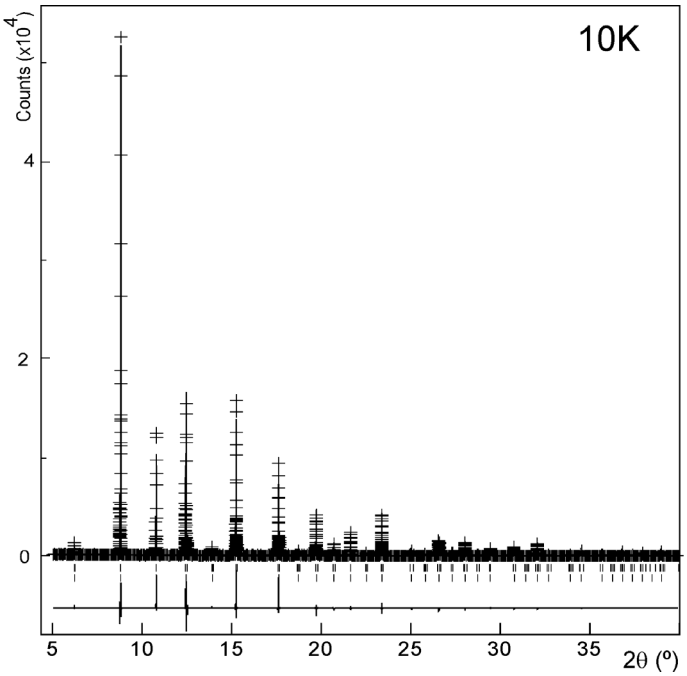

Figure 3. *Rietveld fit of the Cubic $SrCrO_3$ phase measured at 10K.*

References

[1] B. L. Chamberland *Solid State Comm*., **1967**, *5*, 663.

[2] A. J. Williams, A. Gillies, J. P. Attfield, G. Heymann, H. Huppertz, M. J. Martinez-Lope and J. A. Alonso, *Phys. Rev. B*, **2006**, *73***,** 104409.