ESRF	**Experiment title:** **Correlating structures and magnetism in $Sr_2CoO_2Ag_{2-x}Se_2$**	**Experiment number**: CH-4616
Beamline: ID22	**Date of experiment**: from: 1 APR 2016 to: 3 APR 2016	**Date of report**: 22 SEP 2016
Shifts: 6	**Local contact(s)**: Dr A N Fitch	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

The aim of the experiment was to probe the changes in structure accompanying deintercalation of Ag from $Sr_2CoO_2Ag_2Se_2$. This experiment has been accompanied by a complementary powder neutron diffraction experiment at the ISIS facility to probe the evolution of the magnetic ordering.

Figure 1 shows a typical refinement at 5K for the sample with $x = 0$. The structure is modelled in *Immm* below 140 K consistent with the small orthorhombic distortion evident in the analogous $Sr_2CoO_2Cu_2S_2$ [1]

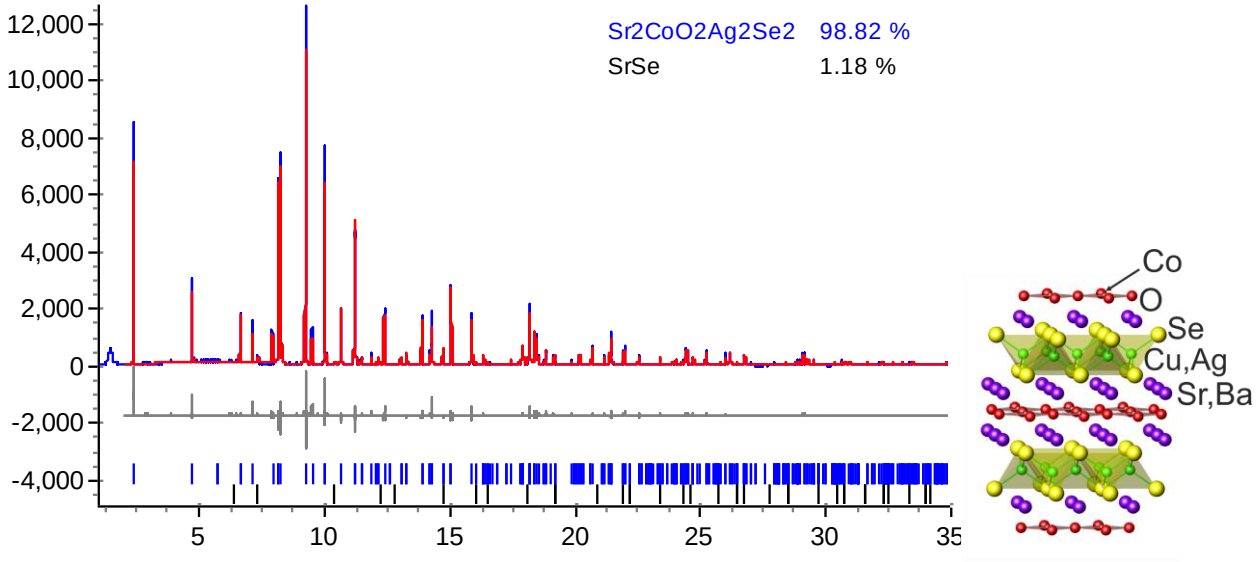

Figure 1. Preliminary Rietveld refinement of $Sr_2CoO_2Ag_2Se_2$.

Probing the change in crystal structure with increasing x initially reveals slight broadening of the 020 reflection, although it is not clear whether this is a consequence of a structural distortion or a compositional inhomogeneity.

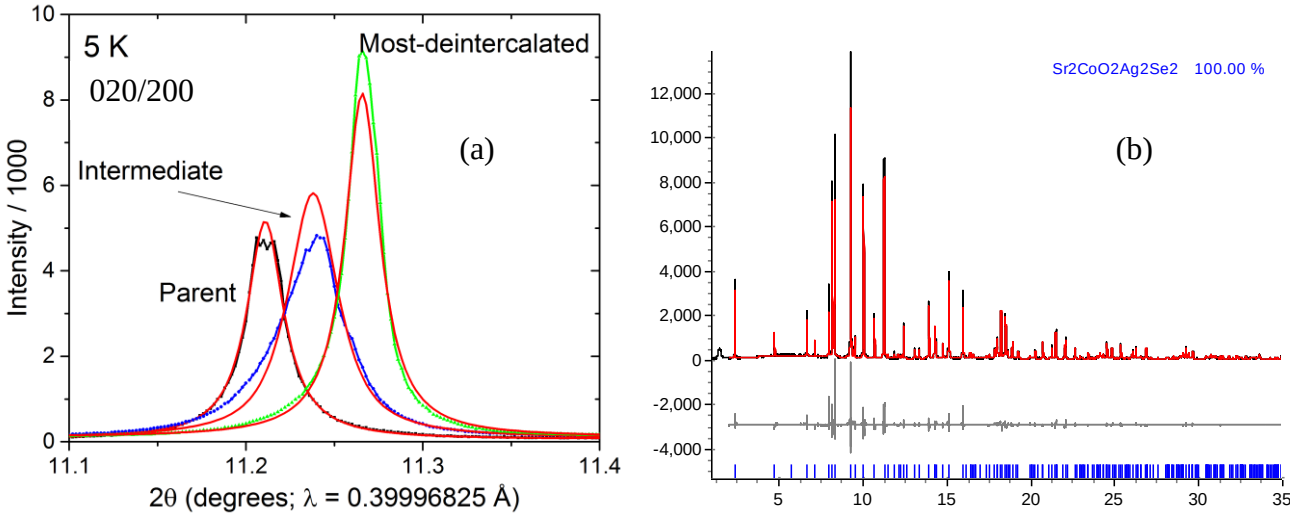

Figure 2 (a). Evolution of the 020/200 reflection(s) in $Sr_2CoO_2Ag_{2-x}Se_2$ for x = 0, 0.15, 0.25. (b) refinement at 5 K for $Sr_2CoO_2Ag_{1.75(2)}Se_2$.

When the deintercalation is carried out to the full extent available chemically "Most-deintercalated" in Figure 2(a) (x = 0.25(1)), the Rietveld refinement (Figure 2(b)) suggests that the tetragonal model in *I*4/*mmm* is appropriate at all temperatures, and that there is no structural distortion. There was also no evidence for superstructure reflections arising from ordering of Ag^+ ions and vacancies. Further refinements are required to model the peakshapes prior to publication of this work.

As a comparison the system $Sr_2CoO_2Cu_{2-\delta}Se_2$ was also probed. In this case the orthorhombic distortion clearly *increases* as Cu is deintercalated (Figure 3). This prompts the question of whether such an increase in the size of the distortion is also evident in $Sr_2CoO_2Cu_{2-\delta}S_2$.

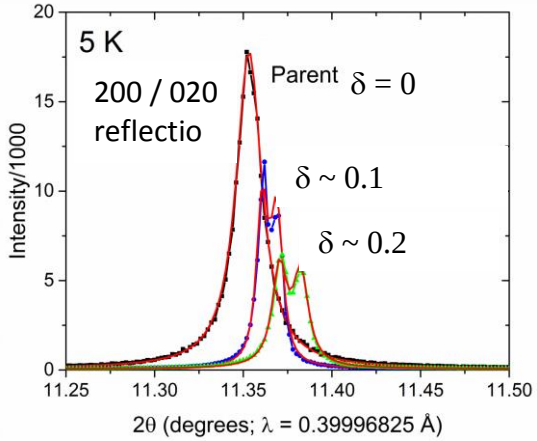

Figure 3. The evolution of the 020/200 reflections in $Sr_2CoO_2Cu_{2-\delta}Se_2$ showing the increasing orthorhombic distortion.

In summary the experiment has answered important questions about this series of oxide chalcogenides and has also posed new questions about the evolution of the crystal structures with composition. The high resolution of ID22 is important for probing the details of these structures.

[1] Smura, C. F. *et al. J. Am. Chem Soc.* **2011**, *133*, 2691-2705.