

Abstract No. Igar0394

Crystal Structures of Sr₂MWO₆ (M=Zn, Ni, Co, Mg, Ca, Cd) Double Perovskites at Different Temperatures.

M.Gateshki, J.M. Igartua, (UPV/EHU, 644 PK Bilbao 48080 Spain).

Beamline(s): X7A

Introduction: Due to the strong cubic pseudosymmetry, that causes overlapping of the diffraction lines, the real symmetry of double perovskite compounds is often overestimated or misassigned. This is the reason why phase transitions in double perovskites are relatively less studied, although it is known that the perovskite structure can be easily distorted and many compounds with that structure present some kind of phase transition. The materials from the Sr₂MWO₆ family are especially suitable for the study of phase transitions since they are easily synthesized and present a great variety of structural distortions. In order to distinguish among the different possible structures high-resolution powder-diffraction measurements were necessary.

Methods and Materials: Powder sample of Sr₂MWO₆ (M=Zn, Ni, Co, Mg, Ca, Cd) were prepared by solid-state method from high purity oxides. X-ray diffraction data were obtained at NSLS X7A beamline using the position sensitive detector and the detector with Ge (220) analyzer crystal. A Si(111) monochromator crystal was used and the wavelength of 0.79997 Å was calibrated using a CeO₂ standard.

The samples measured with the PSD were placed in a quartz capillary and rotated during the experiment. For the samples measured with the analyzer detector the flat plate geometry was used. The experimental details are summarized in Table 1. The refinement of the crystal structures was performed with the FullProf program.

Results: The high temperature phase of all compounds is cubic with space group Fm-3m. The compounds with M=Ca and Cd change their symmetry to monoclinic, P2₁/n at low temperatures. The Zn and Co materials have two phase transitions changing their symmetry first to tetragonal (I4/m) and then to monoclinic (P2₁/n). When M=Ni and Mg the structure changes to tetragonal (I4/m) and retains this space group down to 20 K. These results are preliminary and further refinement work is necessary.

Conclusions: The high resolution powder diffraction data collected at X7A beamline allowed us to resolve the reflections that in the laboratory measurements appear as overlapped and to obtain refinements with good reliability factors. We propose new structural models for the compounds with M=Ca and Cd. This is the first time the monoclinic phases of Sr₂ZnWO₆ and Sr₂CoWO₆ are refined.

Acknowledgments: This work was supported by the Euskal Herriko Unibertsitatea under project No. UPV0063.310-13564/2001. Authors thank Dr. B. Noheda and Dr. T. Vogt for their assistance with the beamline.

Compound	Detector	Geometry	Temperature			Phases
			Displex	Air	Furnace	
Sr ₂ ZnWO ₆	Analyzer	flat plate		RT		P2 ₁ /n
	PSD	capillary			200° C	I4/m
	PSD	capillary			540° C	Fm-3m
Sr ₂ NiWO ₆	Analyzer	flat plate	20K	RT		I4/m
	Analyzer	flat plate			540° C	I4/m
	PSD	capillary				Fm-3m
Sr ₂ CoWO ₆	Analyzer	flat plate	200K			P2 ₁ /n
	PSD	capillary			540° C	Fm-3m
Sr ₂ MgWO ₆	Analyzer	flat plate	20K	RT		I4/m
	Analyzer	flat plate			420° C	I4/m
	PSD	capillary				Fm-3m
Sr ₂ CaWO ₆	PSD	capillary		RT		P2 ₁ /n
	PSD	capillary			300° C	P2 ₁ /n
	PSD	capillary			540° C	Fm-3m
Sr ₂ CdWO ₆	PSD	capillary		RT		P2 ₁ /n
	PSD	capillary			300° C	P2 ₁ /n
	PSD	capillary			540° C	Fm-3m

Table 1.