

Abstract No. Igar0351

Cation Ordering in $\text{La}_2\text{NiRuO}_6$

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Beamline(s): X7A

Introduction: The question of the B-cation ordering in $\text{La}_2\text{NiRuO}_6$ is long standing and it has been a subject of some discussion in the literature. In (1) this compound is reported to have double perovskite structure with completely ordered B-site cations ($P2_1/n$ space group), while the authors of (2) claim that such order does not exist, which leads to $Pbnm$ space group. Both works are based on neutron powder diffraction measurements, that in principle, allow more accurate determination of the positions of the oxygen atoms than the X-ray diffraction. However, due to its relatively low resolution the neutron powder diffraction technique is not always capable of distinguishing between ordered and disordered structures.

The ordering of the B-cations in double perovskite compounds lowers the symmetry of the structure and is expressed by the appearance of superstructure reflections with indices prohibited in the disordered supergroup. In compounds with cubic or tetragonal symmetry ($a^0a^0a^0$ and $a^0a^0c^-$ octahedral tilts in Glazer's notation) the presence of the superstructure reflections is easily established, but in compounds with a^+b^- tilt the superstructure reflections are strongly overlapping with other reflections permitted in the disordered supergroup. The superstructure reflections usually observed in ordered compounds with a^+b^- tilt are (101) and (103). In the case of $\text{La}_2\text{NiRuO}_6$ the superstructure reflections are overlapping with (011) and (013).

Methods and Materials: A detector with Ge (220) analyzer crystal and a Si(111) monochromator crystal were used and the wavelength of 0.8005 Å was calibrated using a CeO_2 standard. The sample was placed in a quartz capillary and rotated during the experiment.

Results and Conclusions: The comparison between the diffractograms obtained with the two different sources at room temperature is shown in Fig.1 (since different wavelengths were used, 1.54 Å for the laboratory measurement and 0.8 Å for the synchrotron one, the results are represented in the d-space). From the synchrotron measurement it is clear that the peak at $d=4.55$ Å, in the laboratory data, is actually a superposition of two reflections. The indexing procedure identified these reflections as (101) and (011). (The presence of the (101) reflection reveals at least partial order.) The Rietveld analysis of the diffraction data revealed that the Ni^{2+} and Ru^{4+} cations are almost completely ordered.

The symmetry usually attributed to a disordered double perovskite compound with a^+b^- tilts is the orthorhombic $Pbnm$. The only subgroup of $Pbnm$ that allows ordered arrangement of the B-cations is the monoclinic $P12_1/n1$. Thus, the ordering leads to a monoclinic unit cell. In the present study, as in the previously reported (1, 2), evidence of a monoclinic distortion in $\text{La}_2\text{NiRuO}_6$ was not found.

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 help.

References:

1. P.A. Seinen, F.P.F. van Berkel, W.A. Groen, *Mat. Res. Bull.* **22**, 1987, 535-542
2. P.D. Battle, C.W. Jones, *Mat. Res. Bull.* **22**, 1987, 1623-1627
3. J.M. Igartua, M.I. Aroyo, E. Kroumova, J.M. Perez-Mato, *Acta Cryst.* **B55**, 1999, 177-185

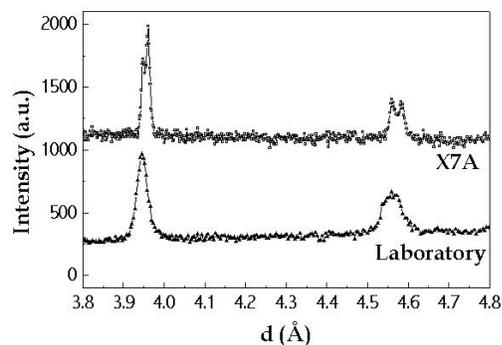


Figure 1. Comparison between the diffractograms obtained with the two different sources at room temperature.