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Neutron and X-ray powder diffraction data to determine the structural properties of novel layered perovskite PrSrMn$_2$O$_{5+\delta}$

Shammya Afroze $^{a,b}$, Nico Torino $^b$, Paul F. Henry $^{b,c}$, Md Sumon Reza $^a$, Quentin Cheok $^a$, Abul K. Azad $^{a,*}$

$^a$ Faculty of Integrated Technologies, Universiti Brunei Darussalam, Jalan Tungku Link, Gadong, BE 1410, Brunei Darussalam
$^b$ Department of Chemistry and Chemical Engineering, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden
$^c$ ISIS Pulsed Neutron & Muon Facility, Rutherford Appleton Laboratory, Harwell Campus, OX11 0QX, United Kingdom

**Abstract**

The data presented in this article are related to the formation of a novel layered perovskite oxide material, PrSrMn$_2$O$_{5+\delta}$, through a solid-state synthesis route. Here, we present the high-resolution neutron powder diffraction and the X-ray powder diffraction data at room temperature. The new perovskite material crystallizes in the orthorhombic symmetry. Interpretation of this data can be found in a research article titled “Insight of novel layered perovskite PrSrMn$_2$O$_{5+\delta}$: A neutron powder diffraction study” (Shammya et al., 2019) [1].

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**Keywords:**
Perovskite oxide
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Neutron powder diffraction
X-ray diffraction
1. Data

The new layered perovskite material, PrSrMn$_2$O$_{5+d}$, was synthesized by solid-state reaction to investigate the structural behavior. X-ray and neutron powder diffraction data were presented at room temperature in Figs. 1 and 2. The XRD pattern of the sample was shown the same crystalline nature of the ceramic material. The XRD pattern was obtained at room temperature for the above sample. To understand the structure of the sample behavior, neutron powder diffraction was also carried out on PrSrMn$_2$O$_{5+d}$ sample at room temperature. A small impurity phase was detected and the percentage of impurity was ~2% for MnO$_2$. The neutron diffraction pattern is perfectly fitted with the orthorhombic layered perovskite structure in the $Pmmm$ space-group yielding, $a = 3.8907$ (1) Å, $b = 3.8227$ (1) Å, and $c = 7.6846$ (2) Å, with dimensions $a_p \times a_p \times 2a_p$. The dimensions were chosen on the basis of X-ray and neutron powder diffraction studies.

The impurity phase for MnO$_2$ also obtained the same crystalline symmetry (orthorhombic symmetry with space group, $Pnma$). The XRD and neutron diffraction patterns are perfectly matched with cell parameter, $a = 9.2451$ (1) Å, $b = 3.1108$ (1) Å and $c = 4.3475$ (2) Å. What are also presented in the article are the detailed neutron powder diffraction data and atomic coordinates (Table 1).

2. Experimental design, materials, and methods

2.1. Materials and methods

PrSrMn$_2$O$_{5+d}$ was prepared by solid-state reaction, using carbonate and oxides: Pr$_6$O$_{11}$ ($\geq$99.99%, Aldrich), SrCO$_3$ ($\geq$99.9%, Aldrich) and MnO ($\geq$99.5%, Aldrich). The obtained powders were annealed at...
1000 °C for 10 hours. Stoichiometric mixtures were prepared by manually grinding the reactants in an agate mortar-pestle, with ethanol as a suspending agent. The finely mixed powders were pressed into pellets and fired at 1200 °C in α-alumina crucibles for 12 hrs, then intensively grounded and pelletized again. The pellet was finally re-sintered for another 12 hrs at 1400 °C, with intermediate grinding and pelletizing. The samples were exposed to a stepwise temperature programme, using the method described in a previous study [2,3].

2.2. Neutron powder diffraction

Neutron powder diffraction data were collected on the time-of-flight instrument Polaris at the ISIS neutron and muon source, UK [4]. The samples were loaded into open, cylindrical 8mm external diameter vanadium can. Time-of-flight powder diffraction data were obtained using the raw format.
and analyzed on GSAS-II [5] software. The experiments were carried out under vacuum, while pressure was controlled by an inlet and outlet valve.

2.3. X-ray diffraction

X-ray powder diffraction (XPD) analysis was performed on a Bruker AXS D8 Advance diffractometer (Cu K radiation — $\lambda = 1.54056$ Å). The experiment was conducted with a 0.02° step, between 10° and 79.995°. The instrument equipped with a copper target, a Ge (111) primary monochromator, and a solid-state LynxEye detector. The powder diffraction patterns for PrSrMn$_2$O$_{5+d}$ was generated using the software Fullprof.

CRediT author statement

Shammya Afroze: Sample preparation, Characterization, Writing.: Nico Torino: Data curation.: Paul Henry: Data curation, Data analysis.: Sumon Reza: Writing, Conceptualization, Methodology.: Quentin Cheok: Data curation, Writing- Original draft preparation.: Abul Azad: Conceptualization, Investigation, Supervision.

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| Table 1 |
|---------------------------------|
| Structural parameters for as-prepared PrSrMn$_2$O$_{5+d}$ at RT with orthorhombic structure. |
|---------------------------------|
| | PrSrMn$_2$O$_{5+d}$ at RT |
|---------------------------------|
| **Structure model** | PrSrMn$_2$O$_{5+d}$ |
| **Crystal system** | Orthorhombic |
| **Space group** | Pnmm |
| **Volume (Å$^3$)** | 480.9290 (0) |
| **Density (gm/cm$^3$)** | 6.9870 (1) |
| **Cell parameters** | |
| a (Å) | 3.8906 (1), $\alpha = 90^\circ$ |
| b (Å) | 3.8227 (1), $\beta = 90^\circ$ |
| c (Å) | 7.6846 (2), $\gamma = 90^\circ$ |
| **Atomic positions** | |
| Pr (x, y, z) | (0.5000, 0.5000, 0.0000) |
| Sr (x, y, z) | (0.5000, 0.5000, 0.5000) |
| Mn (x, y, z) | (0.0000, 0.0000, 0.7547) |
| O1 (x, y, z) | (0.0000, 0.5000, 0.2522) |
| O2 (x, y, z) | (0.5000, 0.0000, 0.2517) |
| O3 (x, y, z) | (0.0000, 0.0000, 0.5000) |
| **Structure model** | MnO$_2$ |
| **Crystal system** | Orthorhombic |
| **Space group** | Pnma |
| **Volume (Å$^3$)** | 131.7360 (0) |
| **Density (gm/cm$^3$)** | 1.7500 (1) |
| **Cell parameters** | |
| a (Å) | 9.2451 (1), $\alpha = 90^\circ$ |
| b (Å) | 3.1108 (1), $\beta = 90^\circ$ |
| c (Å) | 4.3475 (2), $\gamma = 90^\circ$ |
| **Atomic positions** | |
| Mn (x, y, z) | (0.1545, 0.7500, 0.9957) |
| O1 (x, y, z) | (0.0128, 0.2500, 0.6998) |
| O2 (x, y, z) | (0.2613, 0.2500, 0.3399) |
give 3 months summer fellowship to work in their laboratories. The author would like to thank the ISIS neutron and muon facility, UK for access to scheduled beam-time (RB1810638, DOI: https://doi.org/10.5286/ISIS.E.RB1810638).

**Conflict of Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

**Appendix A. Supplementary data**

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105173.

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