Synthesis and crystalline structure of manganites

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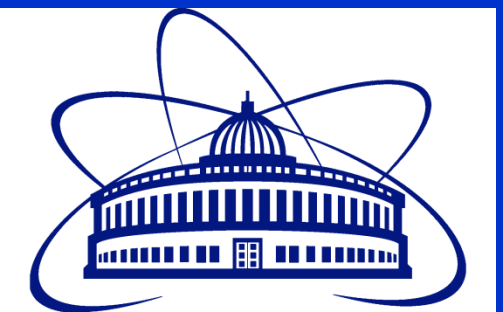


Presentation Outline

- Aim and objectives
- Background
- Materials and Methods
- Results and Discussion
- Conclusion
- References

Aim and objectives

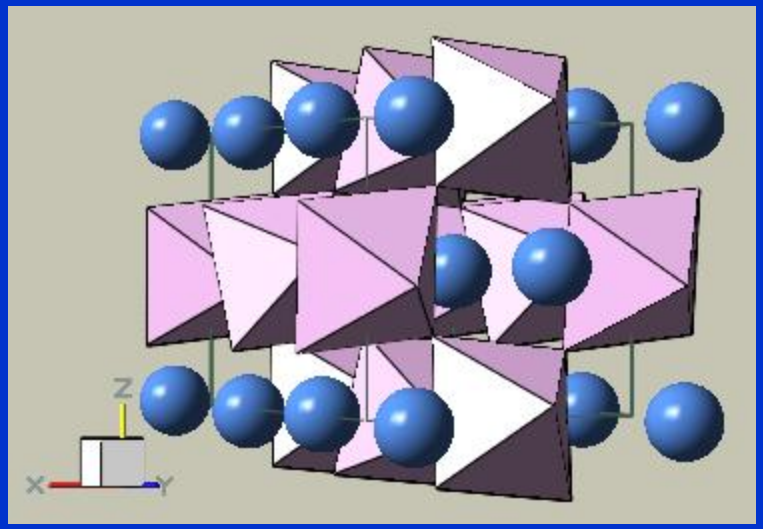
- To synthesize and study the properties of $La_{0.50}Pr_{0.20}Pb_{0.30-x}Sr_xMnO_3$ manganites.
- **Specific Objectives:**

  •To calculate, prepare and obtain manganites corresponding to $La_{0.50}Pr_{0.20}Pb_{0.30-x}Sr_xMnO_3$ manganites, (x=0.0;0.05;0.10;0.15;0.20).

  •To prove the structure of manganites.

  •To obtain lattice parameters, average size of crystalline blocks and microstrains.

Background



$AMnO_3$ compounds having structures based on this architecture are called manganites.. A places are surrounded by 12 O anions and 8 Mn cations, while Mn cations (or other transitional metals) (sitting on the B places) are surrounded by 6 O anions and 8 A cations.

Perovskites - ABO_3

A&B - metallic cations and O is an oxygen. A is a large cation, B is a small cation (e.g. Mn^{3+} and Mn^{4+}) octahedrally-coordinated by oxygen.

A is occupied by large variety of rare earth elements (Nd, Eu, Sm etc.).

Unit cell of manganite

$La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$

Features

Cubic space group:

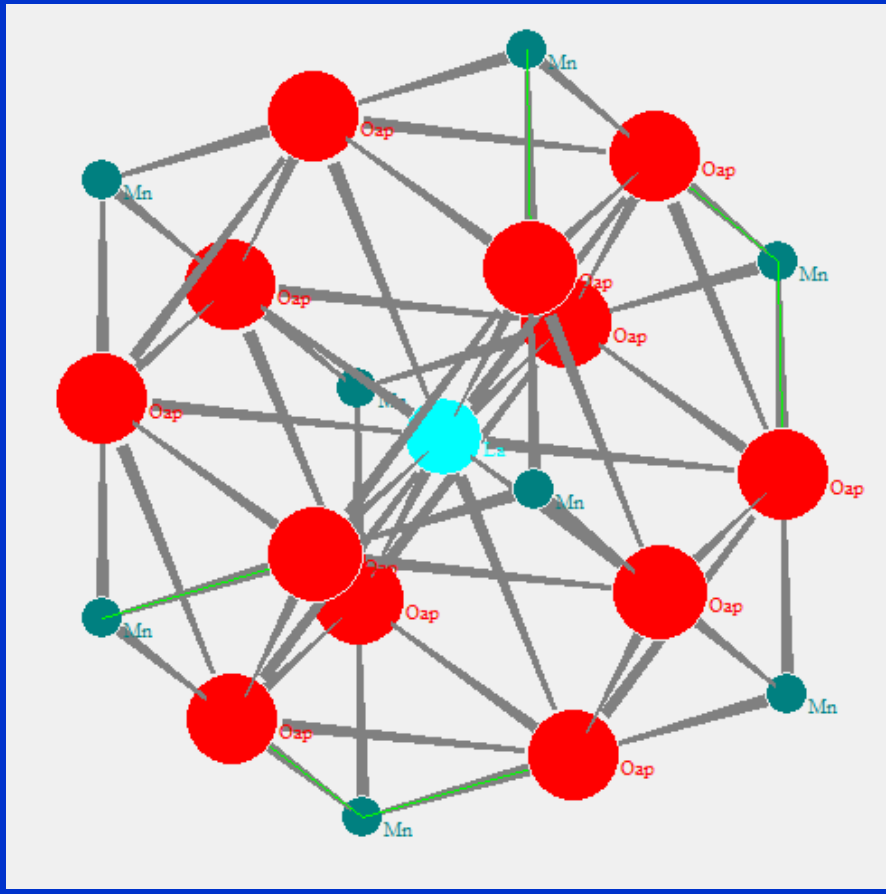
- **P m -3 m**

  -Primitive lattice (P)

  -Mirror plane (m)

  -Centre of inversion and fold axis (-3)

  -Last mirror plane (m)



Unit cell of manganite

$La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$

- **Features:**

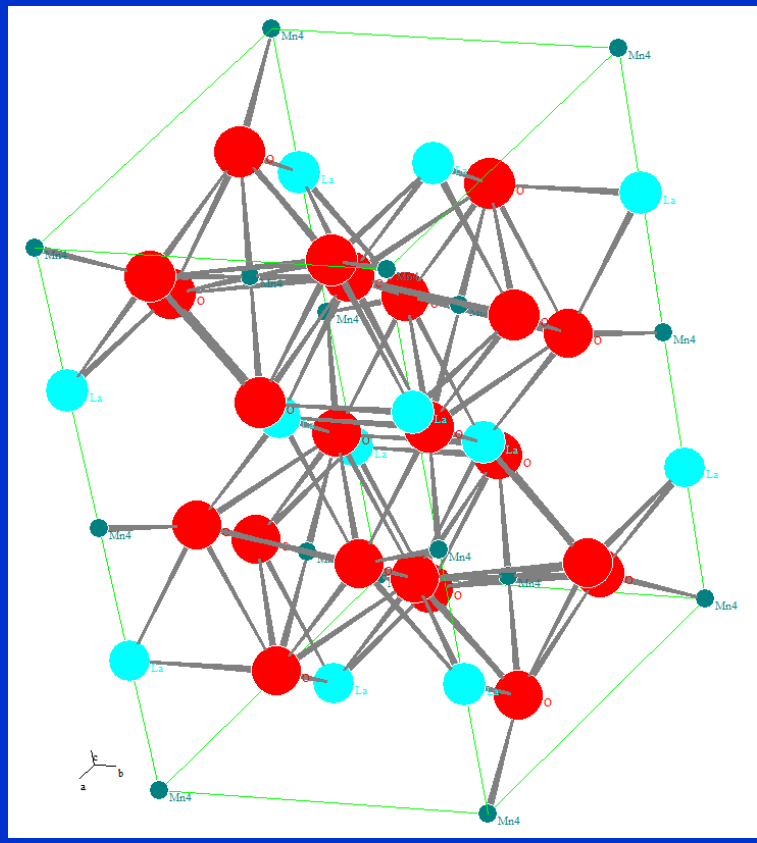
  -Distorted Perovskite

  -Rhombohedral space group: R –3 c

  -Primitive lattice (R)

  -Centre of inversion and threefold axis (-3)

  -Slide plane (c)



Materials and methods

- Preparation of $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$

Weighing of precursors

Mixing and milling of sample

Treatment at low temperature

Preliminary investigations

Grinding/ Polishing

Final sintering at high temperature

Synthesis and Measurement methods

Weighing balance

High Speed Vibrating Ball Mill

Electric Hydraulic Laboratory Press

EQ-Unipol-300 Economy 3" Grinder / Polishing

Metallurgical microscope

X-ray diffractometer

Results and discussion

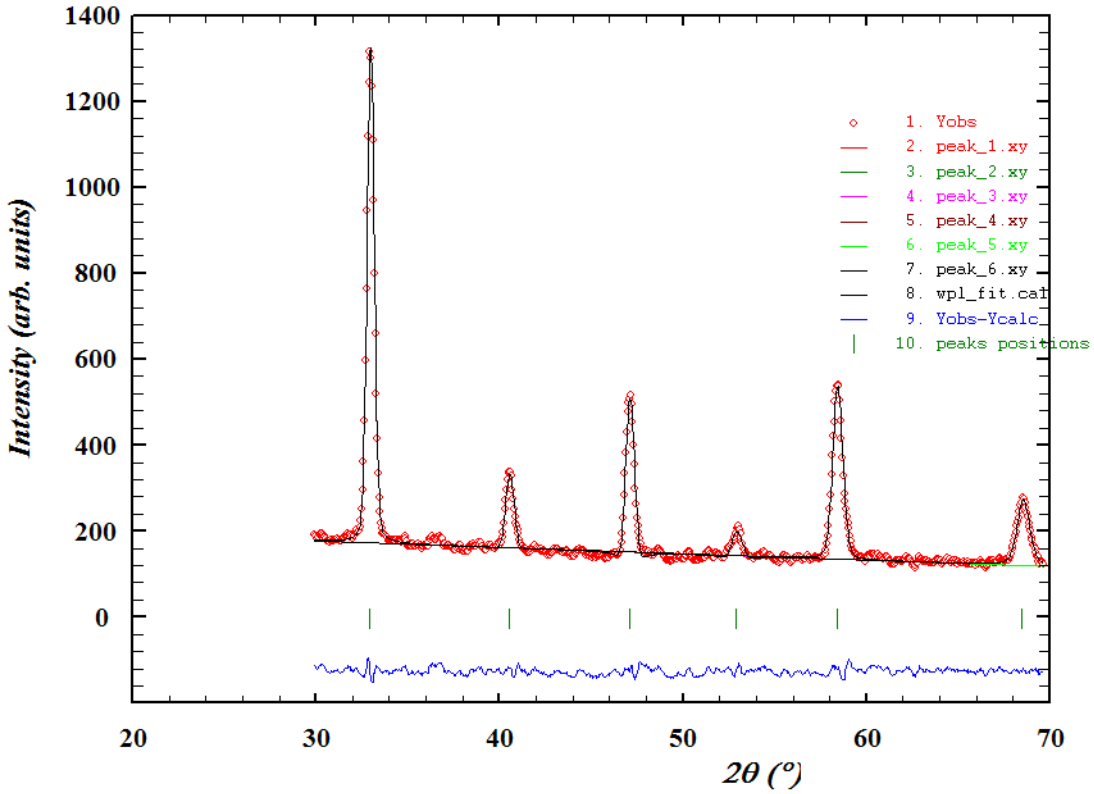


Figure 1: Diffractograms of $La_{0.50}Pr_{0.20}Pb_{0.30-x}MnO_3$ when x = 0 (FullProf method). We obtained the position of the maxima, the average size of the crystalline blocks and the microstrains (red - observed XRD data; black – calculated XRD data; blue - the difference between the observed and calculated data).

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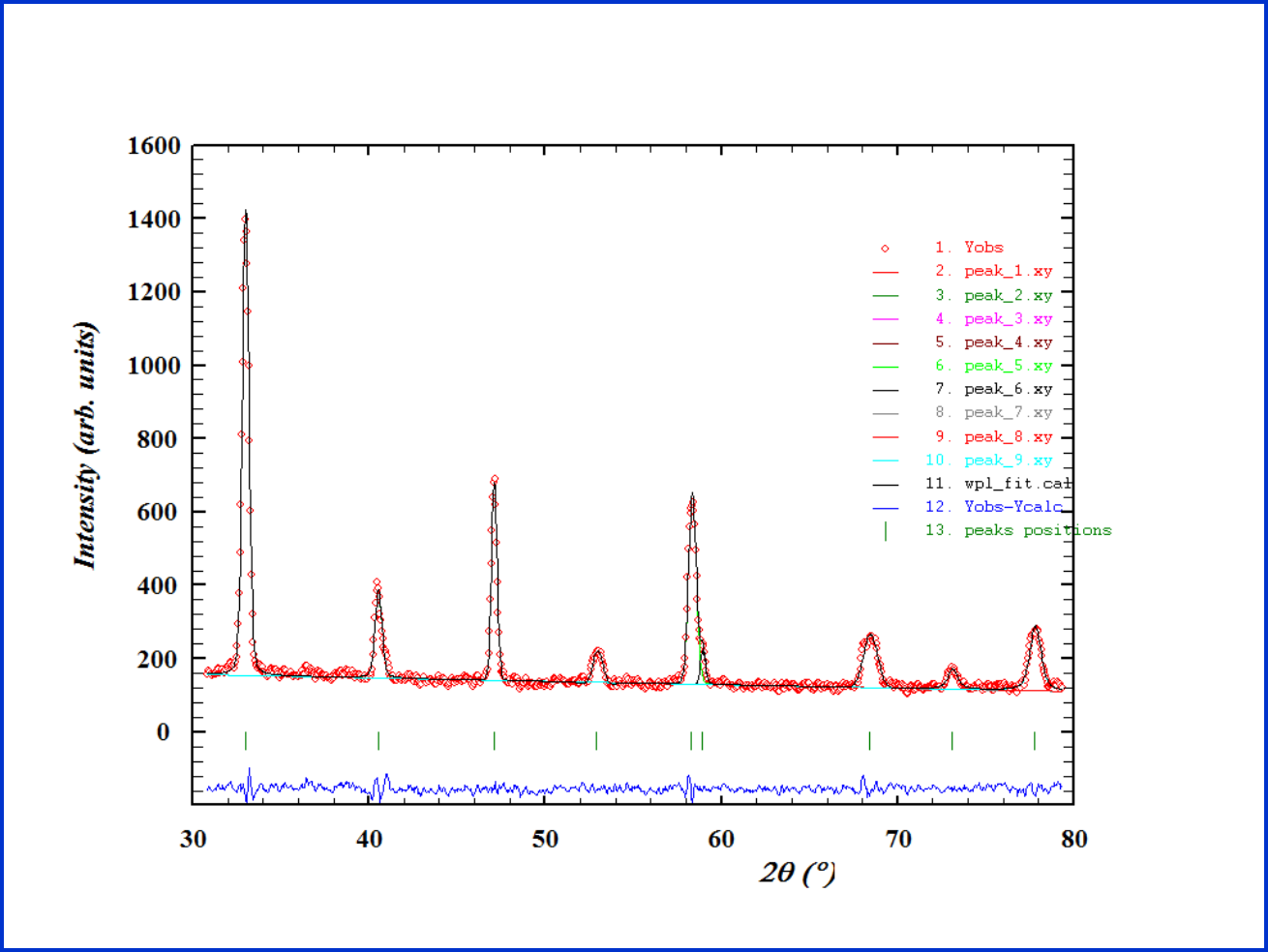

Figure 2: Diffractograms of $La_{0.50}Pr_{0.20}Pb_{0.30-x}MnO_3$ when x = 0.05 (FullProf method). We obtained the position of the maxima, the average size of the crystalline blocks and the microstrains

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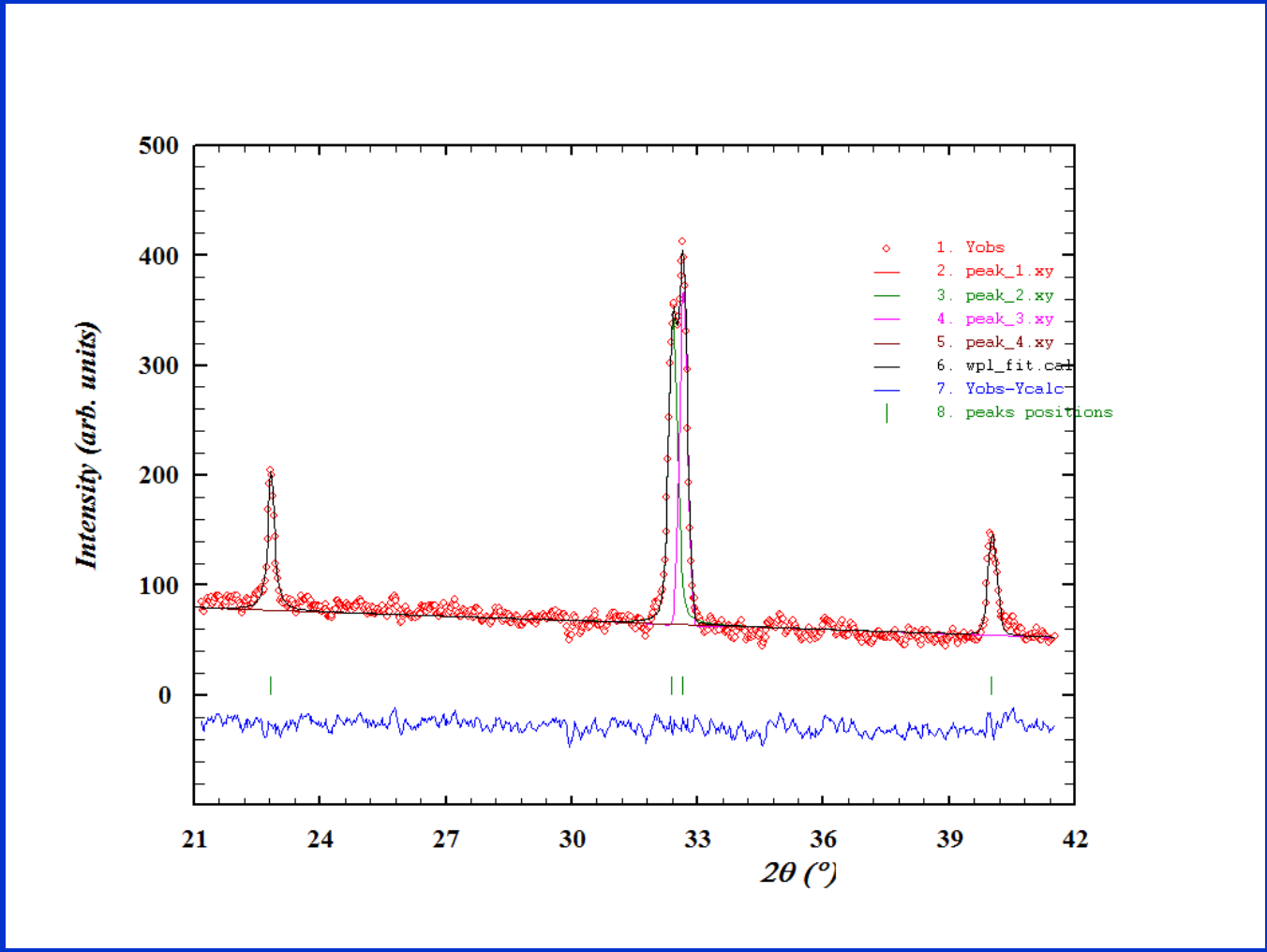

Figure 3: Diffractograms of $La_{0.50}Pr_{0.20}Pb_{0.30-x}MnO_3$ when x = 0.2 (FullProf method). We obtained the position of the maxima, the average size of the crystalline blocks and the microstrains

Summary of crystal structure parameters Powder Cell method

Table 1: Variation of lattice constants (a, b, c), average size of crystal size and microstrain of

- $La_{0.50}Pr_{0.20}Pb_{0.30-x}Sr_xMnO_3$

	Lattice constant		Crystal size	Microstrain	Space group
x	a = b	c	D(Å)	ε	
0.00	3.8954	3.8954	271	0.0020	Pm-3m
0.05	3.9069	3.9069	266	0.0018	Pm-3m
0.10	5.5254	13.4019	201	0.0012	R -3c
0.15	5.5390	13.4174	335	0.0010	R -3c
0.20	5.5398	13.4194	274	0.0011	R -3c

Conclusion

- Samples for $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$ changed the crystallographic structure from SG Pm-3m to R -3 c for $x \geq 0.1$. The unit cell volume and the lattice constants increased with the increase of Sr concentration due to the increase of Mn^{3+} concentration.
- The microstrains suddenly decreased with the changes of the crystallographic structure .
- The average size of mosaic blocks remain practically constant with different Sr concentration.

References

1) The Basic of Crystallography and Diffraction, C. Hammond, Oxford University Press, 2001

2) Modern Crystallography, B.K.Vainstein, Springer-Verlag, 1995

3) Nanoscale Phase Separation and Colossal Magnetoresistance: The Physics of Manganites and Related Compounds, E. Dagotto, Springer-Verlag, 2003

4) http://www.ill.eu/sites/fullprof/

5) www.flnr.jinr.ru

6) Perovskiti Magnetorezistivi: sinteza, proprietati si aplicatii, Mihail-Liviu Craus, Nicoleta Cornei, Mihai Lozovan, Viorel Dobrea, Iassy:Alfa, 2008

7) An introduction to the program FullProf, Juan Rodríguez-Carvajal, Laboratoire Léon Brillouin (CEA-CNRS), CEA/Saclay, 91191 Gif sur Yvette Cedex, FRANCE

Acknowledgements

- I am indebted to Prof Mihail-Liviu Craus and Dr Vitali Turchenko for their guidance & patience.
- Thanks to the Director and staff of JINR for the nice organization of the student practice.
- Thanks to NRF/iThemba LABS for Funding
- Thanks to my fellow students from Egypt: Hawary, Mostafa, Sherifa, Ali and Alaa for their support.

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THANK YOU
Спасибо