JOINT INSTITUTE FOR NUCLEAR RESEARCH
Frank Laboratory of Neutron Physics

CRYSTAL AND MAGNETIC STRUCTURE OF ADVANCED OXIDE MATERIALS: NEUTRON DIFFRACTION STUDIES

Project supervisors:

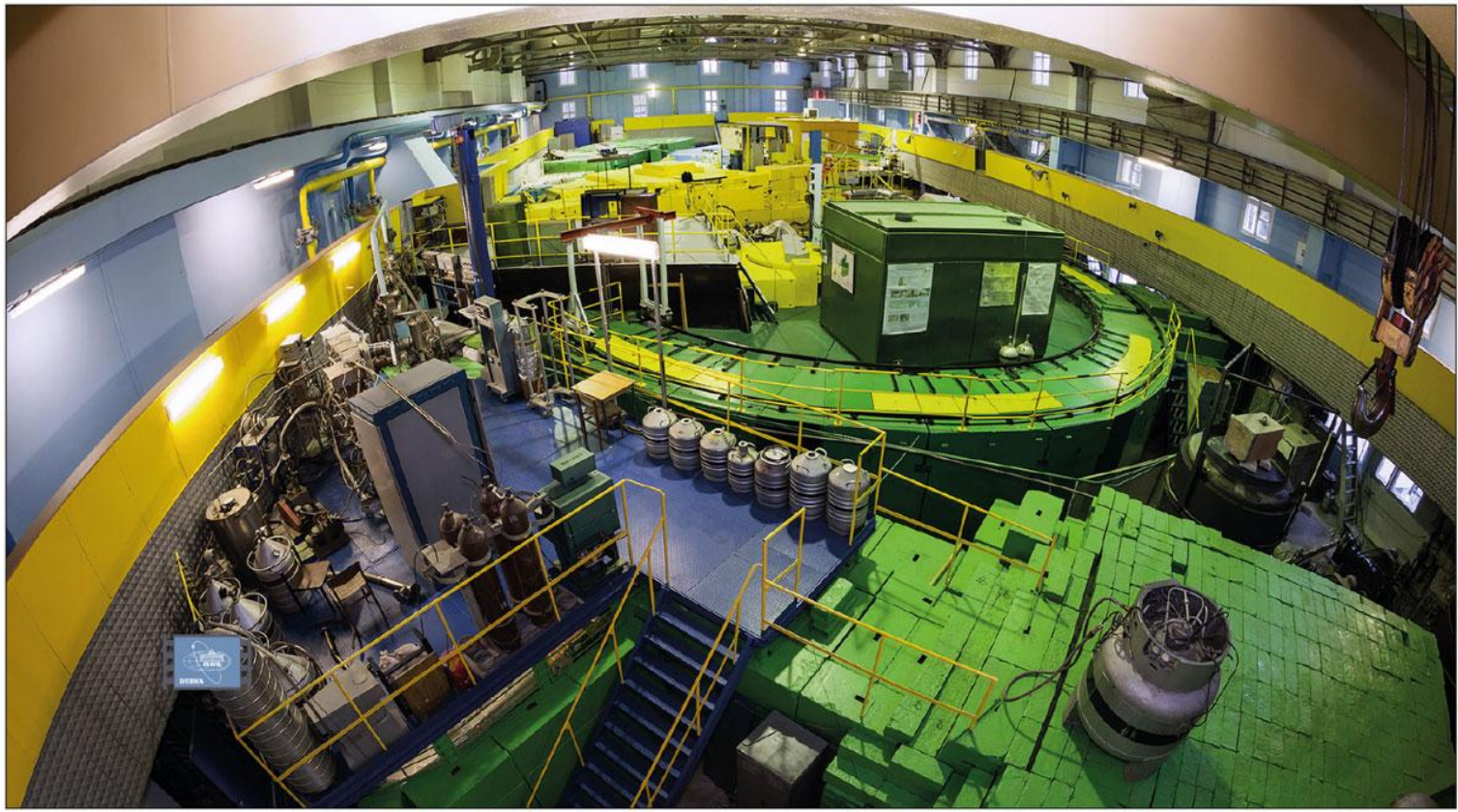
Nadezda Belozerova – Junior Researcher, Condensed Matter Department Frank Laboratory of Neutron Physics, JINR
Dr Sergey Kichanov – Senior Researcher, Condensed Matter Department Frank Laboratory of Neutron Physics, JINR

PhD student:

Nevena Božinović, Researcher at Institute of Nuclear Sciences ,, VINCA'' , National Institute of the Republic of Serbia

Content before introduction:

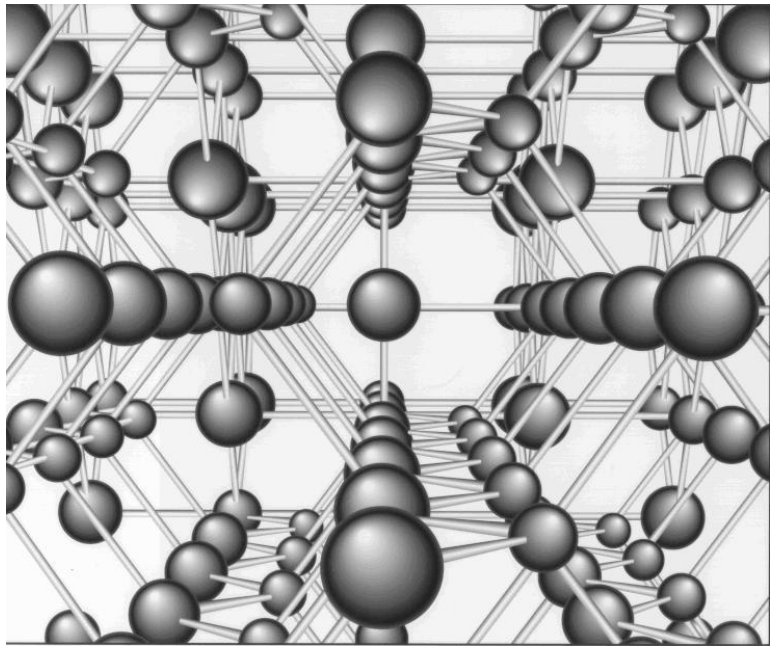
- The basic principles of condensed matter physics
- Diffraction methods (Neutron diffraction)
- Scientific software
- Obtaing data using Rietveld method
- Results and discussion



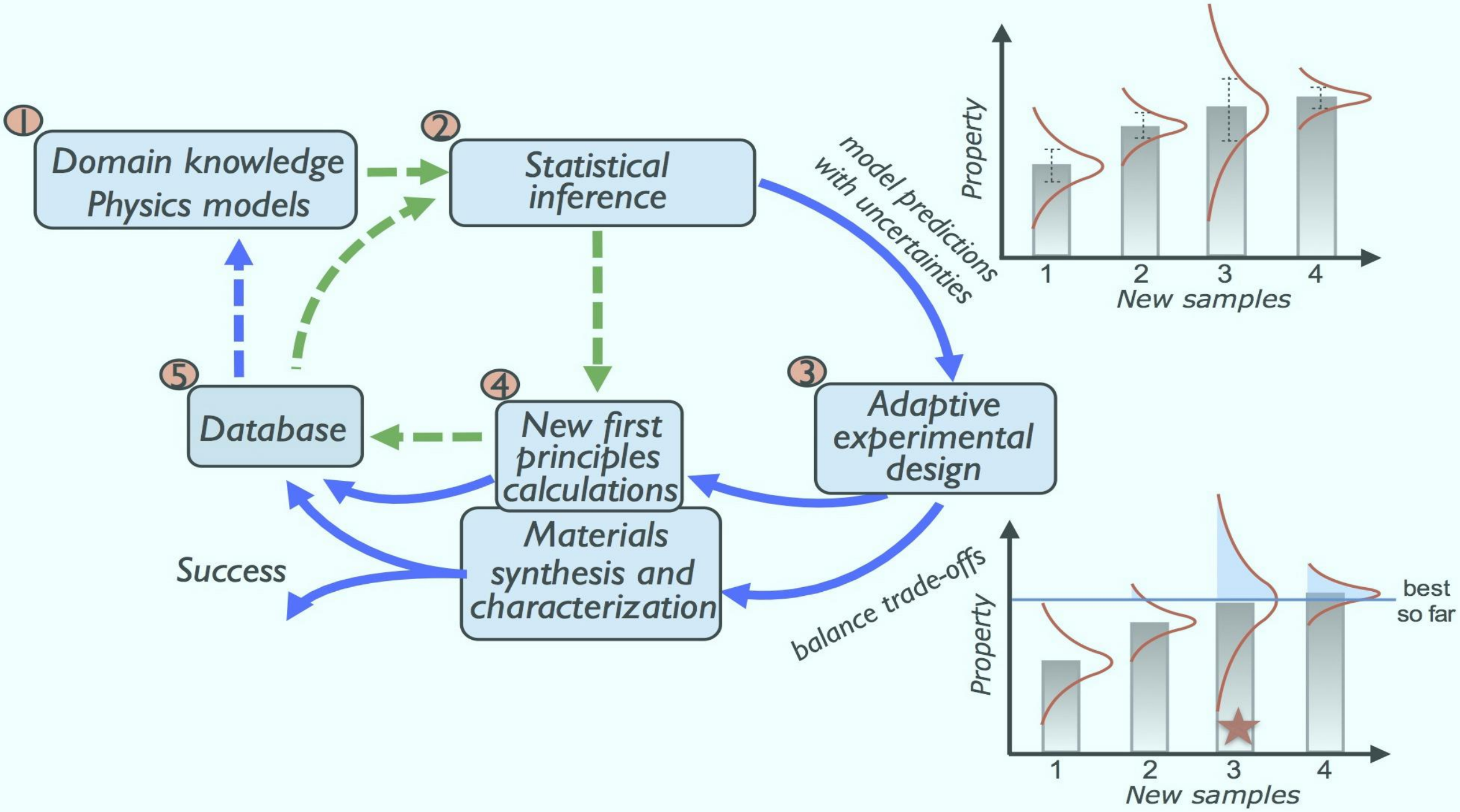
Objective of the project

All aims of the project were achived:

- ✓ The knowledge about the main methods used neutrons as instrument for study condensed matter were obtained,
- ✓ The way how to perform neutron diffraction experiments and treating the experimental data using Rietveld method were found out,
- ✓ Processing of experimental data in the software FullProf was realized,
- ✓ The most important crystal and magnetic structure parameters of the complex oxide $La_{1-x}SrxMnO_3$ by means of FullProf were defined.

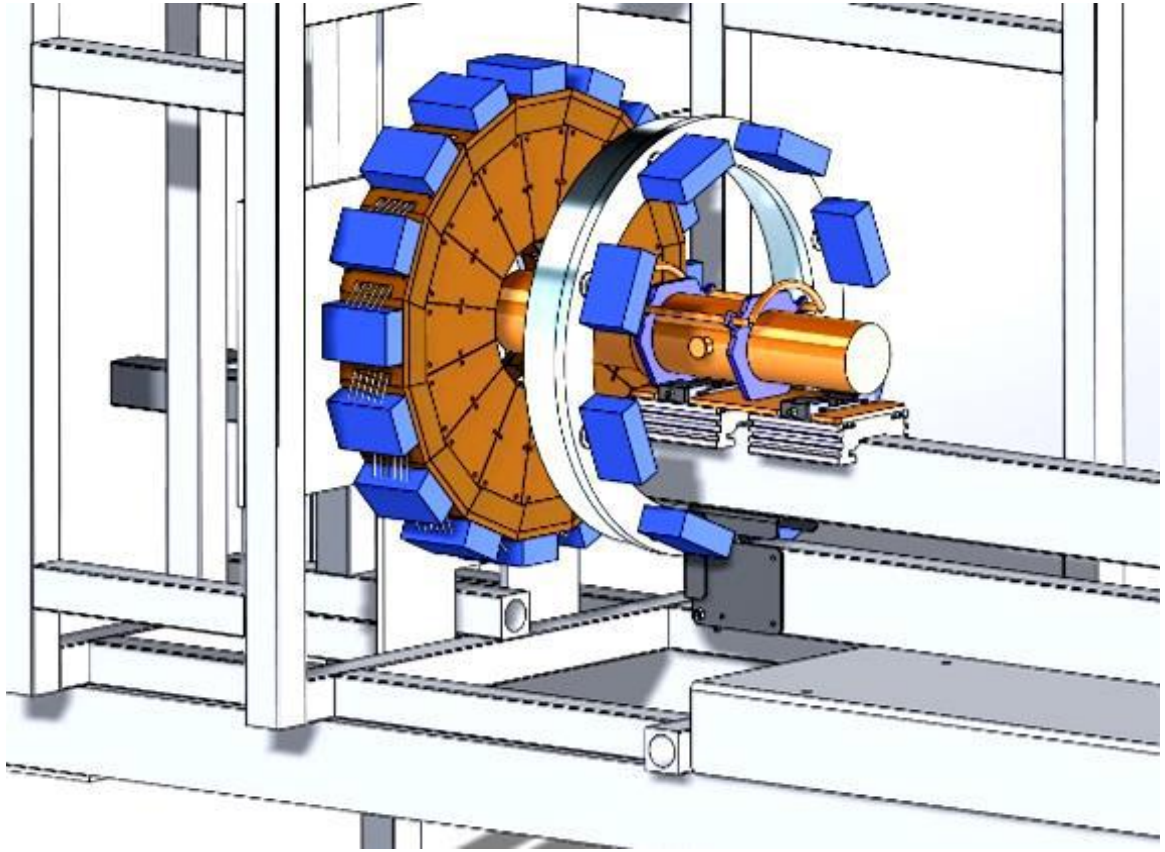


- high temperature superconductivity,
- magnetoresistance effect,
- metal-insulator transition,
- charge and orbital ordering, ferroelectricity, magnetoelectric effect, spin crossover, etc.


1
Domain knowledge
Physics models
2
Statistical
inference
model predictions
with uncertainties
Property
1
2
3
4
New samples
5
Database
4
New first
principles
calculations
3
Adaptive
experimental
design
Materials
synthesis and
characterization
Success
balance trade-offs
best
so far
Property
1
2
3
4
New samples

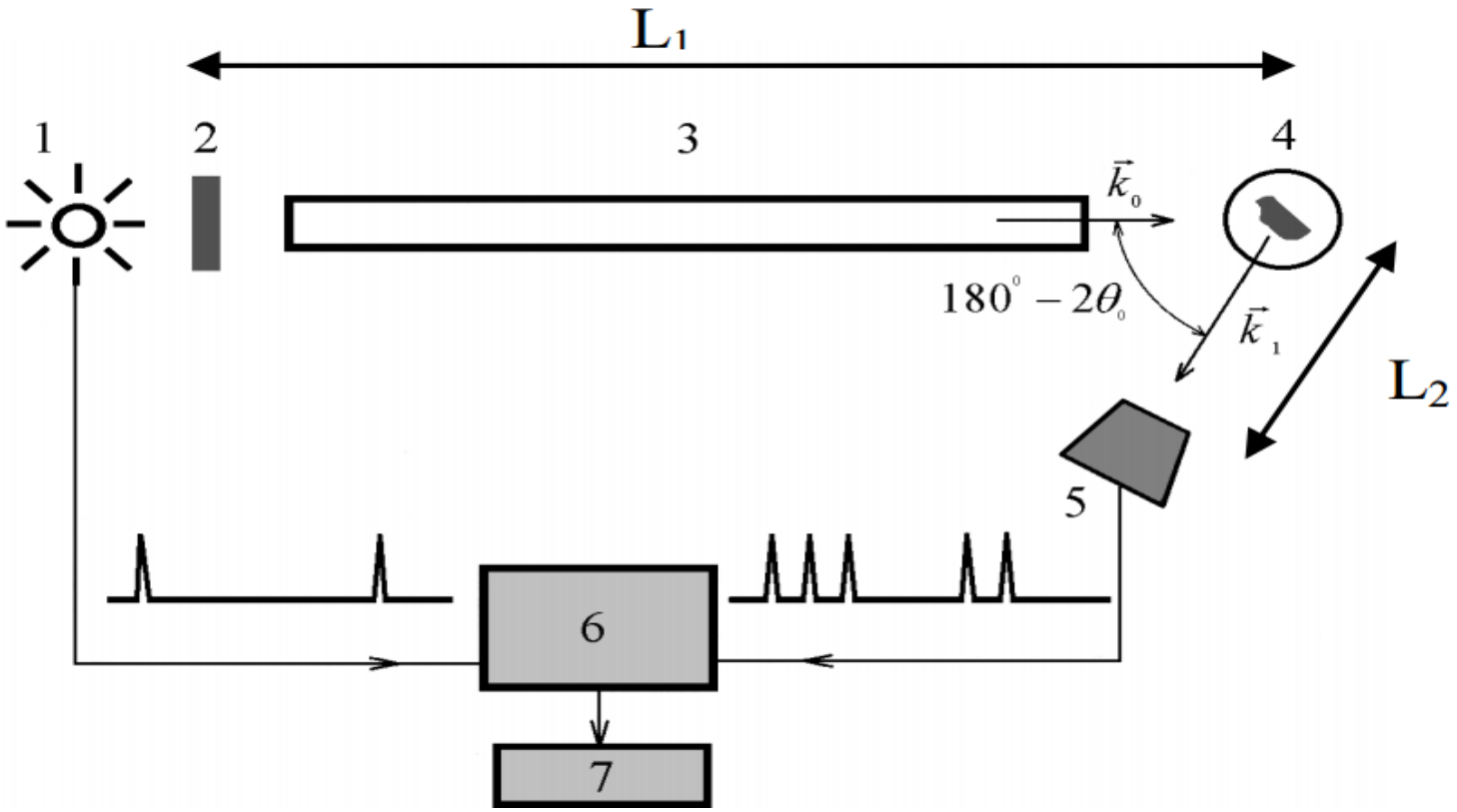
Experimental method: Neutron Diffraction

- Neutron is sensitivity to the light atoms such as oxygen. It is give as opportunity to determine location of oxygen with high precision.
- Neutron intrinsic magnetic moment make neutrons sensitive to the magnetic structure and dynamics of magnetic substances
- The energy of the neutron is comparable with the energy of elementary excitations in the material



Time of flight method (TOF)

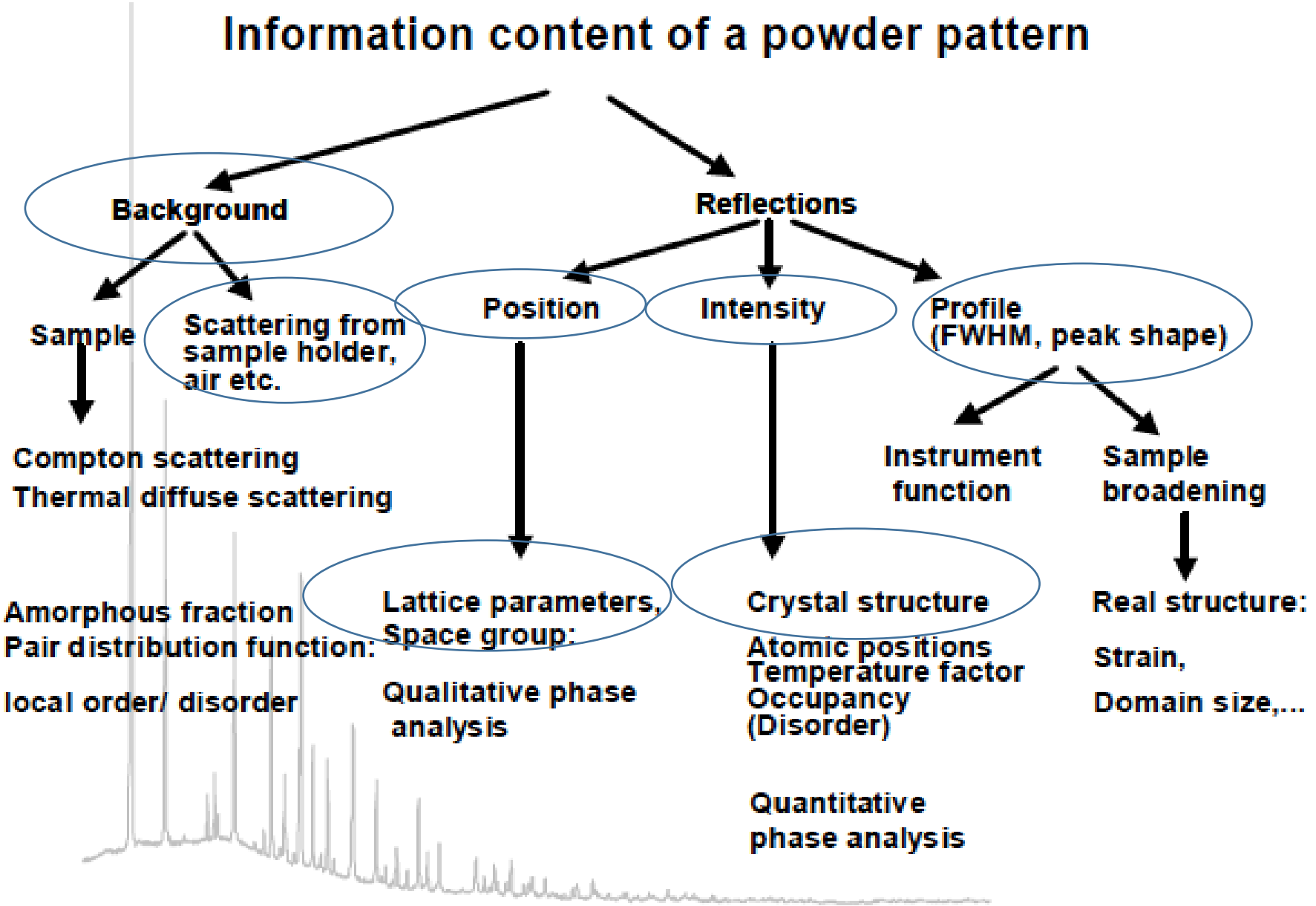
One of the most efficient method in structural neutronography



1) Pulsed neutron source
2) Moderator
3) Flight path of the primary beam
4) Sample
5) Detector
6) Time analyzer
7) RW memory

$$d_{hkl} = \frac{ht}{2m(L_0 + L_1)sin\theta_0}$$

Why do Reitveld Refinement?



Basic refinement procedure of Rietveld method

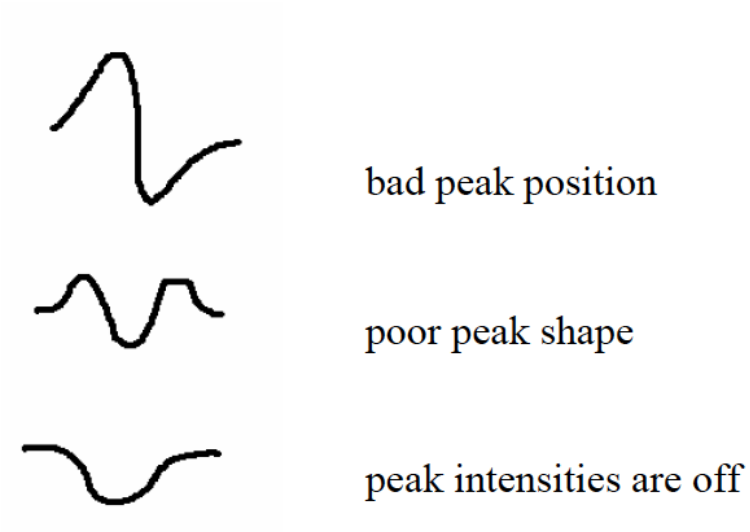
Experimental diffraction pattern

Starting crystal structure (.cif, ICSD)

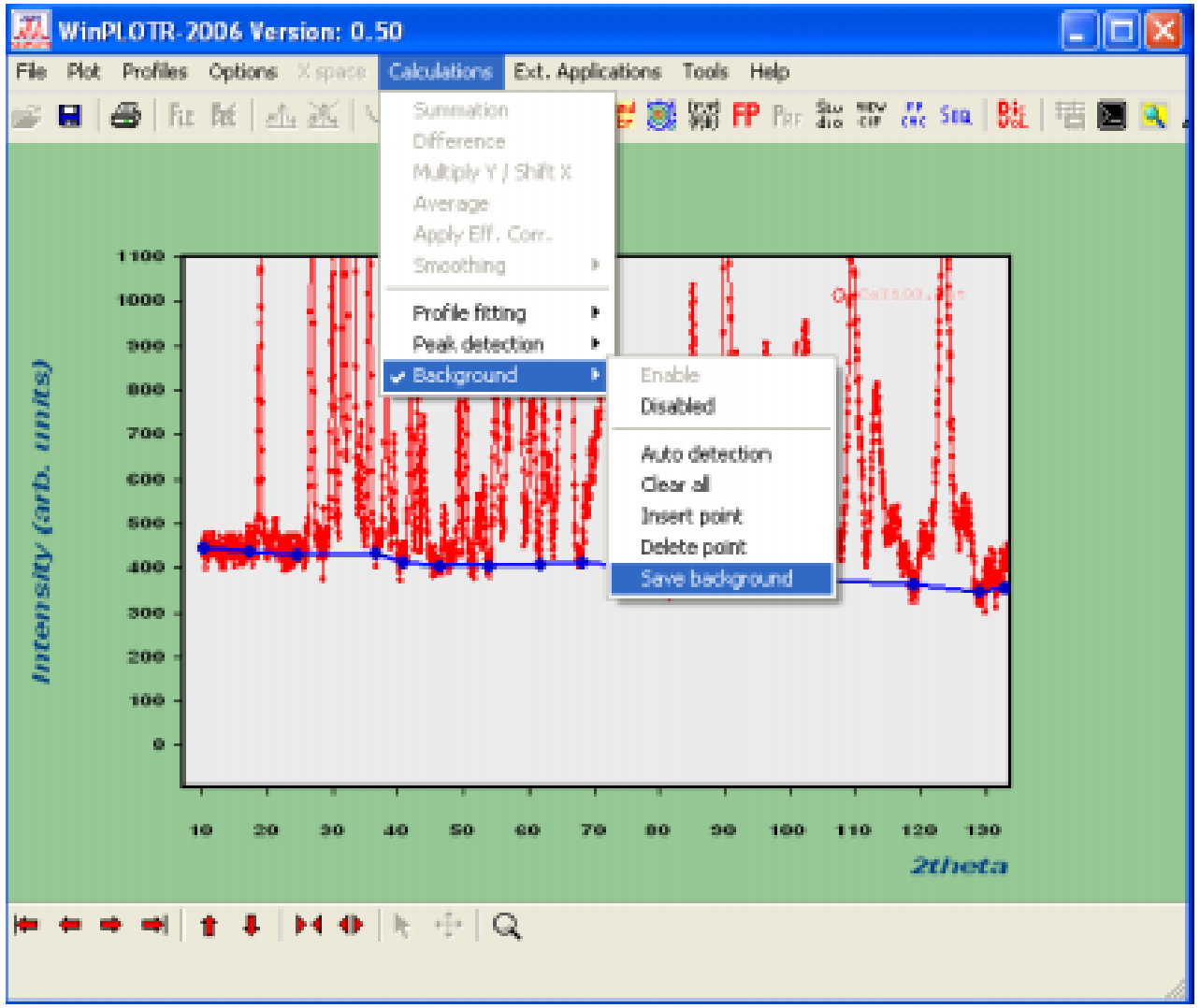
Refinement program: FullProf

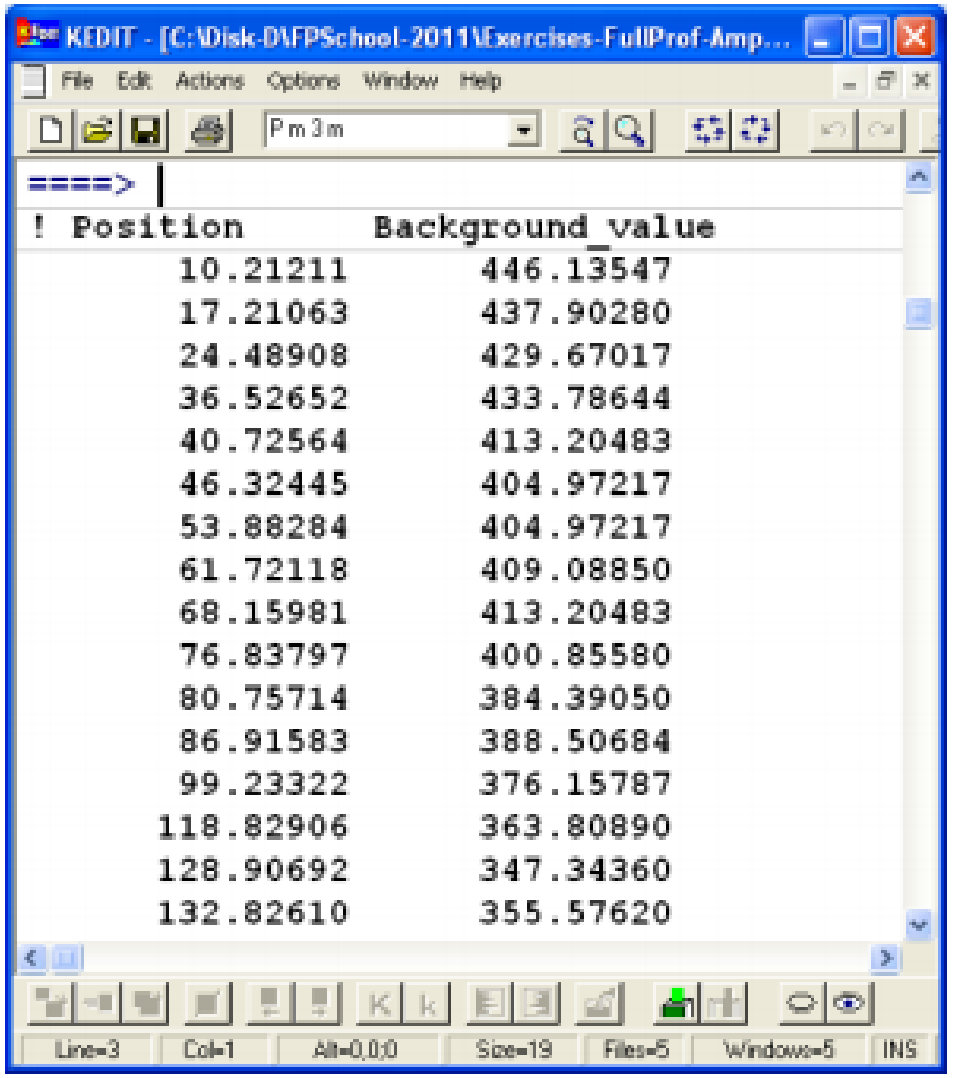
Refine:
- Background
- Lattice parameters
- Peak intensities
- Peak shapes
- Peak positions
- Phase fractions

Assess:
- Goodness of fit/R factors
- Impurity phases
- Peak/background shapes



FullProf Tutoril





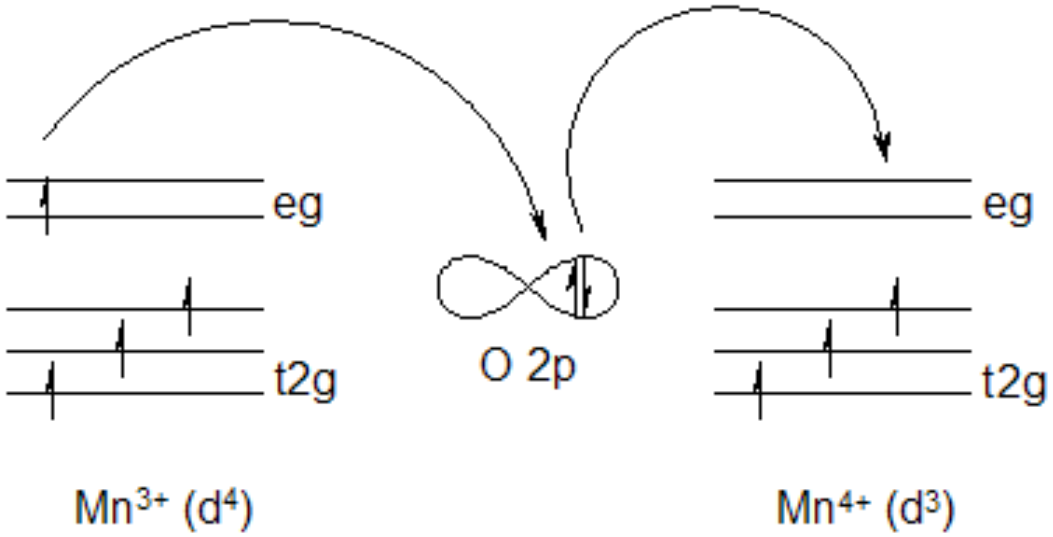
Properties of lanthanum strontium manganite
$La_{1-x}Sr_xMnO_3$ (LSMO)

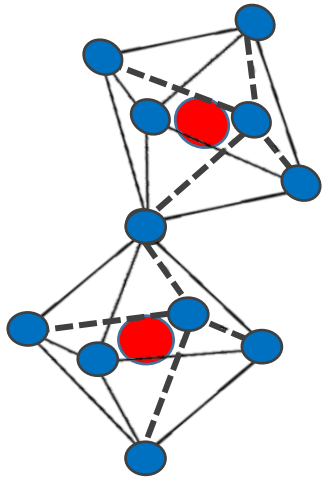
- Perovskite based crystale structure with general form ABO_3

Complex oxide of manganese La0,53 Sr0,47MnO3, T =15K, T= 320 K

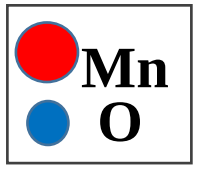
- Space group symmetry: R – 3C

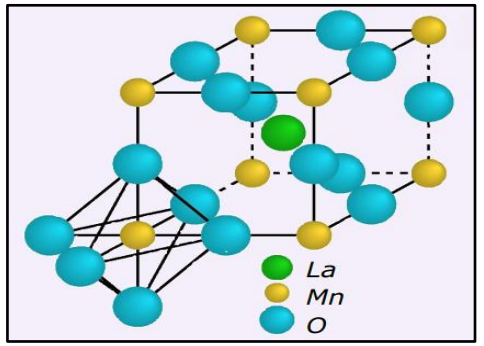
	x	y	z
La/Sr	0,00	0,00	0,25
Mn	0,00	0,00	0,00
O	x	0,00	0,25

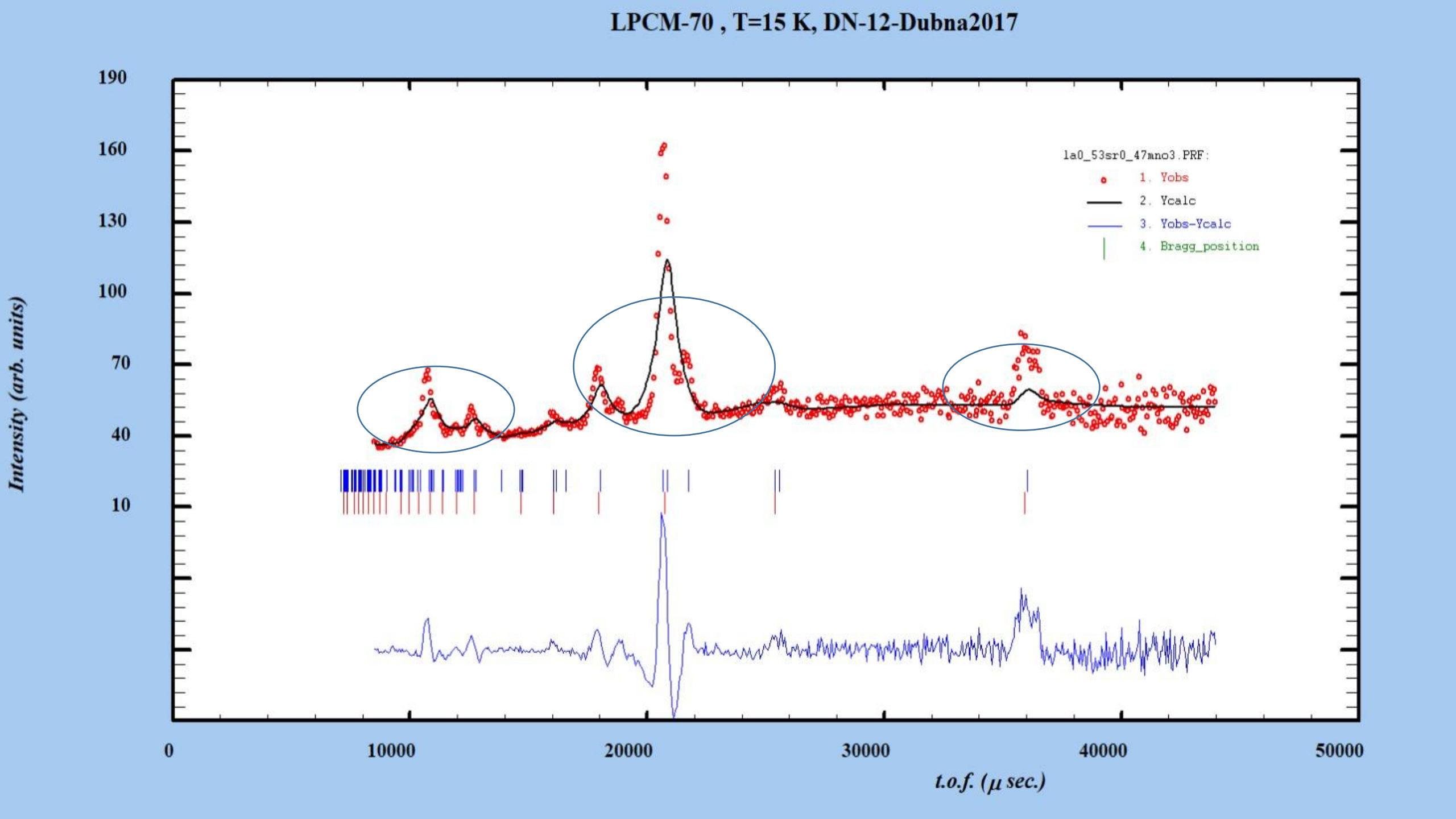




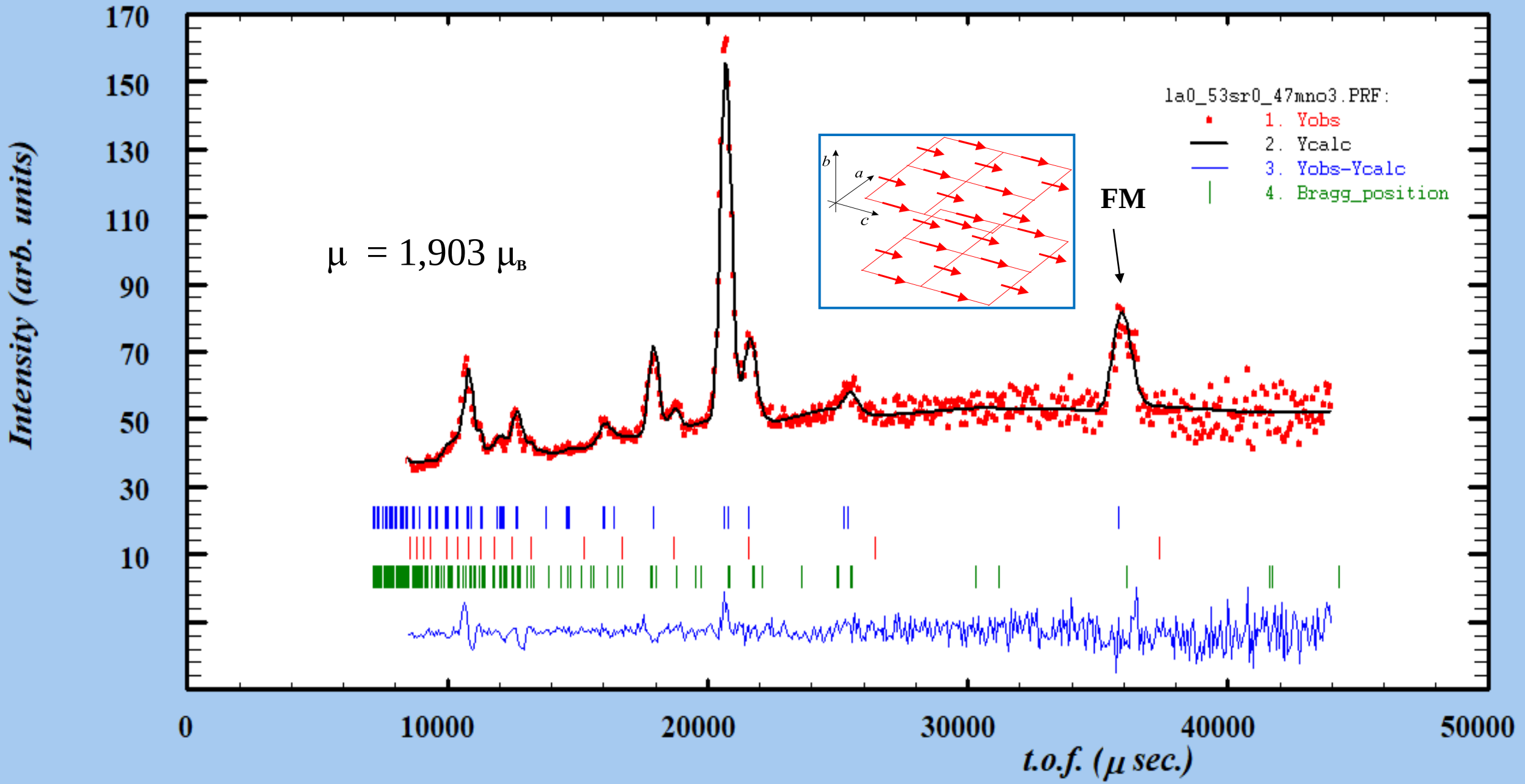
MnO_6 octahedron



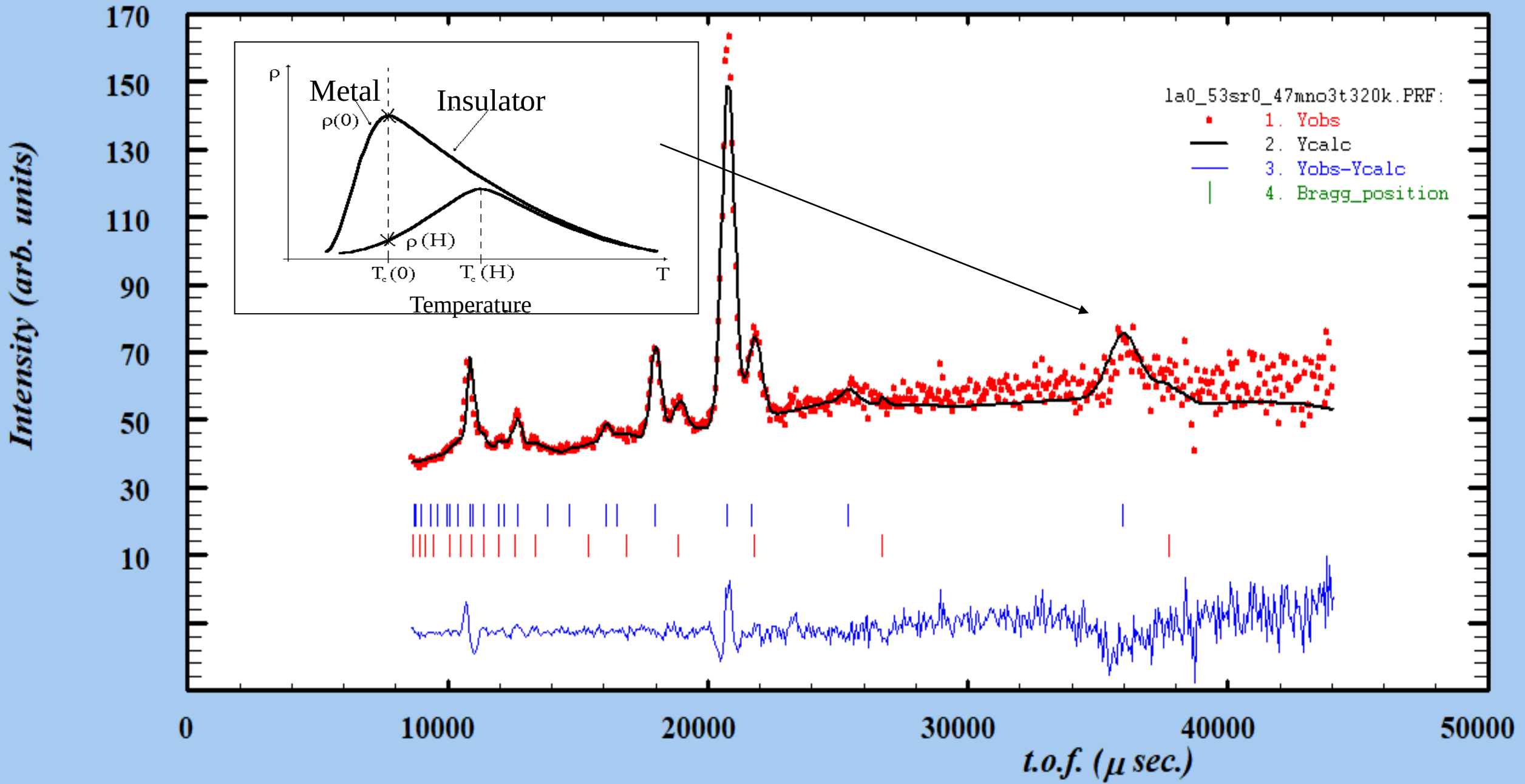


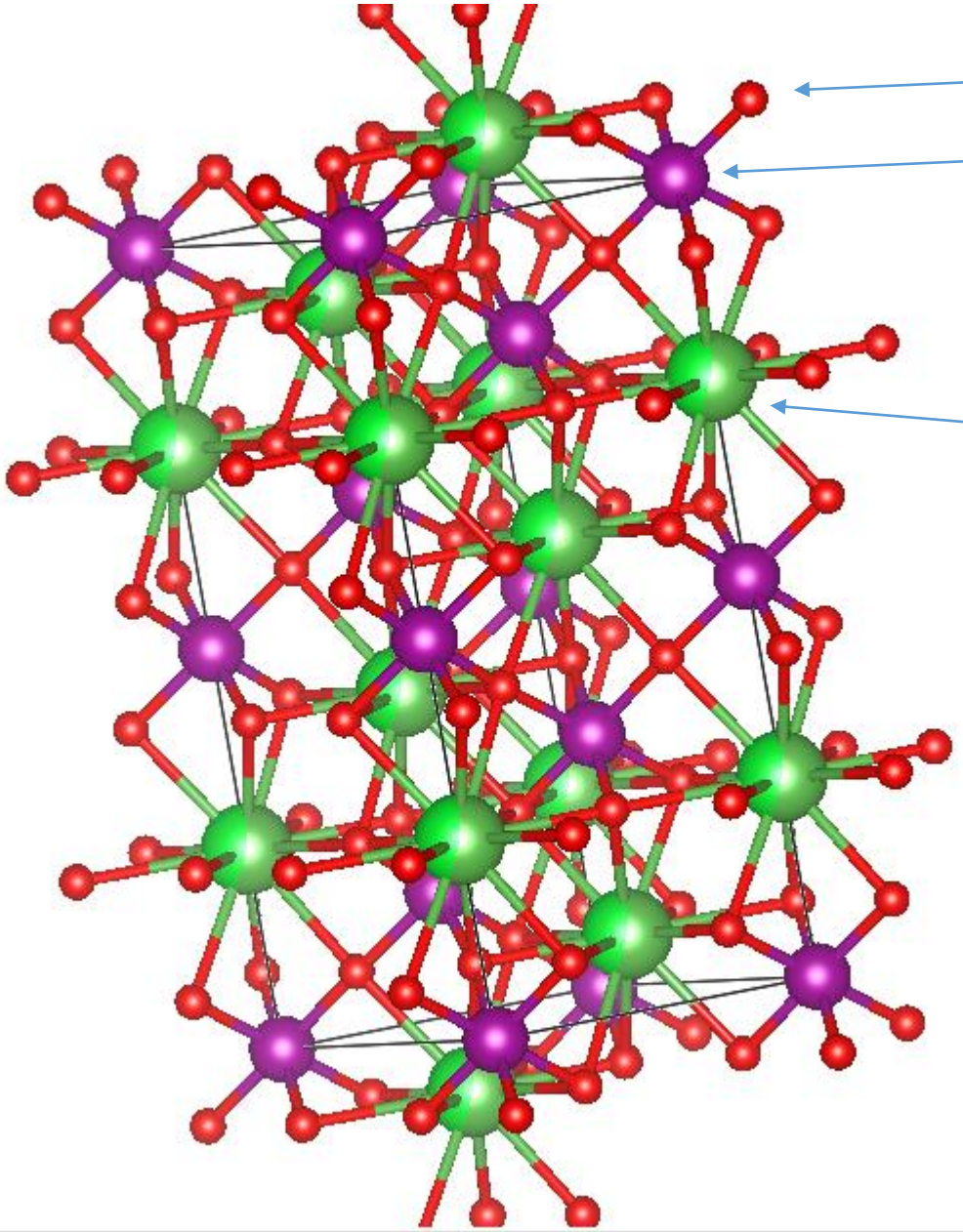

LPCM-70 , T=15 K, DN-12-Dubna2017
la0_53sr0_47mno3.PRF:
1. Yobs
2. Ycalc
3. Yobs-Ycalc
4. Bragg_position
Intensity (arb. units)
190
160
130
100
70
40
10
0
10000
20000
30000
40000
50000
t.o.f. (μ sec.)

LPCM-70 , T=15 K, DN-12-Dubna2017



LPCM-70 , T=320 K, DN-12-Dubna2017





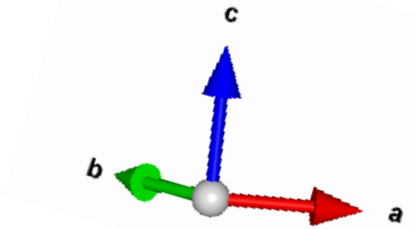


Table: Crystal structure parameters of $La_{0,53}Sr_{0,47}MnO_3$ obtained at temperature T – 320K

Lattice parameters	**[Å]**		
a,b	5,414 (1)		
c	13,258 (1)		
Atomic coordinates	**X**	**Y**	**Z**
La/Sr	0,0000	0,0000	0,2500
Mn	0,0000	0,0000	0,0000
O	**0,4725**	0,0000	0,2500
Calculated angle Mn – O – Mn			
α	171, 093 °		
Calculated distance between Mn – O	**[Å]**		
d	1, 9193		

SUMMARY OF THE PROJECT

The aim of study was:

- ✓ to get to know the main methods used neutrons as instrument for study condensed matter,
- ✓ find out how to perform neutron diffraction experiments and treating the experimental data using Rietveld method,
- ✓ how to realized processing of experimental data in the software FullProf,
- ✓ to define the most important crystal and magnetic structure parameters of the complex oxide $La_{1-x}Sr_xMnO_3$ by means of FullProf.

THANK YOU FOR YOUR ATTENTION ☺