Crystal and Magnetic Structure of Advanced Oxide Materials: Neutron Diffraction Studies

Supervisors

Prof. Sergey Kichanov & **Dr. Bulat Bakirov**

Dubna, Russia, 15 – 03 June 2023

Teamwork

Ahmed Farrag Mohamed
South Valley University

Ahmed Abdellattife Ahmed
Ain-Shams University

Mahmoud Ali Salim
Helwan University

Moamen Ragab Ali
National Institute of Standards

Outline

1 AIM AND OVERVIEW

2 CRYSTAL AND MAGNETIC STRUCTURE

3 RIETVELD REFINEMENT

4 RESULTS AND DISCUSSIONS

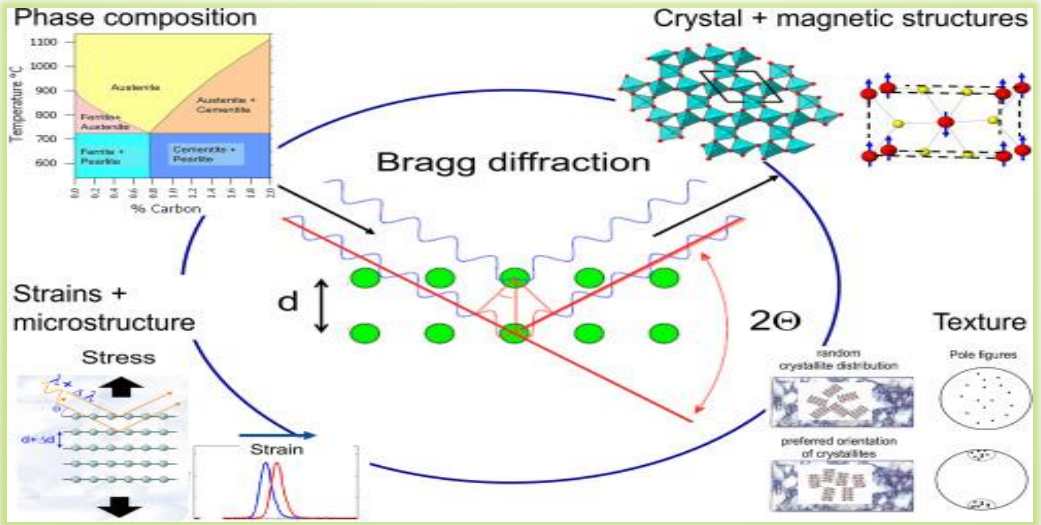
5 CONCLUSIONS

6 ACKNOWLEDGEMENTS

Aim of Practice

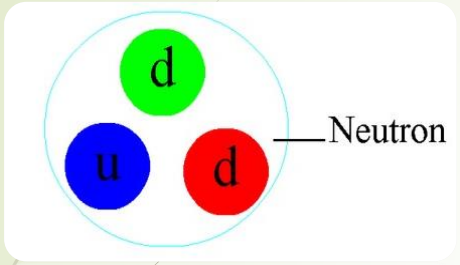
- Study structural and magnetic properties of doped ferrite $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ using neutron diffraction method at high pressures up to 4.7 GPa and in temperature range 300–425 K;

- Obtain the lattice parameters, magnetic moments of iron ions as functions of temperature and pressure.



Overview

What is neutron?!



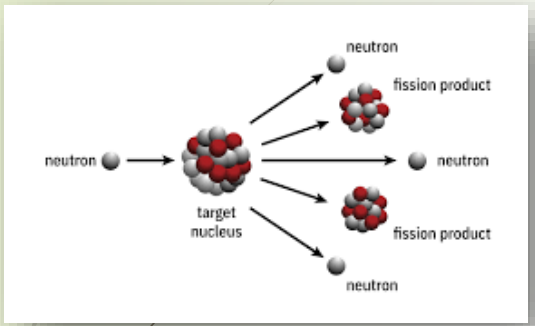
$m_n \approx 1.675 \cdot 10^{-24}$ g
$\mu_n \approx -1.9131 \cdot \mu_N$
$\mu_N = eh/2m_pc$
$J = 1/2$

Neutron types

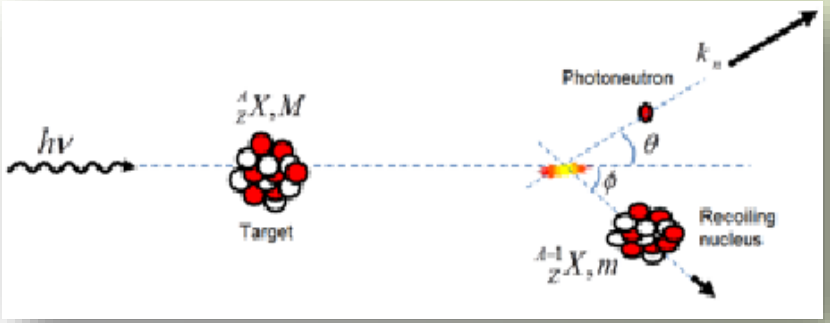
Type of neutrons/ Characteristics of neutrons	Ultracold	Cold	Thermal	Epithermal
Energy, meV	0.25 μeV	1	25	1000
Temperature, K	3mK	12	290	12000
Wavelength, Å	570	9	1.8	0.29
Velocity, m/s	6.9	440	2200	14000

Overview

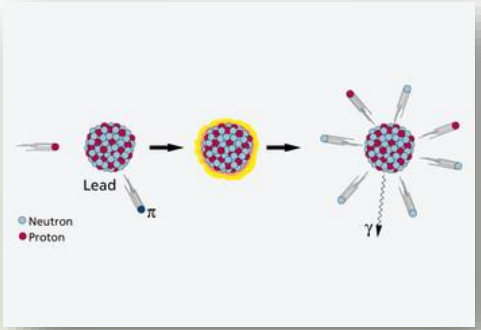
How can we obtain neutron?!



1. Fission reaction



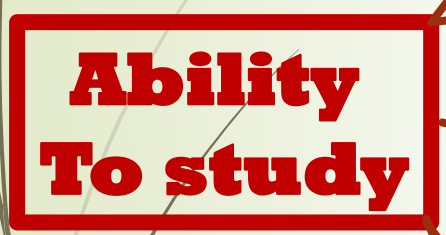
2. Photonuclear reaction



3. Spallation reaction

Overview

Why neutrons?!



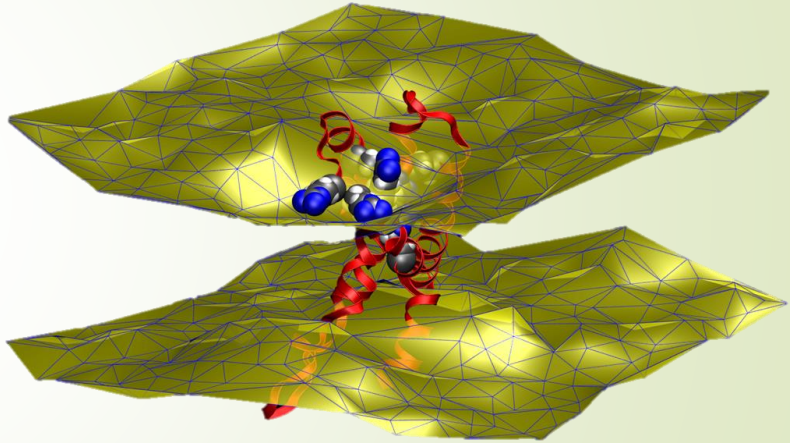
- The bulk properties of objects;
- Localize light atoms accurately;
- Structure of condensed matter and its changes under the influence of external influences;
- Atomic and molecular dynamics;
- Aagnetic structure and magnetic dynamics.

Overview

What is the Neutron Diffraction?!

- Application of neutron scattering to the determination of the atomic and/or magnetic structure of a material.

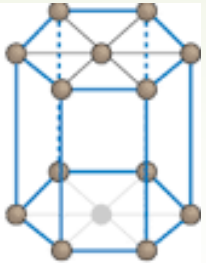
- A sample to be examined is placed in a beam of thermal or cold neutrons to obtain a diffraction pattern that provides information of the structure of the material.



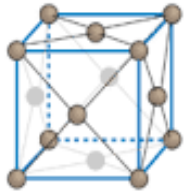
Crystal structure

The 7 crystal systems :

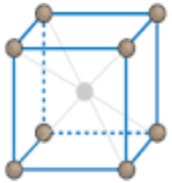
Cubic, Hexagonal, Tetragonal, Trigonal, Orthorhombic, Monoclinic, Triclinic.



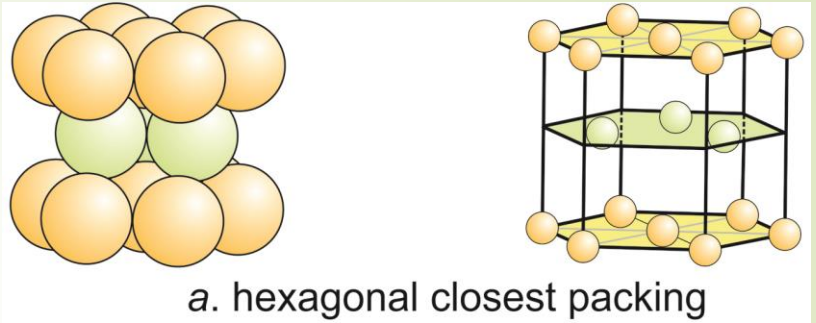
Hexagonal
Ti, Zn, Mg, Cd



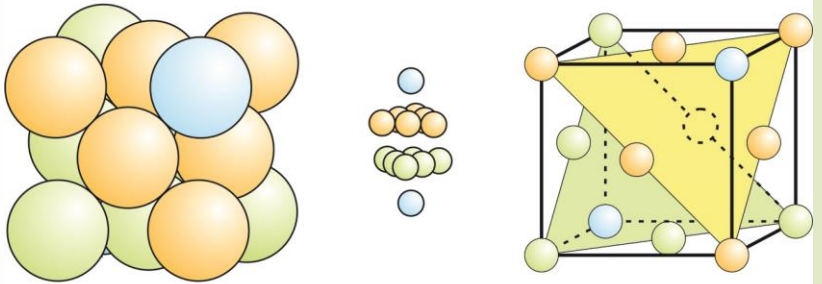
Cubic face centered (fcc)
Al, Ni, Aq, Cu, Au



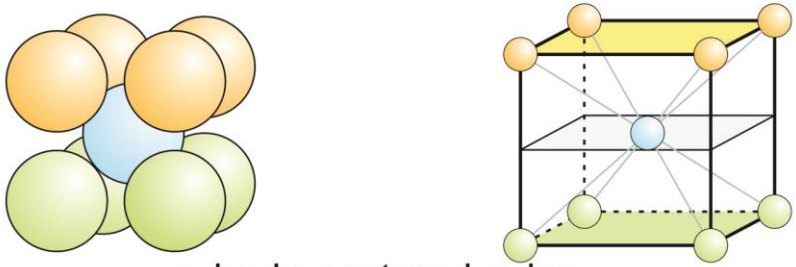
Cubic body centered (bcc)
Fe, V, Nb, Cr



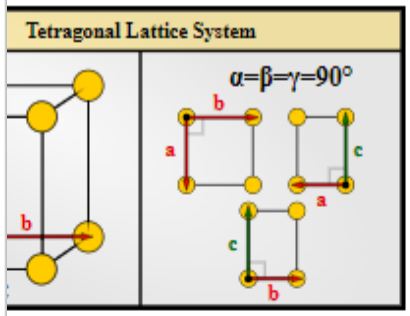
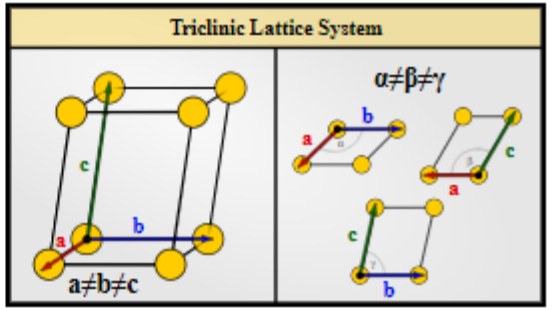
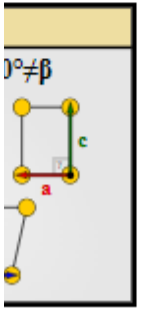
a. hexagonal closest packing

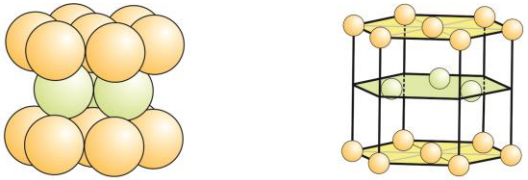


b. cubic closest packing

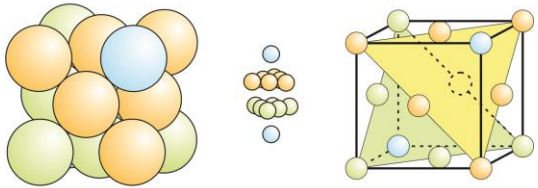


c. body-centered cube

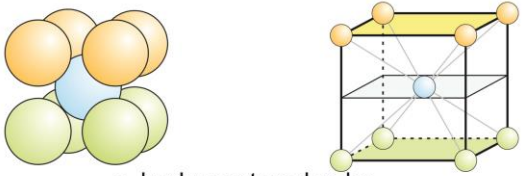
Basic Lattice Systems			Basic Lattice Systems			
Cubic	Tetragonal	a=	Cubic	Tetragonal		
Hexagonal	Orthorhombic	a≠	Hexagonal	Orthorhombic	α≠β≠γ	
Rhombohedral	Monoclinic	a≠	Rhombohedral	Monoclinic	Triclinic	



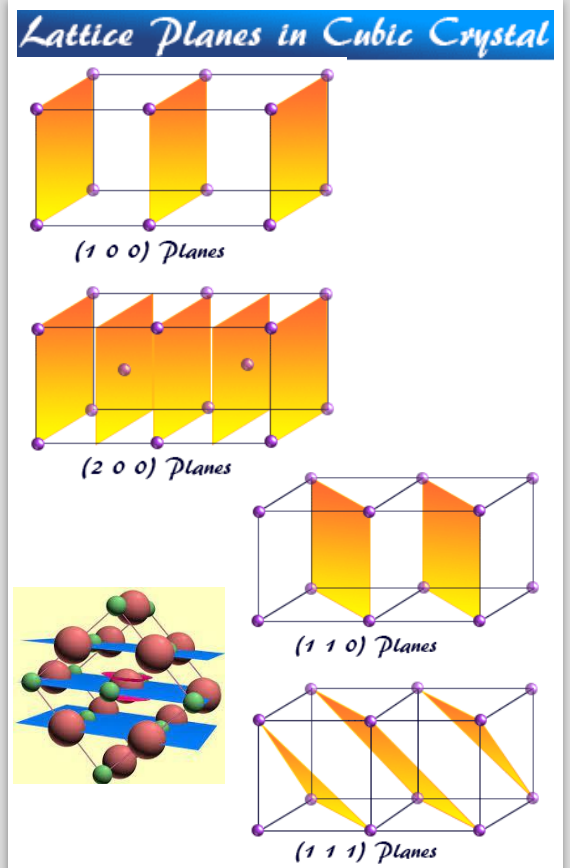
a. hexagonal closest packing

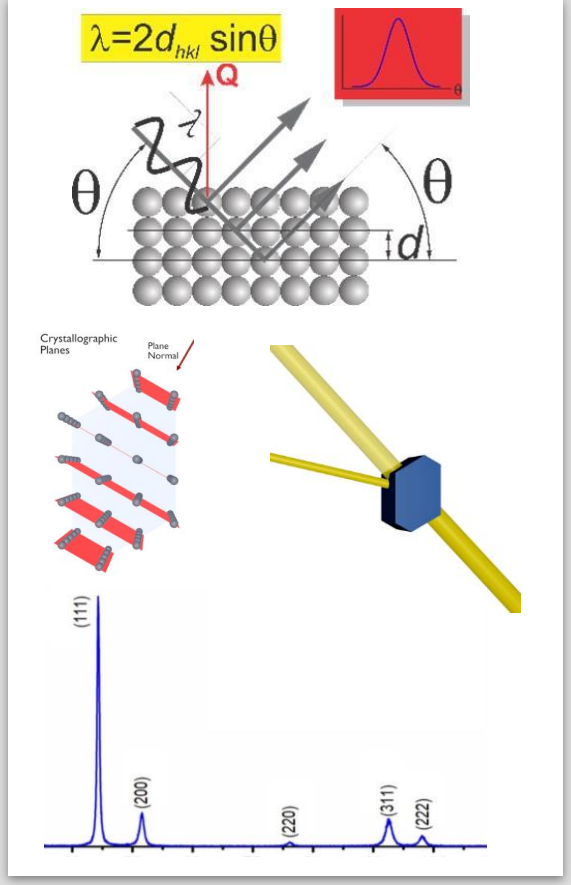


b. cubic closest packing

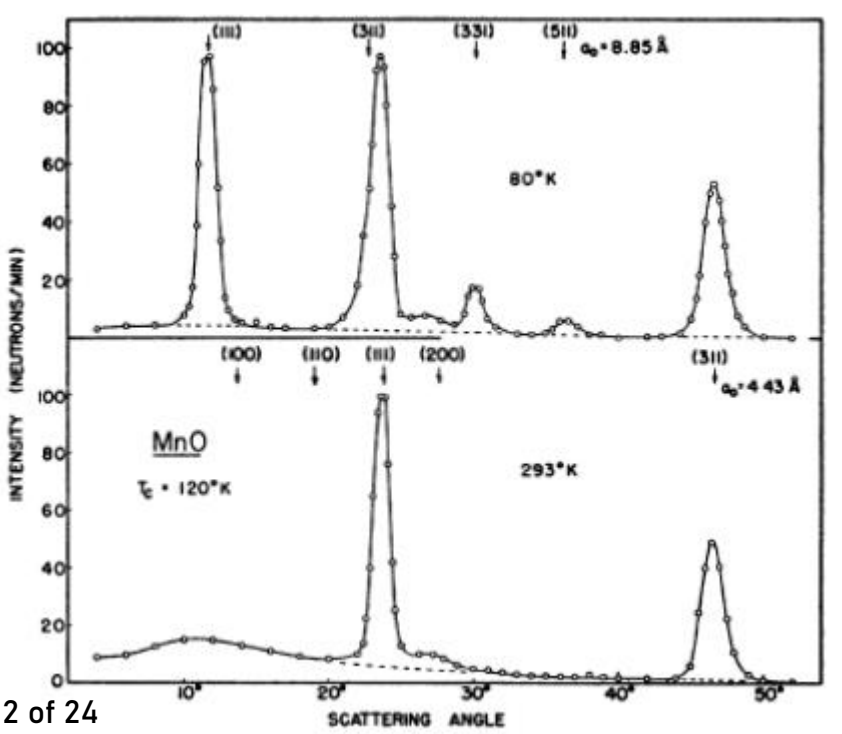


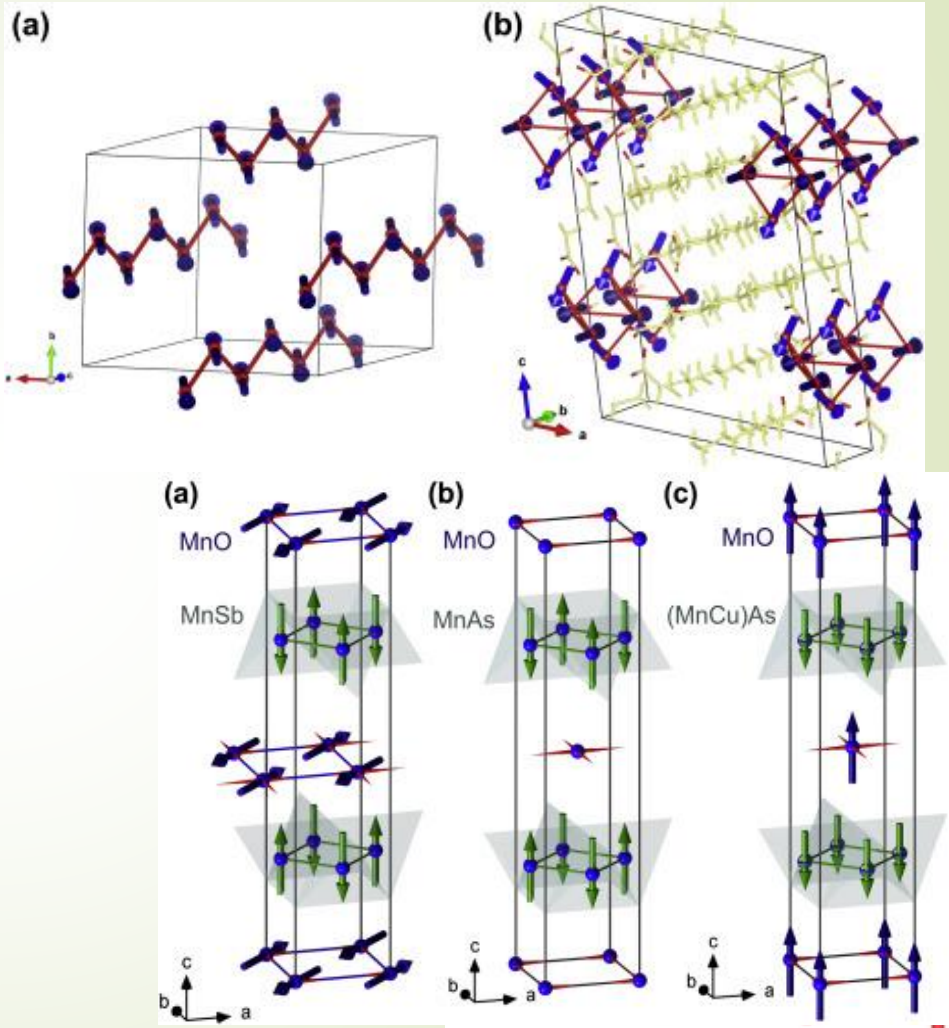
c. body-centered cube

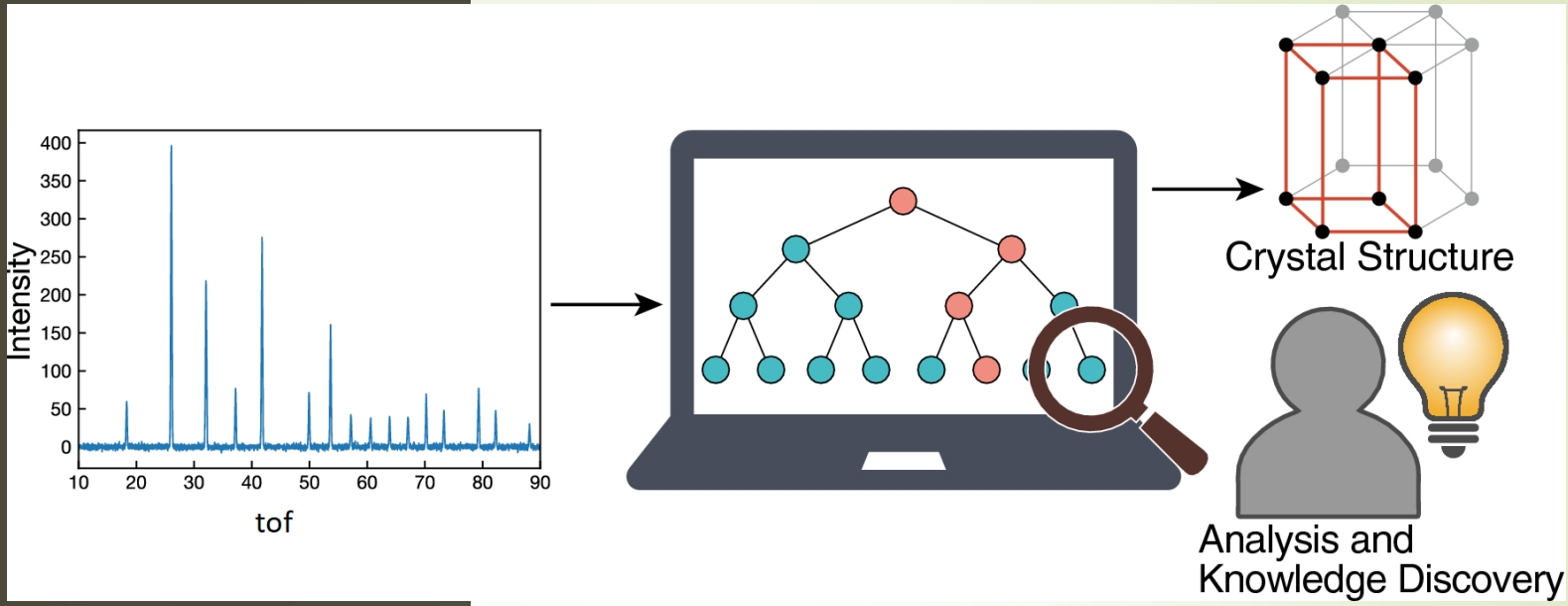




Magnetic structures







Phase analysis

Rietveld Refinement

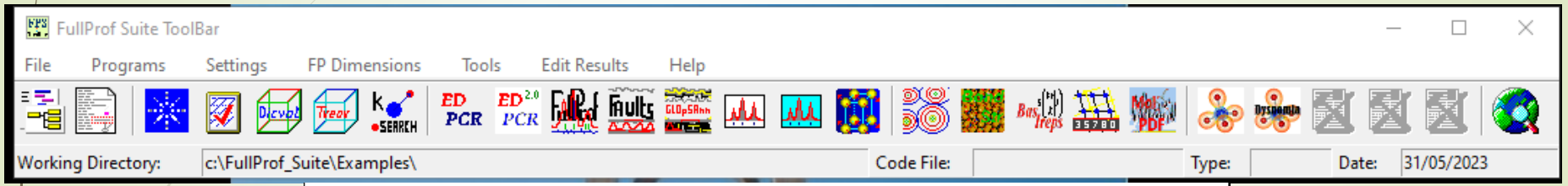
Refinement technique, most commonly employed today, is based on the idea suggested in the middle 1960's by Rietveld method that is known as full pattern refinement or whole-pattern fitting.

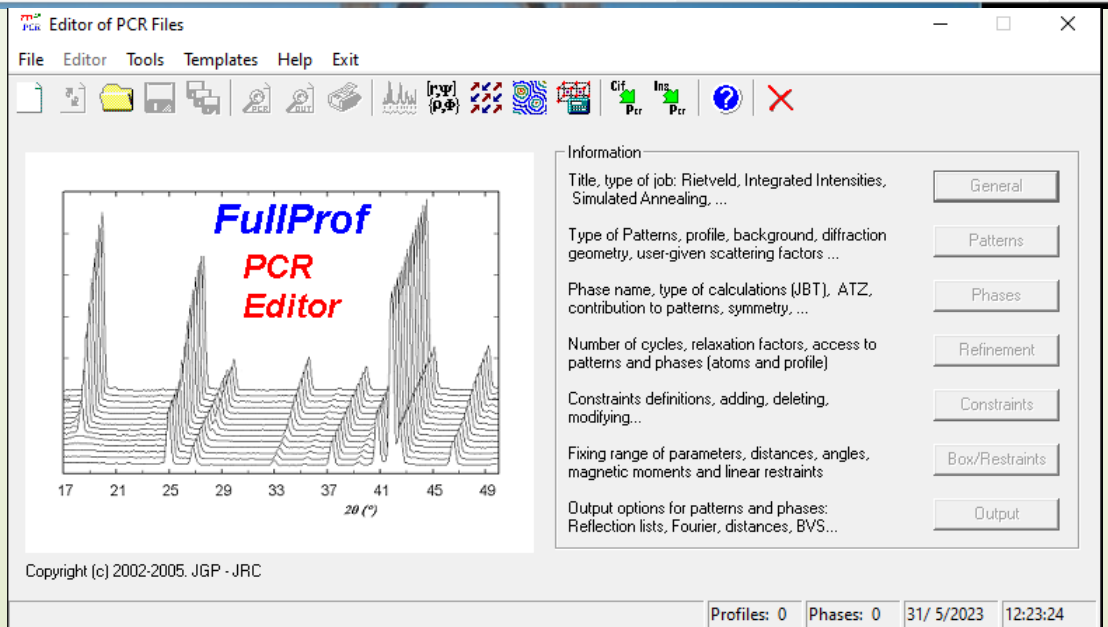
Available Rietveld Refinement Softwares

- GSAS & FullProf
- MAUD & Rietica
- Rietan & BGMN
- PSSP

Rietveld Refinement

FullProf program





Rietveld Refinement

Features of FullProf

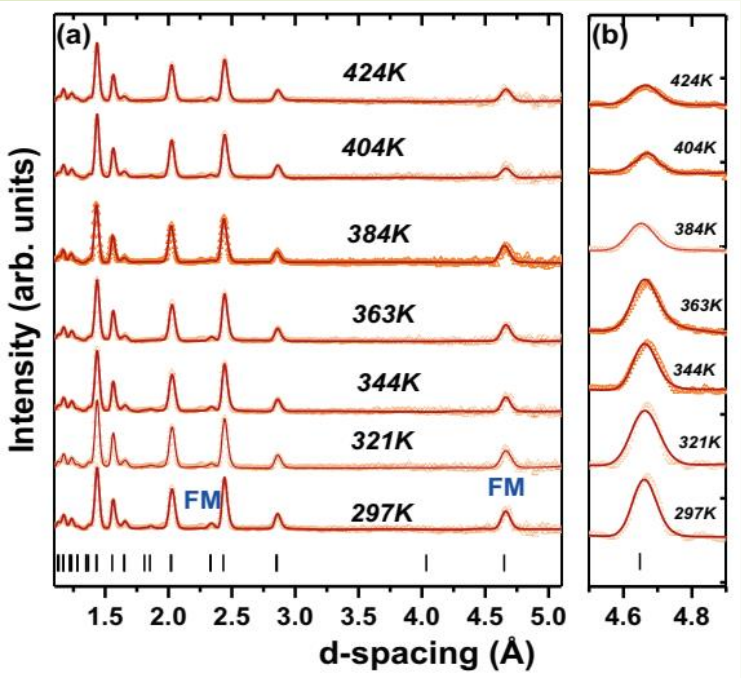
- Calculation of X-ray and synchrotron data.
- Neutron diffraction data: obtained by the constant wavelength method and the time-of-flight method.
- Data obtained on single- and polycrystals.
- One or two wavelengths of radiation. The scattering variable can be 2Q angle in degrees, in microseconds (time-off light method), and as energy in KeV.

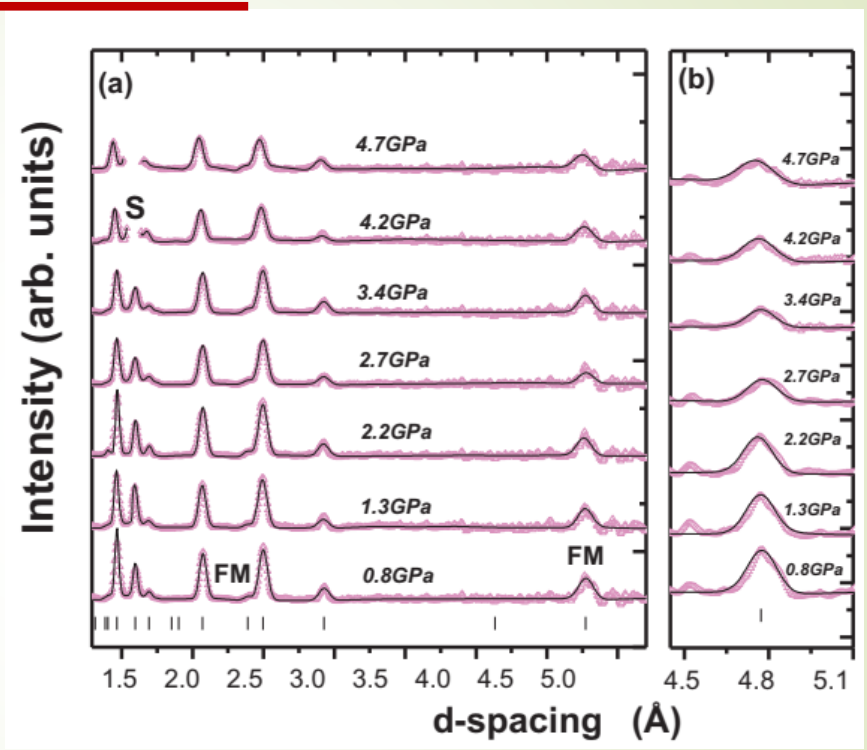
Rietveld Refinement

Features of FullProf

- Selection of functions for describing the shape of reflections: Gaussian, Lorentzian, modified Lorentz, Psefdo-Voit, Pearson-2, Thompson-KochNastings.
- Choice of background in the diffraction pattern: fixed and refined.
- Calculation of up to 16 different phases.
- Accounting for texture, correction for the absorption of incident radiation.
- Calculation of the crystal structure.
- Calculation of the magnetic structure: commensurate and incommensurable.

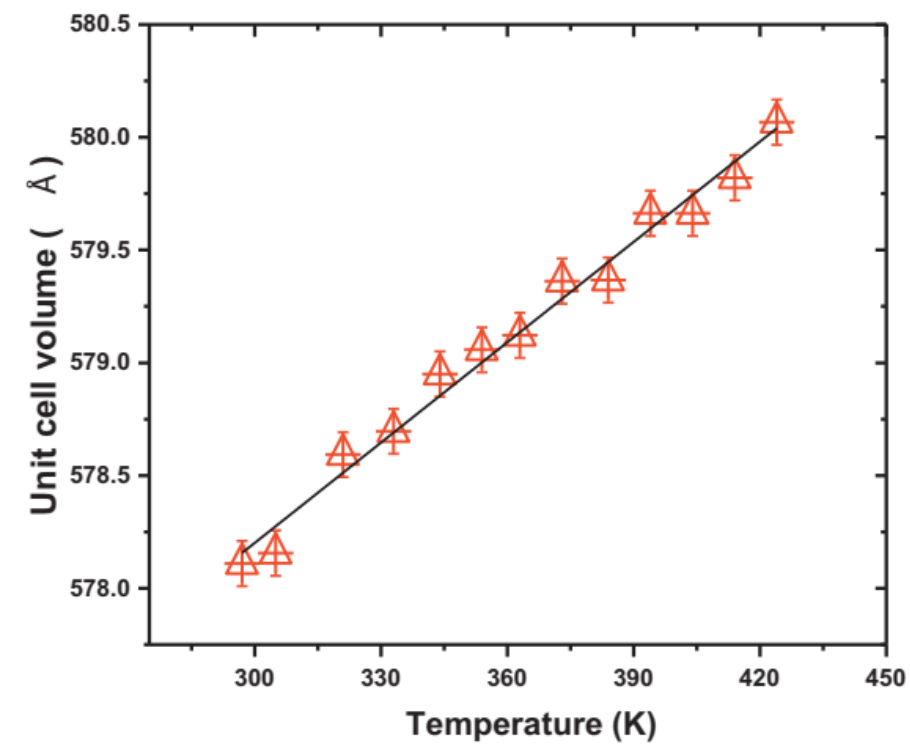
Results and Discussions





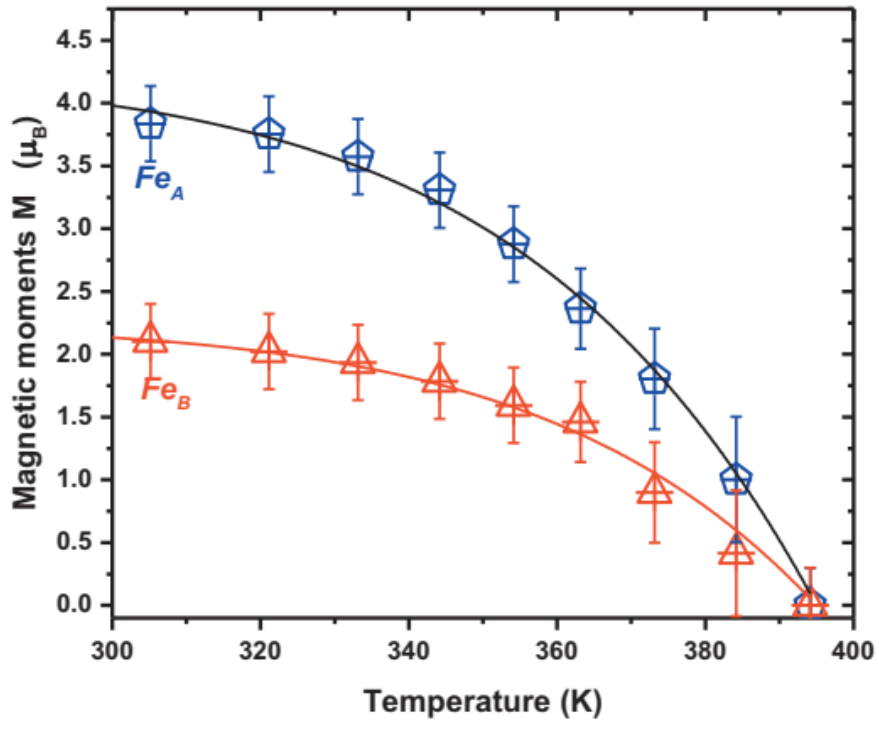
Neutron diffraction patterns of compound measured at selected temperatures up to 424 K, different pressures up to 4.7 GPa at room temperature, processed by the Rietveld method

Results and Discussions

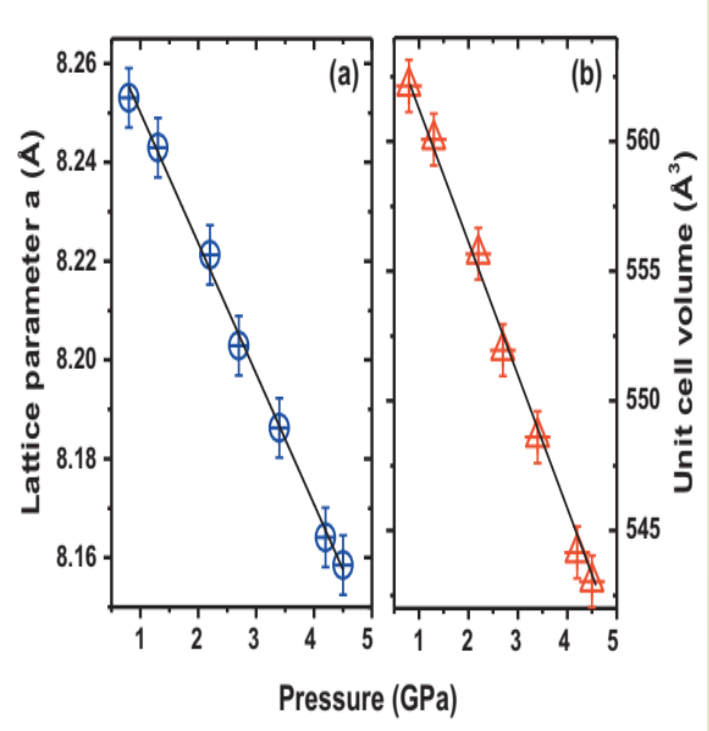


Temperature dependence of the unit cell volume of $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ spinel. The solid line is linear fit of experimental data.

Results and Discussions



Temperature dependences of the magnetic moments of iron ions FeA and FeB located in A and B sites.



The pressure dependence of the cubic lattice parameter and unit cell volume of $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ compound

Conclusions

- Neutron Diffraction mechanism and Rietveld refinement using Fullprof software were studied.
- Crystal and magnetic structure of $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ at high pressure and different temperatures using the neutron diffraction technique were also studied.
- Results revealed that a remarkable instability of the ferrimagnetic state with respect to the application of high pressure.

Web Sources

- https://flnph.jinr.ru/en/
- https://www.sciencedirect.com/science/article/abs/pii/S0304885317328925
- http://ccp14.cryst.bbk.ac.uk/ccp/web-mirrors/fullprof/
- https://www.wikipedia.org/

ASRT-Egypt

JINR-Russia

ASRT-Egypt

Thank You Supervisors

شكراً

Большое спасибо


ANY
QUESTIONS?