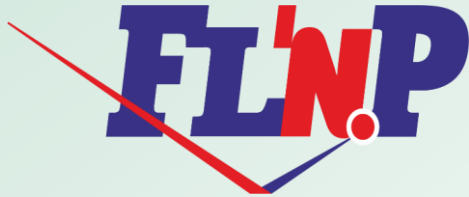


**The XXVI International Scientific Conference of Young  
Scientists and Specialists (AYSS-2022)**



**Phase transition of nanostructured zinc  
ferrite spinel at high pressure**

N.M. Belozerova, D.P. Kozlenko, S.E. Kichanov, E.V. Lukin and  
B.N. Savenko

**Dubna, 2022**

# Plan

## 1. What are complex oxides of iron?

- Ferrites are perspective compounds
- Brief description of structure and physical properties of complex oxides of iron

## 2. Neutron diffraction experiment

- Experimental method
- Crystal and magnetic structure of  $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$  in wide temperature range

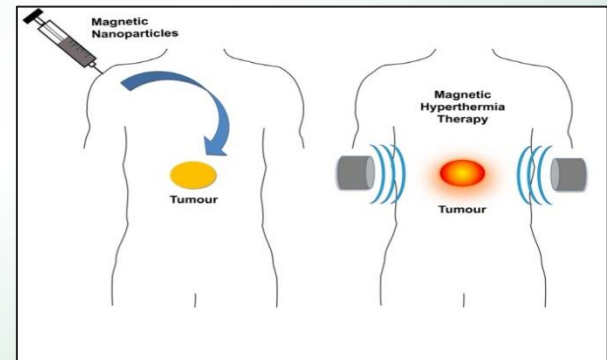
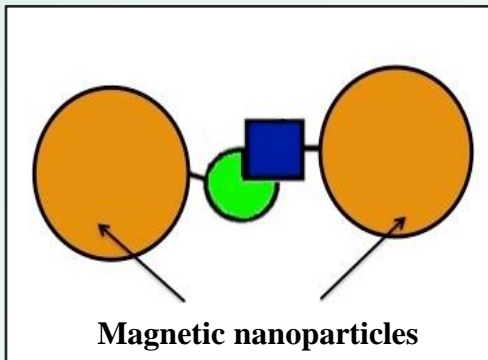
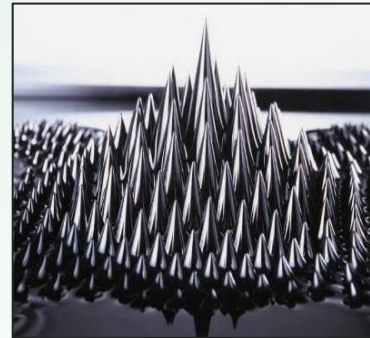
## 3. X-ray diffraction experiment

- Experimental method
- Crystal structure of  $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$  in wide pressure range

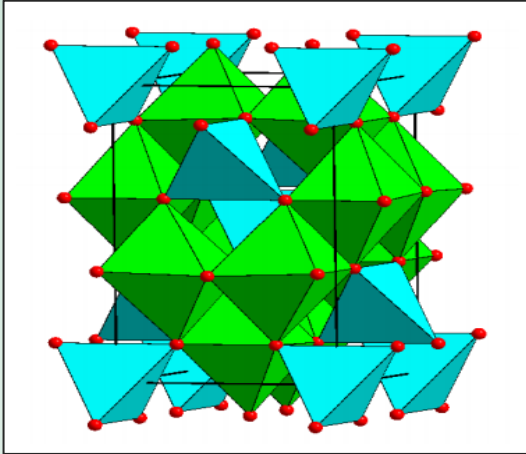
## Summary

# Complex iron oxides applications

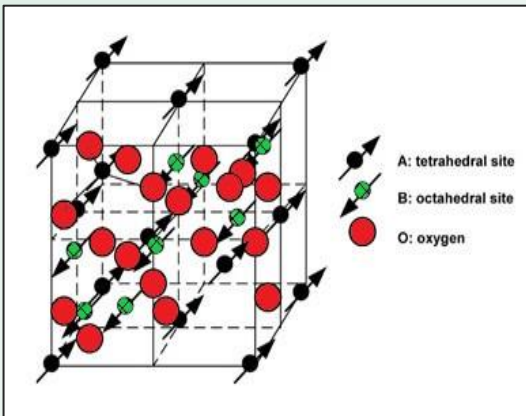
- ✓ Significant saturation magnetization
- ✓ High electrical resistivity
- ✓ Low electrical losses
- ✓ High chemical stability



# Structure and properties of complex iron oxides



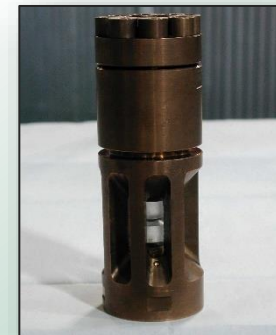
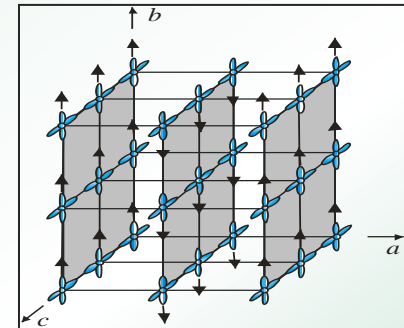
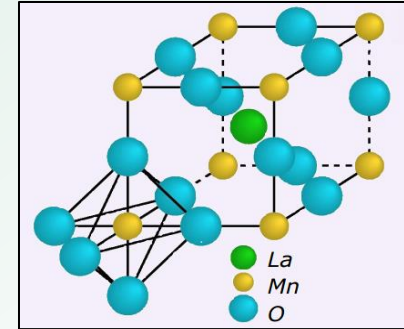
The spinel structure ( $AB_2O_4$ ) is represented by the densest face-centered cubic lattice. Metal cations are distributed between two crystallographic positions: **tetrahedral (A-site)** and **octahedral (B-site)**.



The magnetic properties of spinel ferrites is forming by the exchange interaction between the electrons of the ions in the A and B sublattices. Usually, the **A - B interaction** is the strongest. The **A - A interaction** is almost ten times weaker, and the **B - B interaction** is the weakest. The dominant interaction A - B leads to **ferrimagnetic ordering**.

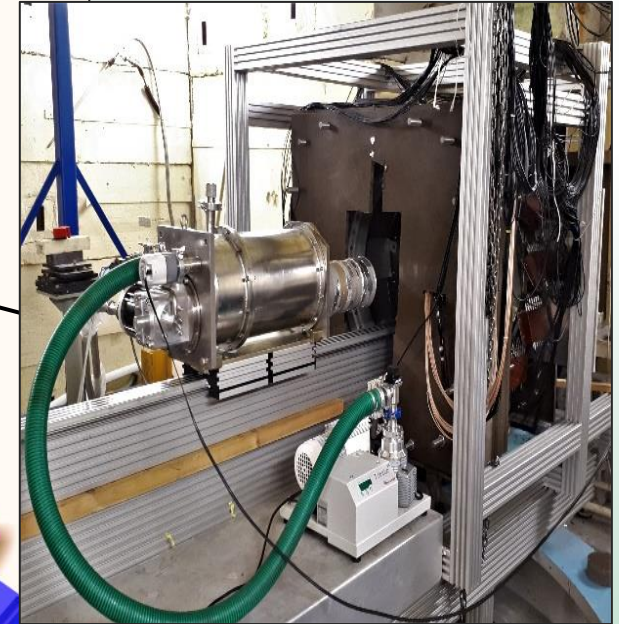
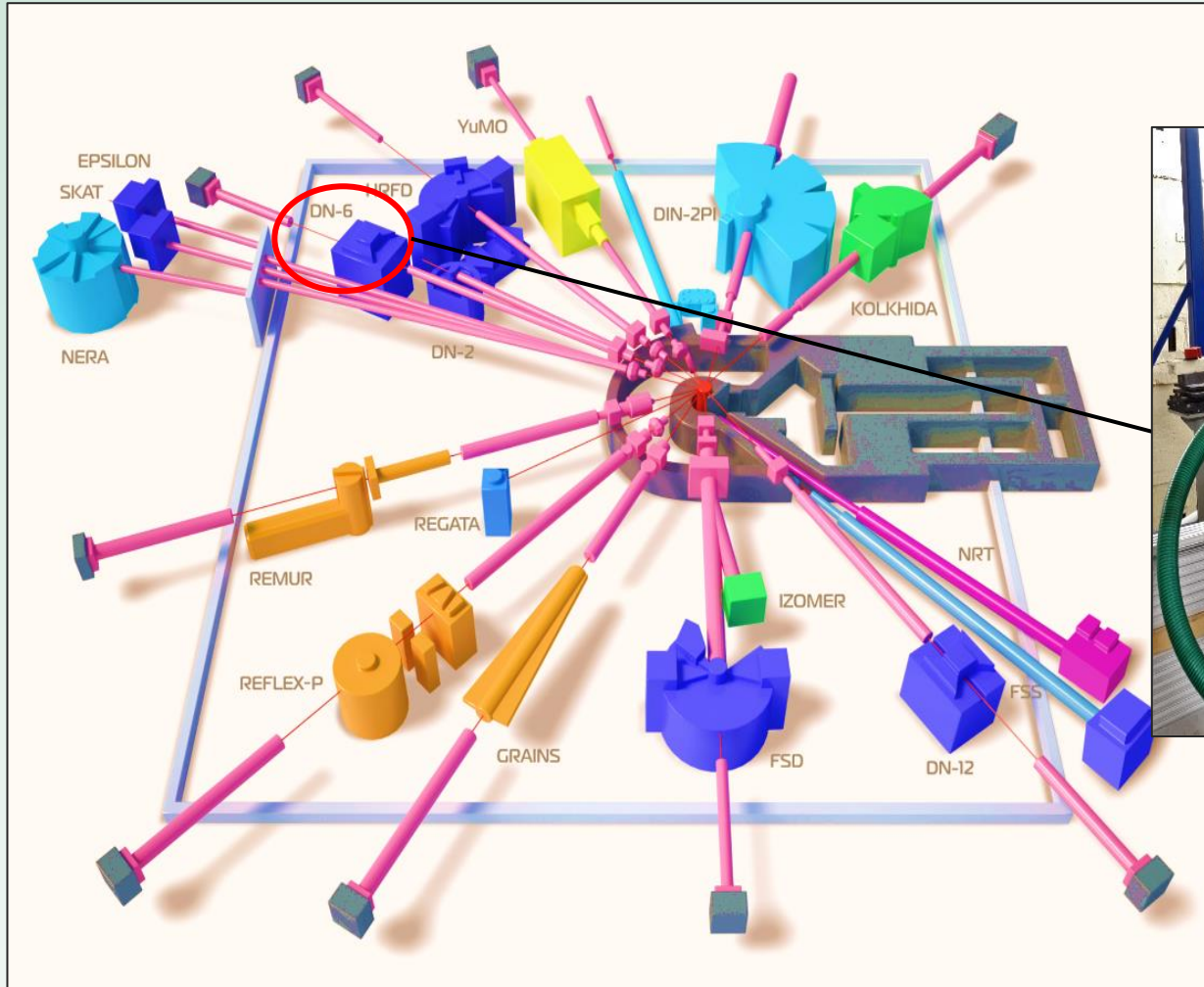
# Experimental method: Neutron Diffraction

- Neutron is **sensitivity to the light atoms** such as oxygen. It is give as opportunity to determine location of oxygen with precision.
- Another advantage of the neutron is **sensitivity to the magnetic structure** and dynamics of the magnetic substance.
- An important is the **high penetrating power of neutrons**, which gives opportunities for working with high-pressure cells and devices for changing the temperature on the sample.

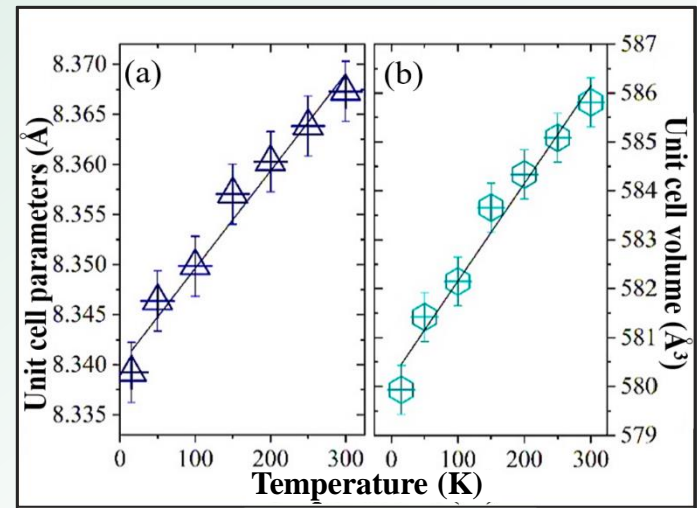
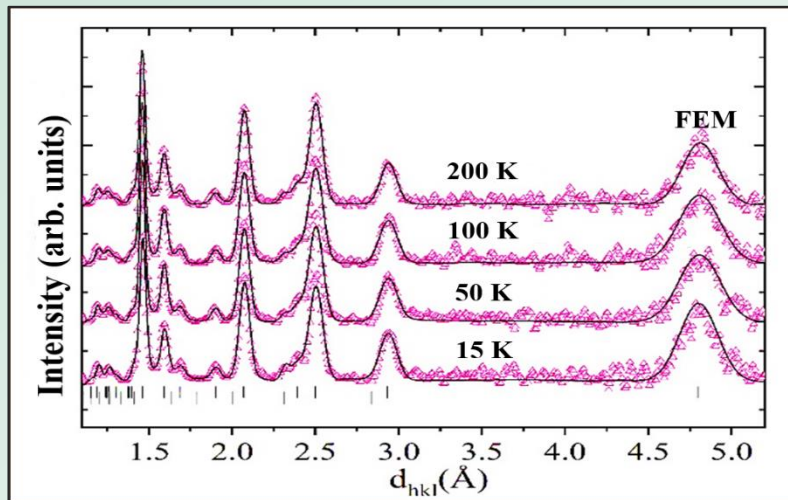




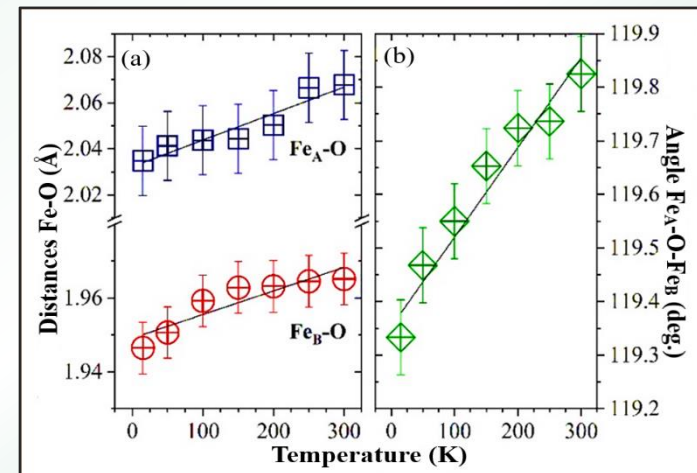
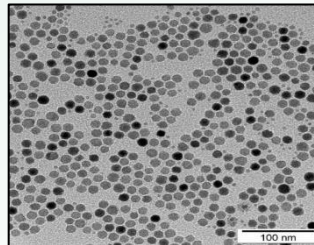
# Experimental method: Neutron diffractometer DN-6



# Crystal structure of ferrite $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$ in wide temperature range

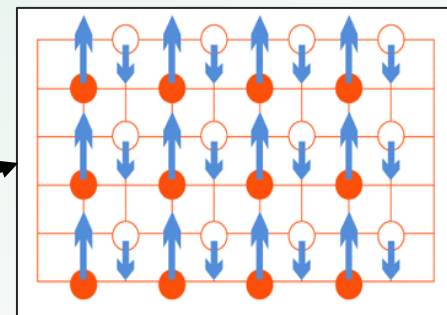
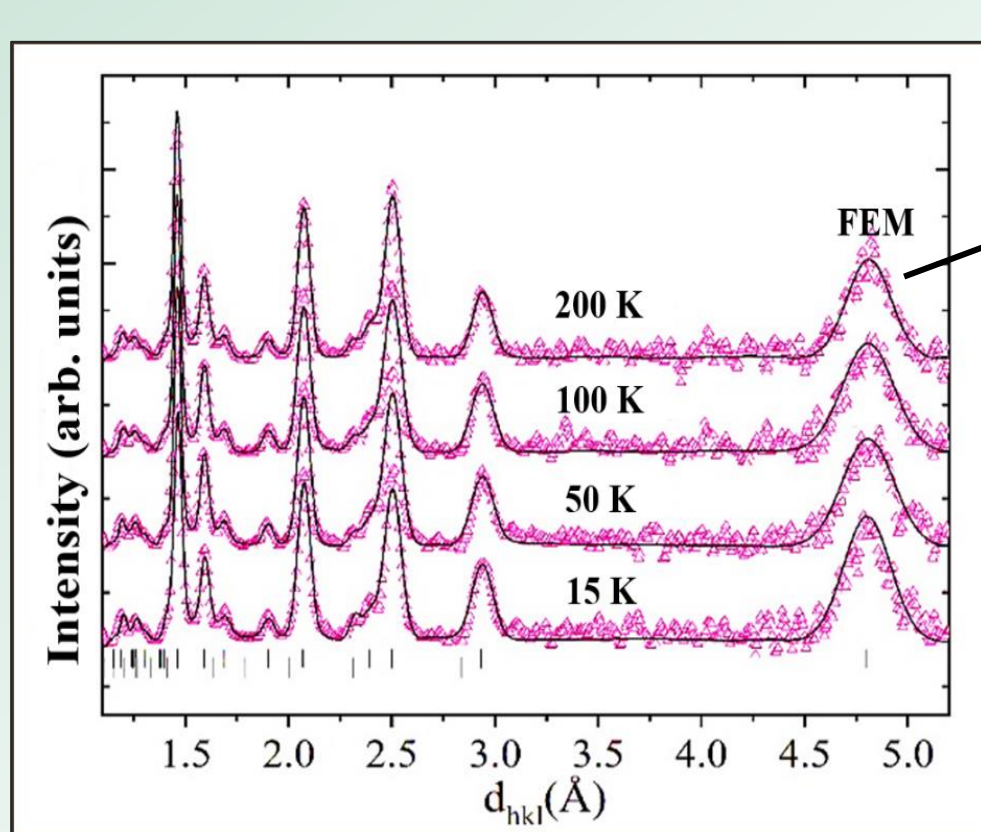


Unit cell parameters		
<b>a, Å</b>		8.331(3)
<b><math>\alpha</math>, K<sup>-1</sup></b>		$1.26(2) \cdot 10^{-5}$
Atomic occupations		
<b>A site:</b>	Zn	0.18(1)
	Fe	0.82(2)
<b>B site:</b>	Zn	0.16(1)
	Fe	1.71(3)
	vacancy	0.13(2)



Belozerova N.M., Kichanov S.E., Kozlenko D.P., et al., Neutron diffraction study of the crystal and magnetic structures of nanostructured  $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$  ferrite. *Journal of Nanoparticle Research*, 22(5), 1-9 (2020).

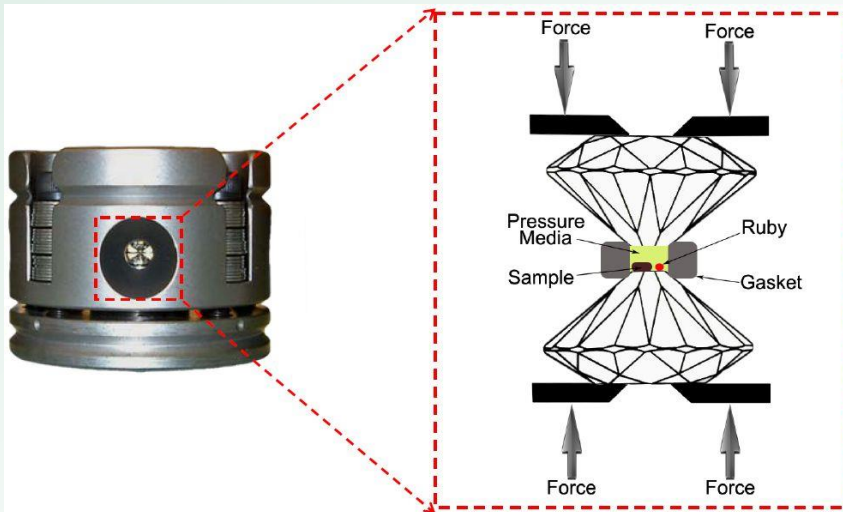
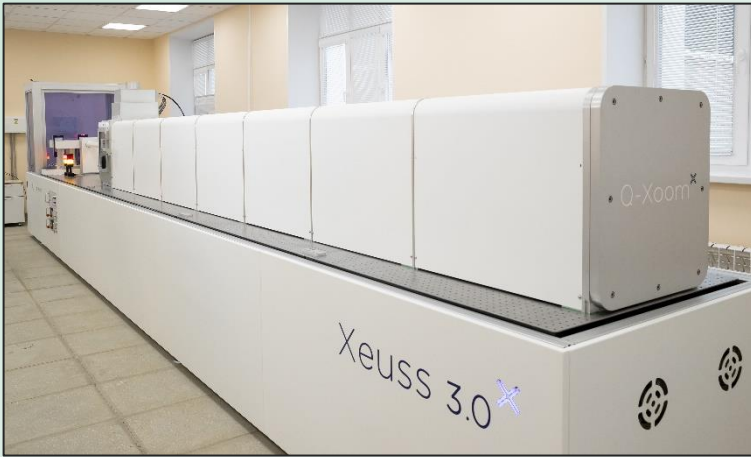
# Magnetic structure of ferrite $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$ in wide temperature range



Magnetic moment			
T=15 K		T=300 K	
$M_A, \mu_B$	3.1(4)	$M_A, \mu_B$	2.7(4)
$M_B, \mu_B$	3.9(4)	$M_B, \mu_B$	3.6(4)

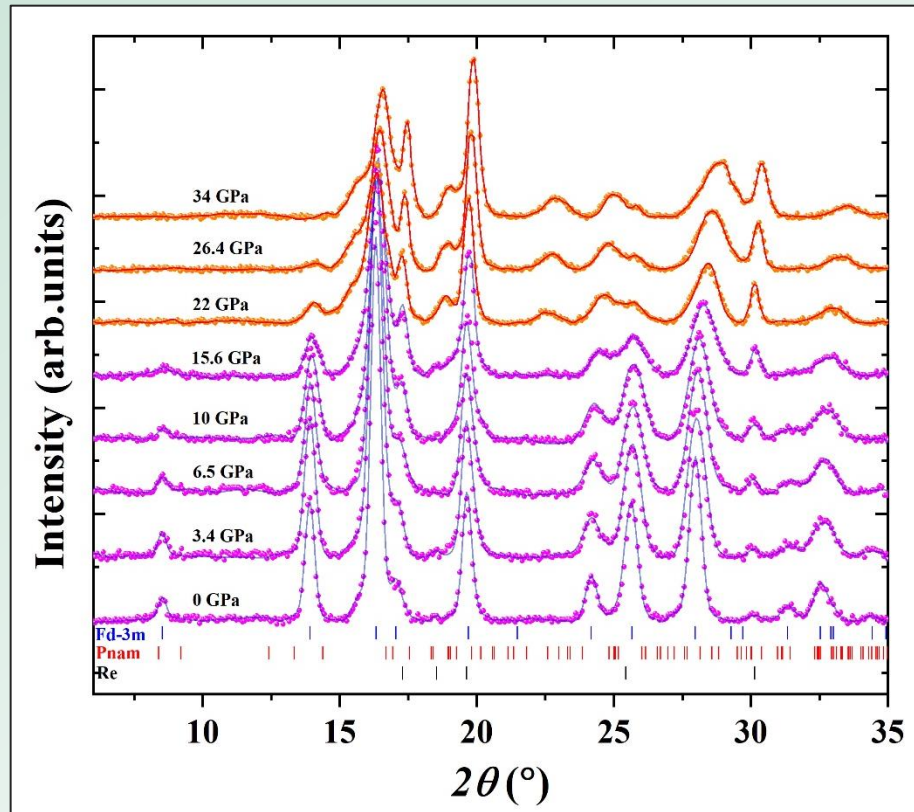


# Experimental methods: X-ray diffraction under high pressure

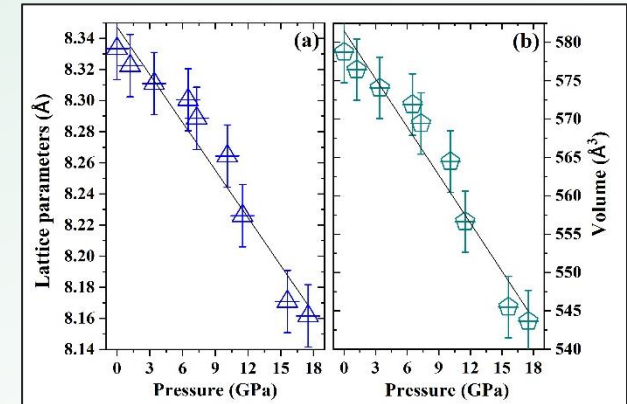


Maximum pressure is **50 GPa**

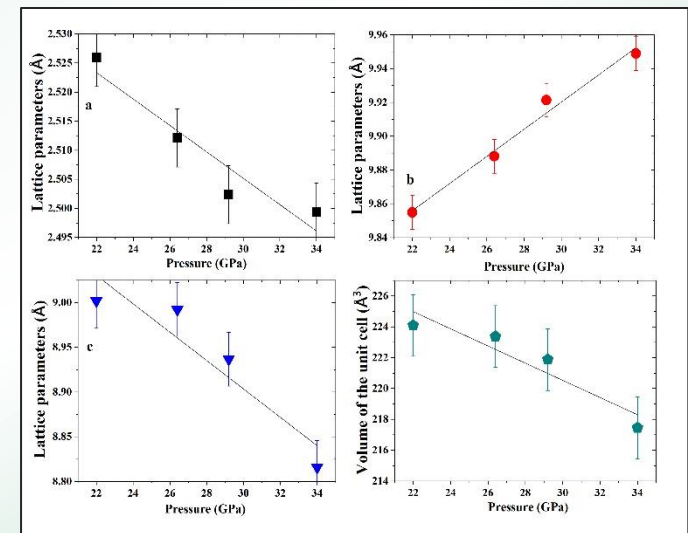
# Crystal structure of ferrite $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$ in wide temperature range



**Fd-3m**



**Pnam**



# Summary

1. **Crystal structure** of ferrite  $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$  presented by the mixed spinel cubic structure with space group Fd-3m **remains stable** in all studied temperature. The most important parameters of crystal structure were obtained.
2. The presence of **vacancies** in octahedral positions of the crystal structure of nanostructured ferrite  $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$  was established.
3. **Magnetic structure** of nanostructured ferrite  $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$  presented by **ferrimagnetic** ordering **remains stable** in wide temperature range.
4. **Phase transition** from initial phase with cubic structure (Fd-3m) to high pressure phase with orthorhombic structure (Pnam) was found in ferrite  $\text{Zn}_{0.34}\text{Fe}_{2.53}\square_{0.13}\text{O}_4$  at pressure above 18GPa.

# Thank you for attention!

**E-mail:**

**nmbelozerova@jinr.ru**

**Used article:**

Belozerova N.M., Kichanov S.E., Kozlenko D.P., et al. Neutron diffraction study of the crystal and magnetic structures of nanostructured  $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$  ferrite// Journal of Nanoparticle Research. – 2020. – T. 22. – №. 5. – C. 1-9.

J Nanopart Res (2020) 22:121  
<https://doi.org/10.1007/s11051-020-04852-4>

RESEARCH PAPER

**Neutron diffraction study of the crystal and magnetic structures of nanostructured  $\text{Zn}_{0.34}\text{Fe}_{2.53}\text{O}_4$  ferrite**

**N. M. Belozerova**  • S. E. Kichanov • D. P. Kozlenko •  
O. Kaman • Z. Jiráček • E. V. Lukin • B. N. Savenko