Research on Magnetic and Nonmagnetic Biomaterials Using Neutron Techniques

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Outline

1) Areas of scientific interest and motivations
2) Tested materials and desired properties
3) Scientific aspects
4) Corresponding neutron techniques

Outlook

As to: Areas of scientific interest and motivations

a_1) magnetic nanoparticles coated by organic shell – spinels- biomedical applications - anticancer therapy (magnetic fluid hyperthermia);

a_2) nonmagnetic nanoparticles – polymers, biomedical applications – anticancer therapy (drug delivery);

b_1) nanofilters – spinles again, pro-ecological and industrial applications;

b_2) multiferroics in the form of cut monocrystalline disks with known orientation, belonging to the group of smart switch -type materials – instrumental and industrial applications.

As to: Tested materials and desired properties

CUBO-FERRITES

Fe_3O_4

ORTHO-FERRITES

Fe_2O_3

SUBSTITUTED:

Ga^{3+}, and M: La^{3+}, Tb^{3+}, Ce^{3+}, Ce^{4+}

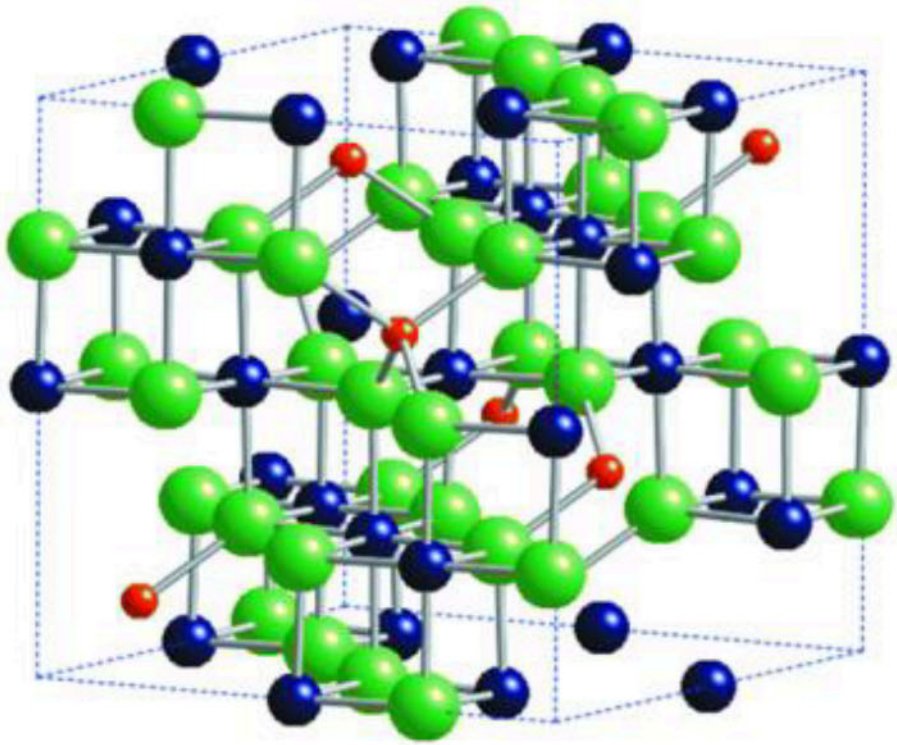
$Ga_xFe_{3-x}O_4$, $0<x<1$

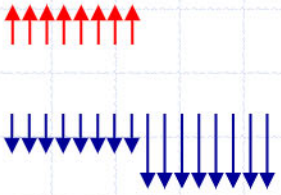
$M_\delta Fe_{3-\delta}O_4$, $0<\delta<0,02$ $Ga_{1\pm\delta}Fe_{1\pm\delta}O_3$

CUBO-FERRITES: Crystal and magnetic structures of gallium ferrites

$Ga_xFe_{2-x}O_4$ $Fd\bar{3}m$ (sg no. 227)

$Ga_xFe_{2-x}O_4 \times 8$





A – tetrahedral coordination:

Fe^{3+}(8a): (⅛, ⅛, ⅛), r_j = 64.5 pm

B – octahedral coordination:

Fe^{3+}/Fe^{2+}(16d): (½, ½, ½), r_j = 78 pm

O^{2-}(32e): (x, x, x), x~0.251, r_j = 140 pm

Ga^{3+}, r_j = 62 pm

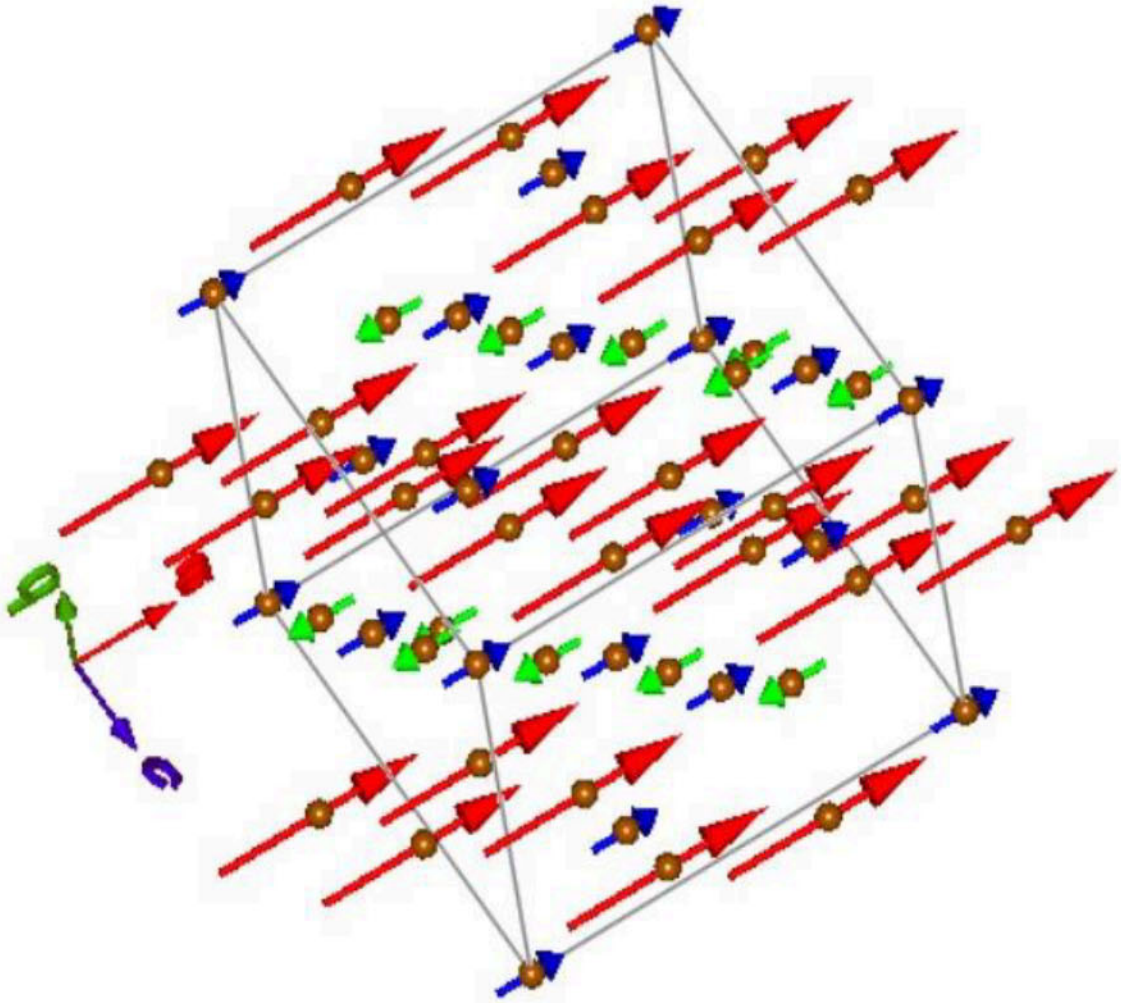
Lyubutin I S et al. J Phys Chem C 120 (44) 25596 (2016)

Rećko K et al. Phase Transitions 91 (2), 128 (2018)

Orzechowska M et al. International Journal of Molecular Sciences, 24 (18), p.14184 (2023)

Ga-SUBSTITUTED CUBO-FERRITES

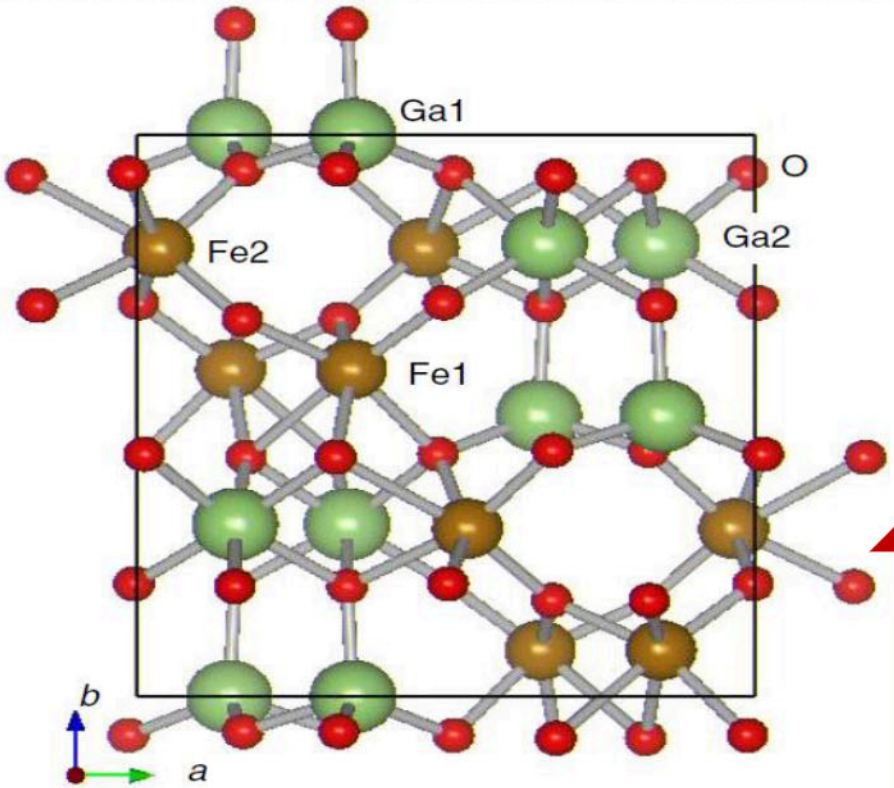
Spin ordering of $Ga_{0.6}Fe_{2.4}O_4$

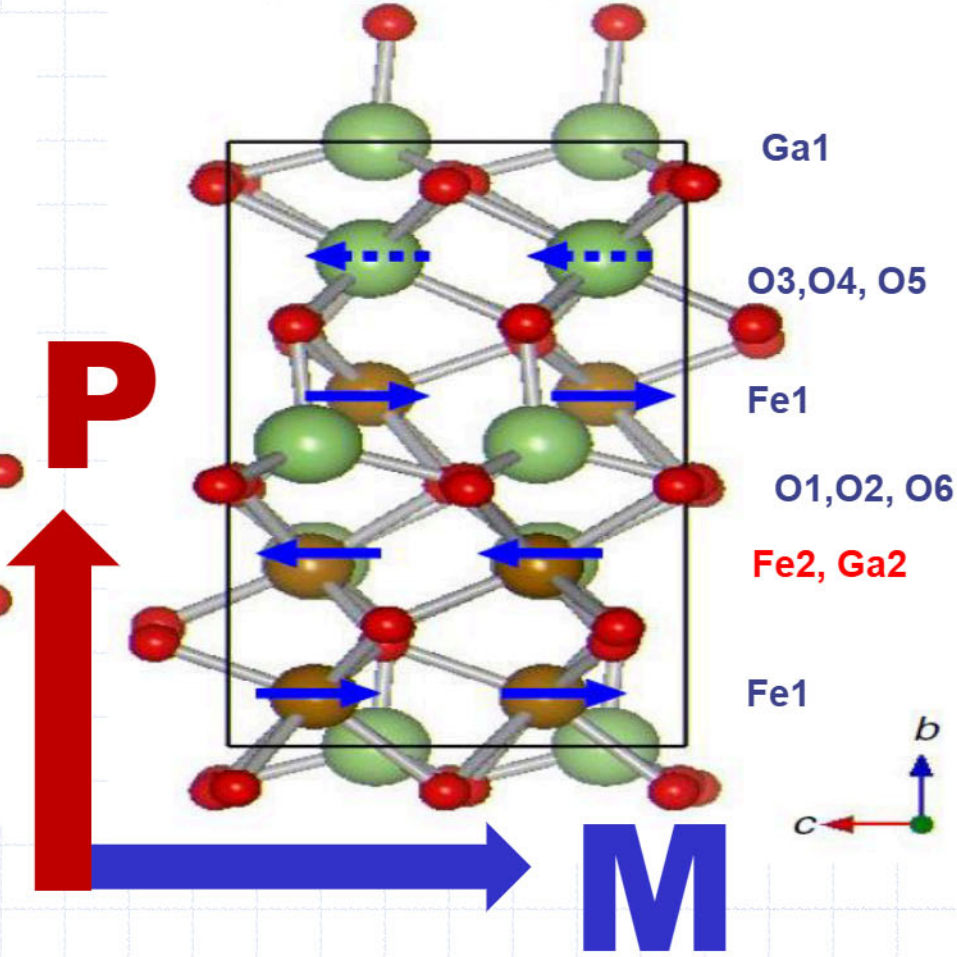


The nanosized (LT) ferrimagnetic and (HT) superparamagnetic particles are magnetocaloric agent with high biocompatibility and SAR coefficient.

Simultaneous analysis of X-ray and neutron diffraction data clearly indicates the preferred location of Ga in the A-tetrahedral sublattice.

ORTHO-FERRITES: Crystal structure $Pc2_1n$ (no. 33)





Polarization vs. the crystal structure

$Pc2_1n$ => $P_z > 0$ (59 $\mu C/cm^2$)

$Pnna$ => $P_z = 0$

$Pna2_1$ => $P_z < 0$ (-24 $\mu C/cm^2$)

3.12 μ_B // [001] $Ga_{1.12}Fe_{0.88}O_3$

3.7 μ_B // [001] $Ga_{0.98}Fe_{1.02}O_3$

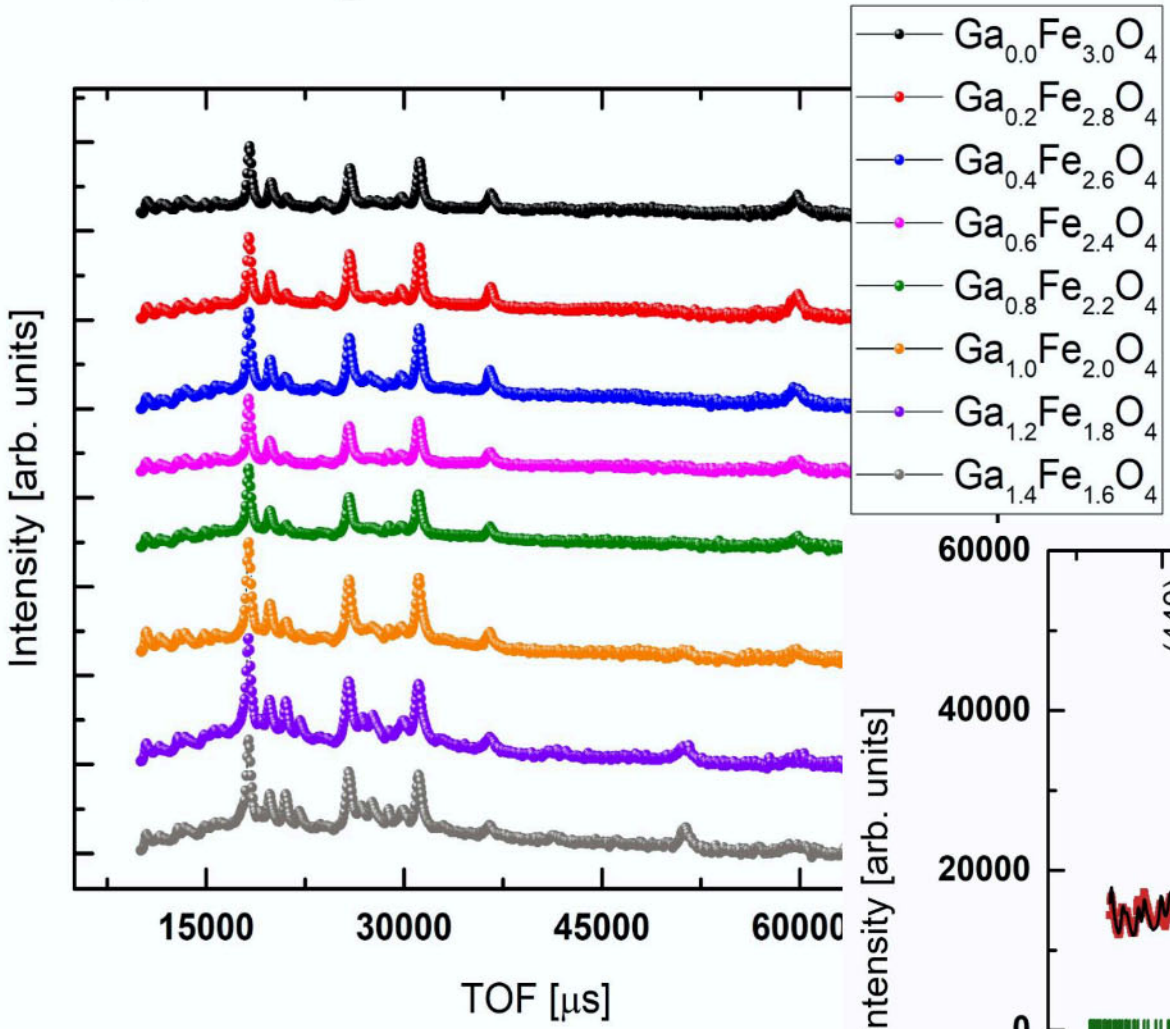
4 μ_B // [101] $GaFeO_3$ (LLB, o. m.)

Daniel Stoeffler, First principles study of the electric polarization and of its switching in the multiferroic $GaFeO_3$ system,J. Phys.: Condens. Matter 24 (2012) 185502

As to: scientific problems

- nanoparticles: spherical shape of core-shell type, in-site occupancy uniform morphology, small size and narrow size distribution, water-dispersible, non-toxic, biocompatible and superparamagnetic at human body temperature and above;
- polymeric drug carriers with lithocholic acid moiety;
- nanofilters: in-site occupancy, and stable magnetic efficiency;
- multiferroics: in-site occupancy, electrical polarization, magnetic polarization, noncolinear magnetic ordering.

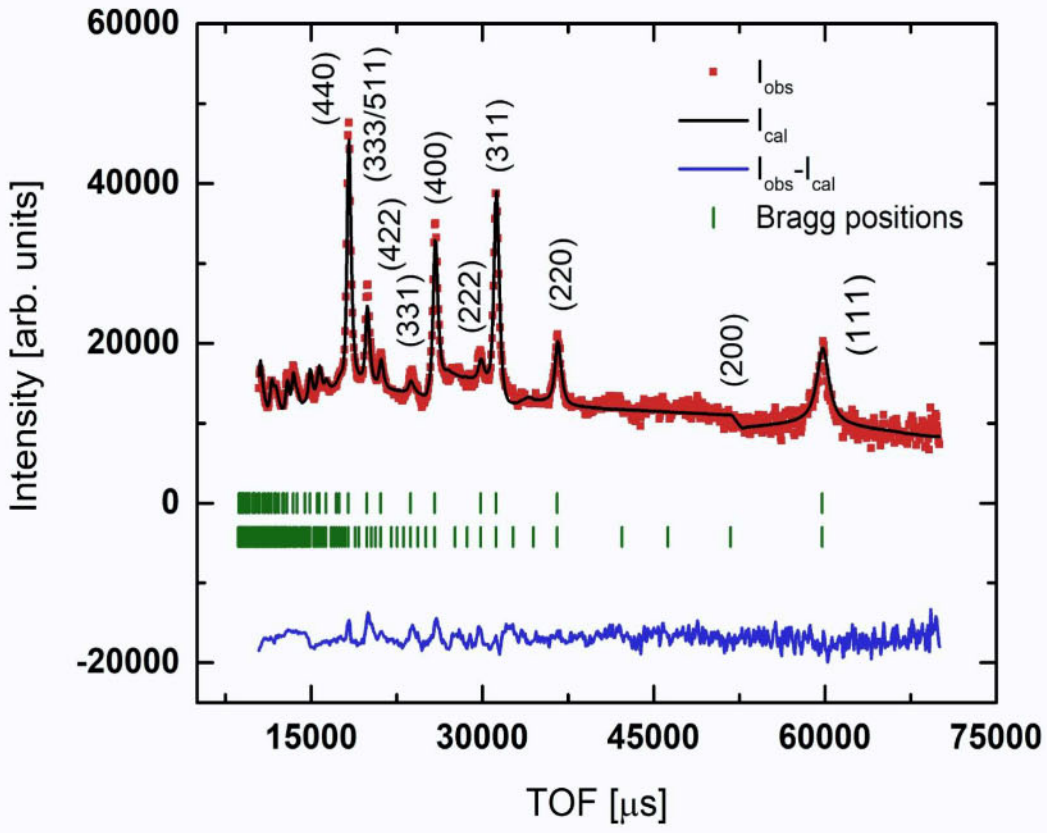
RTD_TOF Diagrams collected at 10 K



$Ga_{0.6}Fe_{2.4}O_4$

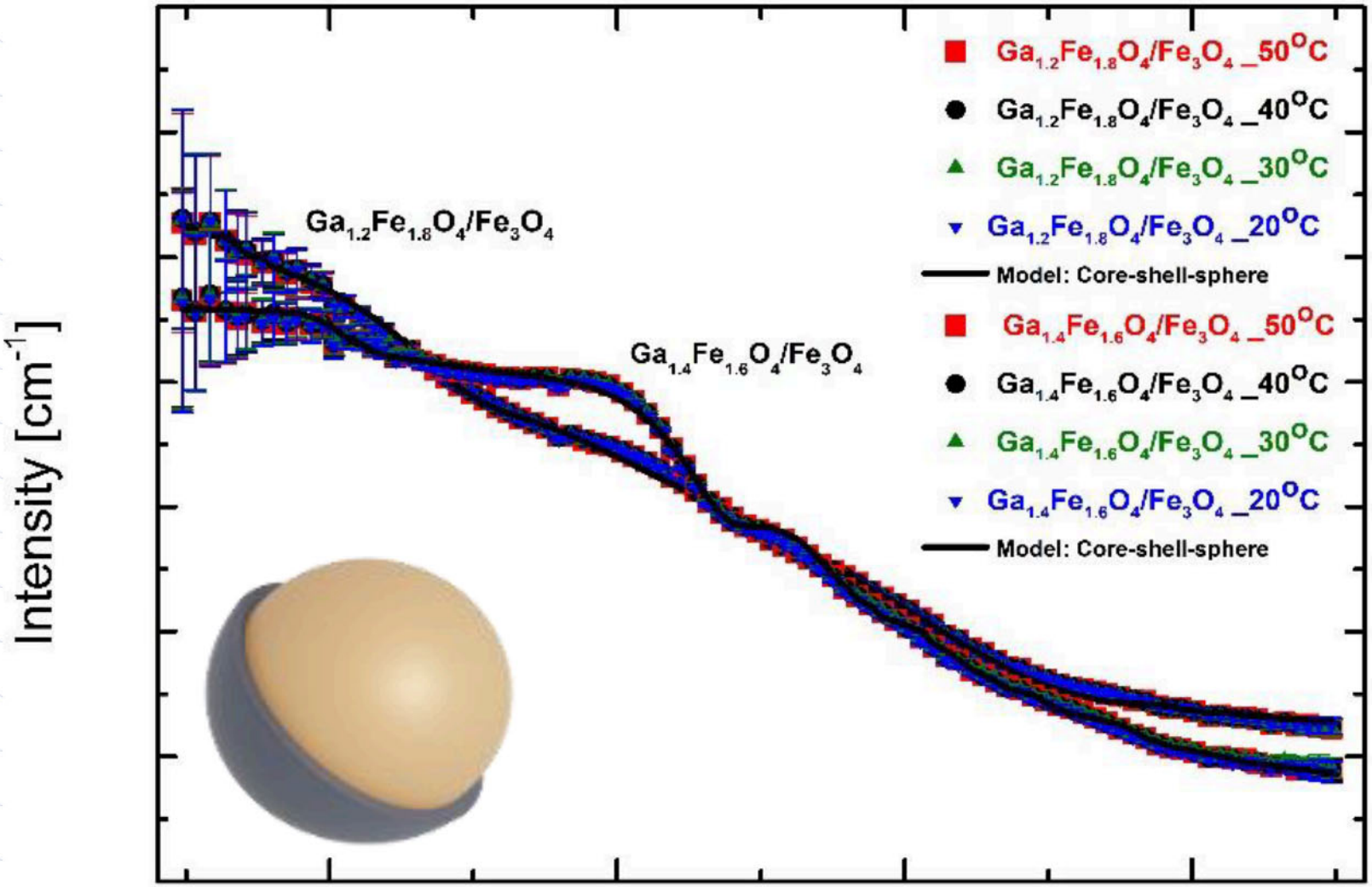
$\mu_{Fe(A)} = -1.09(24)\mu_B$

$\mu_{Fe(B)} = 3.47(56)\mu_B$



Goethite α - FeO(OH),
Pnma (sg. 62)
984 pm, 300 pm, 457 pm

SANS (IBR-2,YuMO, FLNP, Dubna)

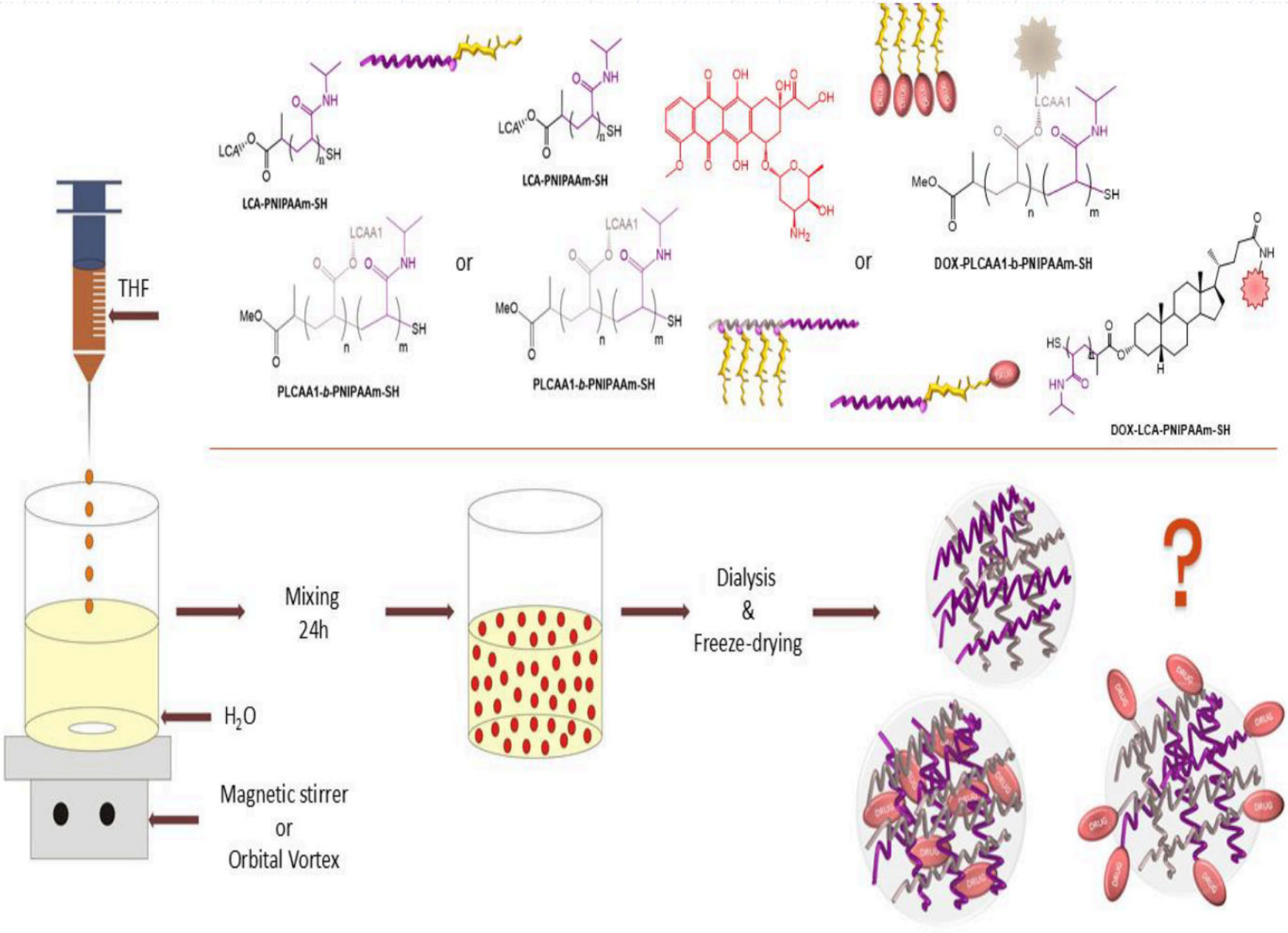


As to: nonmagnetic nanoparticles

Polymeric drug carriers with **lithocholic acid** moiety – what is the organization of polymers in nanoparticles and/or in water solutions?

The current treatments, including classical chemotherapy, are not sufficiently effective, the development of advanced drug-delivery systems **with well-defined interactions with biological membranes** has become essential for achieving targeted and efficient delivery of anticancer agents.

As to: nonmagnetic nanoparticles



As to: nonmagnetic nanoparticles

A set of 24 linear homo- and copolymers, soluble or dispersible in water, was synthesized. The polymers contained LCA-based units either at the ends of the chains or within the side segments of block copolymers. These materials formed stable nanoparticles through nanoprecipitation.

As to: nonmagnetic nanoparticles

SANS provides information about particle size, shape, aggregation, and internal organization. This is crucial for understanding how polymer architecture and the placement of LCA units influence self-assembly. Such knowledge helps to establish **connections between supramolecular structure and functional properties such as stability, and drug-loading capacity.**

In addition, isotopic contrast variation in SANS (for example, through H/D exchange) enables highlighting different parts of the nanoparticles. This allows detailed **analysis of how hydrophobic LCA segments and hydrophilic polymer regions are arranged.**

As to: Corresponding neutron techniques

$Ga_xFe_{3-x}O_4$-based nanoparticles as biomaterials are dedicated to anticancer therapy, primarily in the magnetic range of liquid hyperthermia while the polymeric materials containing lithocholic acid derivatives seem to be promising drug carries . Key structural aspects require high-resolution neutron studies using a dual-spectral powder diffractometer – DREAM.

These nanoparticles possess morphology, shape, size distribution characteristics and disperse well in aqueous or other hydrophilic environments. The unique ability to conduct SANS studies in real-world conditions (liquids) - available at the SKADI station - seems to be powerful tool.

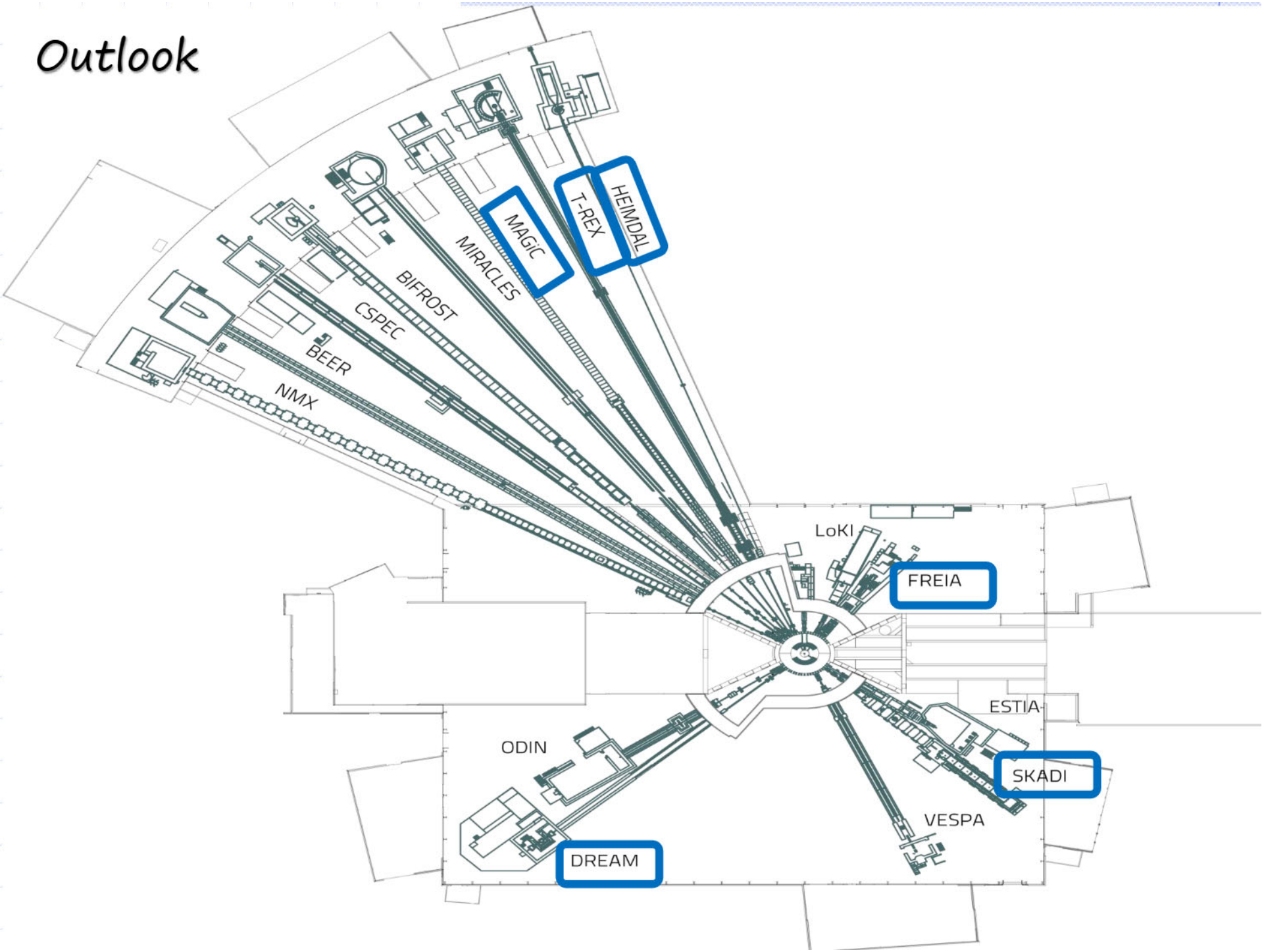
As to: Corresponding neutron techniques

The optimal measurement system seems to be an instrument that combines powder diffraction with SANS scattering, and imaging – HEIMDAL.

Coating deposition or encapsulation efficiency of ferro- and ferrifluids will be available in various media using the FREIA instrument (flux reflectometer).

Presumably, superparamagnetic fluctuations, will be able to determined using unpolarized neutron interference spectroscopy over the wide range generated by T-REX.

Outlook


MAGIC
T-REX
HEIMDAL
MIRACLES
BIFROST
CSPEC
BEER
NMX
LoKI
FREIA
ESTIA
SKADI
VESPA
ODIN
DREAM

Thank you for your time and attention