Kazan Federal University
Zavoisky Physical-Technical Institute
Tatarstan Academy of Sciences

XXIII International Youth Scientific School

ACTUAL PROBLEMS OF MAGNETIC RESONANCE AND ITS APPLICATION

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KAZAN

Program and Proceedings

KAZAN SCIENCE WEEK · 2023 SEPTEMBER 25 – 30

KAZAN FEDERAL UNIVERSITY
ZAVOISKY PHYSICAL-TECHNICAL INSTITUTE
TATARSTAN ACADEMY OF SCIENCES

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Kazan
September 25–30, 2023

KAZAN
2023

UDC 537
LBC 22.334
A19

Supported by a grant from the Russian Ministry of Education and Science for the implementation of activities aimed at supporting student scientific communities.

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A19 **Actual problems of magnetic resonance and its application [Electronic resource]:** program and proceedings of the XXIII International Youth Scientific School (Kazan, September 25–30, 2023) / edited by M.S. Tagirov, E.M. Alakshin. – Electronic text data (1 file: 33 Mb). – Kazan: Kazan University Press, 2023. – 41 p. – System requirements: Acrobat Reader. – Access mode: http://apmra-kzn.com/proceedings/mrschool2023.pdf. – Heading from title screen.

ISBN 978-5-00130-742-6

This collection contains the reports of young scientists submitted to the XXIIII International Youth Scientific School “Actual problems of magnetic resonance and its application”, organized by the Kazan Federal University and the Zavoisky Physical-Technical Institute.

The cover design was developed by D.A. Tayurskii.

UDC 537
LBC 22.334

ISBN 978-5-00130-742-6

Monday, September 25

08:00 – 11:00 Registration (Hotel and entertainment complex «Kazanskaya Riviera», Kazan, Fatykh Amirkhan Ave., 1)

Wednesday, September 25

09:00 – 09:15 Opening Ceremony

09:15 – 09:30 **A.V. Bogaychuk**, "Design of the Halbach array taking into account material imperfections"

09:30 – 09:45 **A.A. Belyaeva**, "Estimating the efficacy of optical flow building techniques based on MRT images"

09:45 – 10:00 A**.M. Garaeva**, "Study of Helium-3 Nuclear Relaxation in Contact with DyF_3 Nanoscale Powders"

10:00 – 10:15 **T.Y. Ivanenko**, "PFG NMR Study of petroleum asphaltene behavior in presence of ionic liquids"

10:15 – 10:30 **D.S. Fedorov**, "Mechanism of sodium diffusion in $Na_{5-x}M_{1-x}Zr_x(MoO_4)_4$ (M= Y, La, Bi; $0 \leq x \leq 0.1$)"

10:30 – 10:45 **Yu.V. Slesareva**, "Investigating Dynamic Effects of Multi-Pulse Protocols on Cu- and Ni-Oxamidato Complexes by Solid-State ^{1}H NMRs"

10:45 – 11:00 **A.L. Valiullin**, "Design of a Gradient Coil System for Nuclear Magnetic Resonance Equipment"

11:00 – 11:30 **Coffee break**

11:30 – 11:45 A.**M. Bulgakova**, "Investigation of signs of biological destruction of muscle tissues by nuclear magnetic resonance"

11:45 – 12:00 **P.A. Gergelezhiu**, "Characterization of ibuprofen by NMR and other complementary methods"

12:00 – 12:15 **E.I. Shamsiyarova,** "Search for complex formation between 5-fluorouracil and β-casein in aqueous solutions by Diffusion NMR"

12:15 – 12:30 **M. Smirnov**, "Application of high-resolution NMR spectroscopy to study the mechanisms of interaction of noble metal nanoparticles with amino acids"

12:30 – 12:45 **T.A. Kazbayev**, "New Aspects of Structural and Molecular Organisation of Oil Resins of Different Genesis from Nuclear Magnetic Relaxation Data"

12:45 – 13:00 **E.S. Kuchaev**, "Structural studies of oligopeptide inhibitor of SrtA by high-resolution NMR spectroscopy"

13:00 – 13:15 **A.A. Khayrullina**, "Search for the optimal gel-forming agent for the study of erythrocytes by NMR"

13:15 – 13:30 **E.R. Khisravashirova**, "NMR study of the interaction of hyaluronic acid molecules with proteins in aqueous solutions"

13:30 – 14:30 **Lunch**

14:30 – 14:45 **T.N. Enderova**, "Comparative study of Topological insulator $Bi_{1.06}Sn_{0.04}Sb_{0.9}Te_2S$ transport properties using DC and microwave measurements"

14:45 – 15:00 **D.E. Zhelezniakova**, "Electron Spin Resonance in $EuSn_2As_2$ Crystal Near the Magnetic Ordering Temperature"

15:00 – 15:15 **A.Kh. Kadikova**, "Structure, magnetic properties and spin-Hall effects in $Pt_{1-x}Mn_x$/Py heterostructures"

15:15 – 15:30 **E.Yu. Sidorova**, "Structural features of kaolinite from the weathering crust according to EPR data"

15:30 – 15:45 **G.D. Ulev**, "Generation and detection of spin current in iridate/manganite heterostructures"

15:45 – 16:00 **P.S. Kudimkina**, "Magnetic properties of $LiCu_3O_3$ studied with ESR"

16:00 – 16:30 **Coffee break**

16:30 – 16:45 **A.I. Shamsieva**, "Approaches to determining the glass transition temperature of polymers by computer simulation"

16:45 – 17:00 **A.A. Evseev**, "*Ab initio* investigation of heterostructures based on ferroelectric and metal with Rashba splitting"

17:00 – 17:15 **A.F. Iafarova**, "Unravelling Magnetic Properties in $LiGdF_4$ via EPR-Spectra Simulation"

17:15 – 17:30 **G.Iu. Andreev**, "Magnetocaloric properties of the $LiGdF_4$ single crystal"

17:30 – 17:45 **A.I. Faskhutdinova**, "Ab initio magnetic properties simulation of nanoparticles $LiTbF_4$, $LiDyF_4$, DyF_3, TbF_3"

17:45 – 18:00 **Y.V. Rebrov**, "High-frequency dielectric anomaly in a quasy-2D square kagomé lattice nabokoite family compounds"

18:00 – 18:15 **S.V. Stazharova**, "Synthesis and magnetic properties of oxides $La_2Zr_2O_7:Nd^{3+}$ and $SrY_2O_4:Sm^{3+}$"

Friday, September 25

13:00 – 13:30 Closing Ceremony (Hotel and entertainment complex «Kazanskaya Riviera», Kazan, Fatykh Amirkhan Ave., 1)

Design of the Halbach array taking into account material imperfections

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Halbach magnet arrays are attractive candidates for generating magnetic field for portable NMR spectrometers. Built from multiple permanent magnets, these devices require neither a power supply nor cryogenic cooling. In comparison to other permanent magnet structures, they are known to give the maximum magnetic field strength per mass of magnetic material and are designed to have minimum stray fields, so that incorporation with other hardware is simplified.

However, in practical engineering implementation, field errors may inevitably exist due to machinery tolerances of manufacture, assembly deviations, and so on. Deformation under various load conditions during operation may also cause significant field impurities, which may worsen the field homogeneity one to two orders compared with the ideal design value.

Therefore, field mapping to analyze of the magnetic field is needed. Then, a field correction procedure called shimming is usually applied to reach a high field homogeneity. There are two commonly used shimming techniques - active shimming and passive shimming. The passive approach involves optimizing the arrangements and sizes of the iron or magnet pieces, so as to compensate for the inhomogeneity of the static field. This method is cheap and flexible but has some problems that have to be considered. The total mass of the iron pieces can be minimized to a very low value by an effective optimization algorithm.

The use of new modern methods and approaches for the experimental evaluation of the imperfection of magnetic materials is proposed in this work. As well as the application of the results obtained in the design of the Halbach arrays.

This work was supported by the Russian Science Foundation (Project No. 23-22-00135).

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Estimating the efficacy of optical flow building techniques based on MRT images

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When obtaining images by MRT scanning, various artifacts appear which negatively influences the results of analysis of the images obtained. The causes of such defects are various. These include the wrong choice of scanning parameters which may lead to convolution effect, or the device defect, in particular, incorrect functioning of the analog-to-digital converter. The results may also be distorted by the artifacts specific for a particular technique of obtaining MRT images, for example, those appearing due to interference of several echoes in a sequence of turbo-spin-echoes. Besides, different tissues have different magnetic susceptibility, under the sufficient magnetic field intensity leading to significant distortions of echo-planar images. This means that using rapid scanning techniques which reduce image irregularity will not always be a priority from the viewpoint of automation of MRT images analyzing.

Let us consider various techniques of building an optical flow by MRT images and estimate their relative efficiency.

Horn-Schunck technique [1] is more sensitive to noise than local method; it also requires constant brightness of the image along the movement trajectory. It is usually hard to fulfill these conditions when obtaining an MRT image.

Lucas-Kanade technique [2] is not as sensitive to noise as point-by-point methods, but it is exclusively local and does not take into account the direction of pixels movement within homogeneous zones. However, this is usually not required when analyzing MRT images. Also, this technique is only applicable for small movements on an object on an image. This limitation can be circumvented by reducing the image resolution, but such reduction is not welcomed in MRT scanning, as it may significantly hinder further analysis of the images.

Phase correlation technique [3] is rather tolerant to noise, occlusions and other defects, characteristic for medical images. This technique is more effective when analyzing a circular rather than linear shift of the object on an image, but this drawback is balanced if the image background is flat and the object is situated far from the edges. In that case the linear shift may be considered equivalent to the circular one, and the technique productivity is not decreased. MRT images, as a rule, satisfy these conditions.

Optimization algorithm [4] is more flexible than the Lucas-Kanade technique, and is already used for correcting patient's movements when obtaining MRT images. It is relatively new and is considered as one of the most promising [5].

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Study of Helium-3 Nuclear Relaxation in Contact with DyF_3 Nanoscale Powders

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Dysprosium fluoride DyF_3 is a dipole ferromagnet with an easy magnetization axis along the [010] axis of the crystal lattice [1]. The compound has unique properties, which allows it to be used as a high-field MRI contrast agent [2] and as an additive to Nd-Fe-B magnets to increase the coercive force [3].

Powders of DyF_3 and LaF_3 with a characteristic particle size of 20 nm were obtained by hydrothermal synthesis according to the nitrate reaction [4], a powder with a size of 220 nm × 150 nm was obtained by the reaction through chloride [5]. Control of the chemical composition and confirmation of crystallinity were carried out using X-ray phase analysis on a Bruker D8 Advance Cu Kα diffractometer, λ=1.5418 Å. Photographs obtained by transmission electron microscopy on a HitachiHT Exalens microscope were used to determine the shape and characteristic size of particles in the obtained powders.

In this work, the rates of longitudinal and transverse relaxation of helium-3 nuclei in contact with DyF_3 (99.67%) and LaF_3 (0.33%) powder in the adsorbed layer, in the bulk of the liquid, and in the case of covering the particles with a helium-4 layer were measured depending on temperature. The relaxation mechanisms of ^{3}He nuclei in contact with DyF_3 particles at 1.5 - 3 K in fields of 173, 287, and 505 mT are considered.

This work was supported by the Russian Science Foundation (Project No. 23-72-10039).

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PFG NMR Study of petroleum asphaltene behavior in presence of ionic liquids

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Abundant worldwide production of light oil along with the depletion of conventional oil resources actually shifted the focus of the petroleum industry and technology toward processing of heavier crude oils and residues. Among the thousands of components presented in crude oil, asphaltenes are highlighted to be the most important group of compounds that undergo deposition during processing, refining, and transportation of heavy oil [1]. Precipitated asphaltenes cause pore throat plugging, decreasing the permeability, changing the wettability of the rock surface, further resulting in damaging the wellbore region and dramatic reduction in the recovery factor. In addition to the downhole problems, asphaltenes form the deposits on the internal surface of the pipelines, pumps, oil tanks and other surface facilities. Consequently, proper understanding of the phase behavior of asphaltenes is an essential step in addressing the flow assurance problem [2].

One of the promising reagents to address the undesired deposition of asphaltenes is ionic liquids (ILs) which can be utilized as a green chemistry alternative to the chemical dispersants. Thus ILs are environment friendly, recyclable, and non-corrosive substances which can keep asphaltene molecules in dispersed state owing to formation of hydrogen bonds and π - π^* interactions with asphaltene PAHs core [3]. In presented report, we investigated the local dynamics of asphaltene molecules in a model solution and in presence of small amount of different ILs ([BMIM]BF_4, [BMIM]TFSI, [$P_{6,6,6,14}$]Cl) via PFG NMR measurements of temperature and concentration dependence of diffusion coefficients (Fig. 1).

a) b)

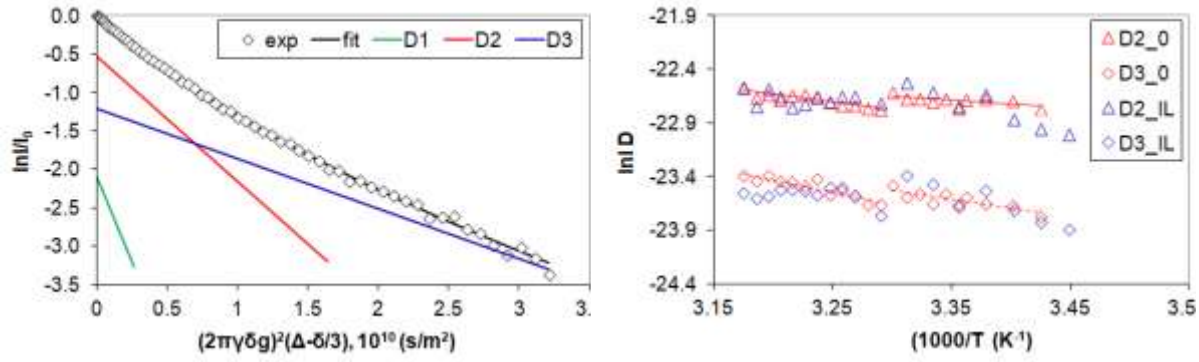

Fig. 1. PGSE signal attenuation decay of 25 g/L asphaltene solution in $CDCl_3$ (a); temperature dependence of diffusion coefficients of neat asphaltene solution in $CDCl_3$ (red symbols) and in presence of 1 vol.% of [BMIM]BF_4 (blue symbols) ionic liquid (b)

This research was performed using the equipment of Krasnoyarsk Regional Research Equipment Centre of Siberian Branch of Russian Academy of Sciences with the financial support of Russian Science Foundation (Project No. 21-13-00171).

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Mechanism of sodium diffusion in $Na_{5-x}M_{1-x}Zr_x(MoO_4)_4$ (M = Y, La, Bi; $0 \le x \le 0.1$)

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Development of the technologies for energy storage and conversion requires a search for compounds with high diffusion of alkali and alkaline-earth ions. Here, the results of comprehensive studies are presented, including synthesis, powder X-ray diffraction, experiments on impedance and ^{23}Na NMR spectroscopy, as well as ab initio calculations, which were carried out to explore the sodium diffusion in scheelite-like $Na_5M(MoO_4)_4$ with M = Y, La, Bi, and in related solid solutions $Na_{5-x}M_{1-x}Zr_x(MoO_4)_4$ ($0.05 \le x \le 0.1$), which were synthesized for the first time.

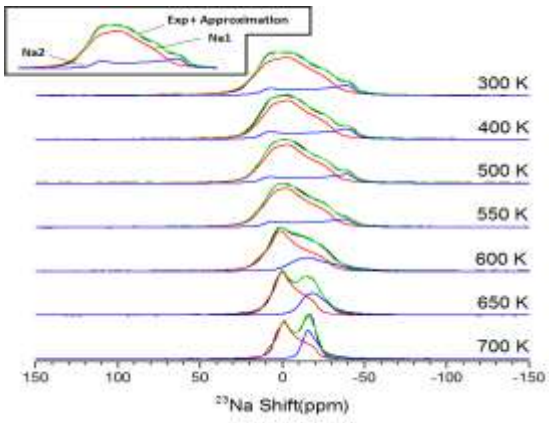

Fig. 1. ^{23}Na NMR spectra acquired for the $Na_5La(MoO_4)_4$ in the temperature range 300 – 700 K

The crystal structure, transport properties, and diffusion mechanism in scheelite-like $Na_5M(MoO_4)_4$ and $Na_{5-x}M_{1-x}Zr_x(MoO_4)_4$, ($M$ = Y, La, Bi; $0 < x \le 0.1$) were studied using a combination of experimental methods and ab initio calculations. Solid solutions $Na_{5-x}M_{1-x}Zr_x(MoO_4)_4$ (M = Y, La, Bi, and x = 0.05 - 0.1) were synthesized for the first time using ceramic technology by annealing stoichiometric mixtures of $Na_5M(MoO_4)_4$ and $Na_4Zr(MoO_4)_4$. X-ray diffraction analysis showed that all samples crystallize in the scheelite-like structure (space group $I4_1/a$, $Z = 4$).

From impedance spectroscopy data and temperature variation of the ^{23}Na NMR spectra (Fig. 1.) we established that Na-ion mobility increases in the sequence Y → La → Bi and with increasing x. The highest ion conductivity is found for $Na_{4.9}Bi_{0.9}Zr_{0.1}(MoO_4)_4$, for which the value $\sigma \sim 10^{-4}$ S/cm at T = 450 °C. According to DFT calculations and ^{23}Na NMR data, the mechanism of sodium-ion diffusion is determined by atomic jumps between equivalent Na2 (16f) positions and through the "two-site-exchange" Na2 ↔ Na1 ↔ Na2, while direct jumps between Na1 (4a) sites are less probable. The energy barrier for both Na-ion jumps is approximately equal to 1 eV, and the ion jump frequency reaches the value $10^3 – 10^4$ s^{-1} at $T \approx 650$ K for $Na_5Y(MoO_4)_4$, and at $T \approx 500$ K for $Na_{4.9}Bi_{0.9}Zr_{0.1}(MoO_4)_4$.

This work was carried out in accordance with the state assignment by the Ministry of Science and Higher Education of the Russian Federation: themes No. 1222021000035-6, 23031300049-8, AAAA-A19-119031890025-9, AAAA-A21-121011890009-6 and project M 3-22.

Investigating Dynamic Effects of Multi-Pulse Protocols on Cu- and Ni-Oxamidato Complexes by Solid-State ^{1}H NMR

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The potential of metal-oxamidato complexes is noteworthy for quantum computing applications and creating new materials in spintronics. Our investigation aims to compare the properties of the magnetic Cu(II)-oxamidato complex and its diamagnetic Ni(II)-containing analog by ^{1}H NMR spectroscopy. The presence of magnetic ions enhances the inhomogeneous broadening and accelerates the relaxation processes. These properties alter the performance of the Carr-Purcell-Meiboom-Gill (CPMG) protocol, which is commonly used to extend the coherence lifetime by suppressing spectral diffusion [1]. Therefore, we used an improved CPMG pulse protocol proposed in [2] to mitigate unwanted echoes. Our experiments reveal the existence of a transient phenomenon that needs to be considered in the design of quantum computing protocols.

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Design of a Gradient Coil System for Nuclear Magnetic Resonance Equipment

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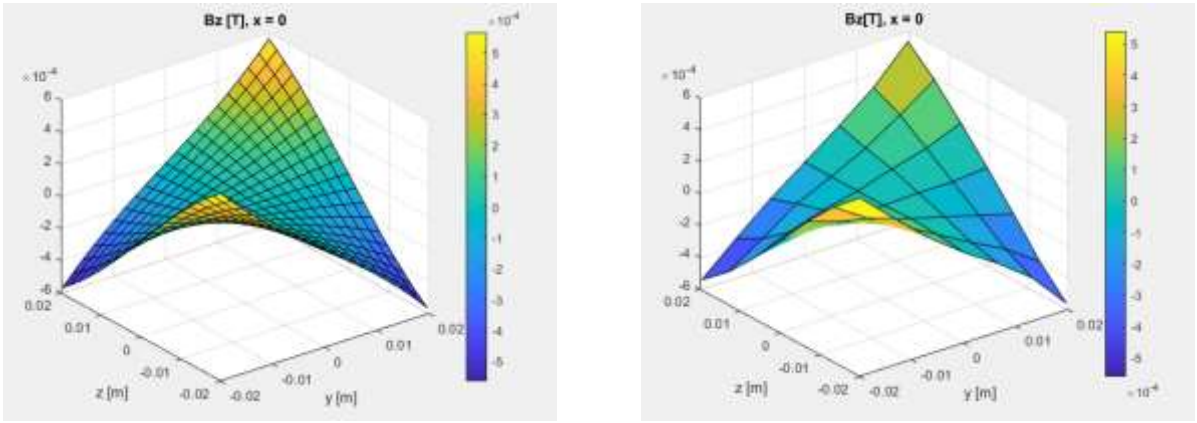
In the technique of magnetic resonance imaging, gradient systems are used to create a space-varying magnetic field encoding a nuclear magnetic resonance (NMR) signal. Linear gradients bijectively encode the study sample, allowing its images to be obtained using classical techniques [1]. However, the creation of nonlinear gradients is also promising, which are used in such areas of MRI as Patlock [2]. The purpose of this work is to calculate and optimize gradient coils for a system with a vertically directed external field, as well as to measure the field created by coils on manufactured models.

Calculation and optimization of gradient coils were performed in the MATLAB. In the developed program, using the Bio-Savard-Laplace law and the finite element method, a magnetic field is calculated at each point of the region of interest (ROI). Thus, coil configurations were obtained to create linear (G_x, G_y, G_z) and quadratic (G_{xy}, G_{yz}, G_{xz}) gradients, according to which the models were made. The calculated and measured magnetic field maps for a coil with a G_{yz}, gradient are shown in Fig. 1.



A) B)

Fig. 1. Magnetic field maps for a coil with a G_{yz} gradient: A) calculated; B) measured

The results of measuring the magnetic field generated by the manufactured models coincide with the result of computer simulation of coils, deviating by no more than 5%. From the data obtained, it can be concluded that the calculation of magnetic fields in the developed program gives reliable results, which allows it to be used in the development of gradient systems based on Golay coils in NMR technology.

This work was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities number FZSM-2023-0016.

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[2] Schultz G. Magnetic resonance imaging with nonlinear gradient fields: signal encoding and image reconstruction. – Springer Science & Business Media, 2013.

Investigation of signs of biological destruction of muscle tissues by nuclear magnetic resonance

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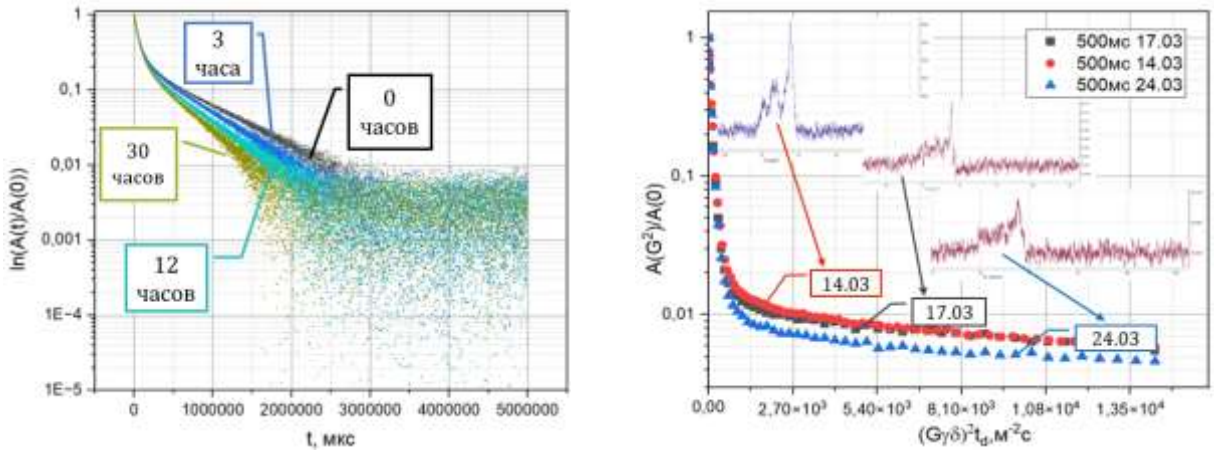
In modern medicine, there is a wide range of methods and approaches for assessing cell viability. It includes both experimental methods, andcomputer modeling [1,2]. However, the search for new methods forassessing destructive processes in tissues is an urgent task. The aim of this work is to assess the sensitivity of nuclear magnetic resonance (NMR) methods to biological tissue destruction.

Studies were carried out in the field of spin-spin relaxation and self-diffusion using the following devices: an NMR-relaxometera Chromatek Proton 20 M using the Carr-Purcell-Mayboom-Gill sequence, a digital NMR-spectrometera «AVANCE 400 III TM» (Bruker) using the stimulated echo sequence. The study samples were muscle tissues of laboratory mice (soleus, diaphragm) with the addition of a contrast agent.

In the course of the study, a change in the shape of the transverse magnetization declines was detected depending on the storage time of the sample, and changes in the diffusion attenuations and spectral lines were also recorded. The observed changes are shown in Figure 1.



A) B)

Fig. 1. Attenuations obtained as a result of studying the signs of biological destruction of muscle tissues: A) relaxation; B) diffusion, with the image of characteristic spectral lines

The results obtained indicate the sensitivity of the NMR method to destructive processes in tissues, which makes it possible to consider NMR methods in assessing cell viability.

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Characterization of ibuprofen by NMR and other complementary methods

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Ibuprofen is a nonsteroidal anti–inflammatory drug that is very popular among pharmaceuticals. From a structural point of view, the skeleton of the ibuprofen molecule is an aromatic acid skeleton that contains an additional chiral center [1]. An important role for the assimilation of medicines is played by the acidity (or pH) of the medium into which the drug enters. Depending on the acidity of the medium, the mechanism of interaction of drugs with cellular receptors may change, which greatly affects the effectiveness of drugs (exposure time, excretion from the body). It should be noted that when the acidity changes, the shape of the molecules also changes, taking various forms from neutral and protonated to anionic.

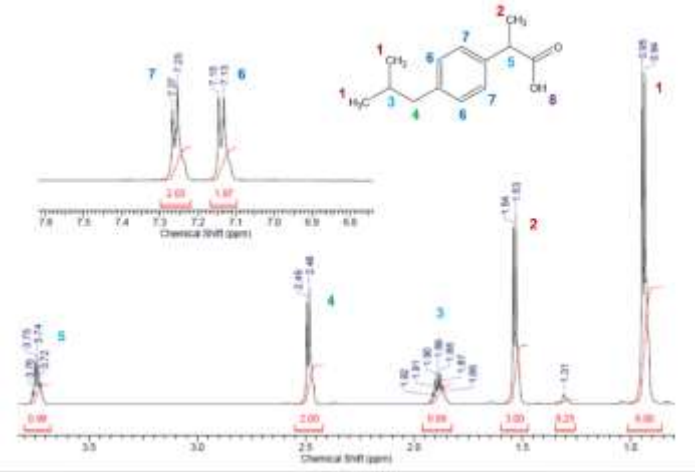

Fig. 1. NMR spectrum of ibuprofen

To determine the purity of the synthesized ibuprofen sample, we obtained the NMR spectrum on the AVANCE III 600 MHz NMR spectrometer (Bruker) at the Federal Research Center "Kazan Scientific Center of the Russian Academy of Sciences". We compared the obtained spectrum with the Database for Organic Compounds SDBS [2]. According to the data from the database, the NMR spectrum was obtained at 400 MHz. Our ibuprofen sample was prepared under the same conditions: dissolved in deuterochloroform in the same proportions as in the database. The spectrum obtained by us, with the interpretation is shown in Fig. 1. Signals at 7.28 ppm refer to the solvent deuterochloroform, the rest correspond to ibuprofen.

It can be concluded that the sample contains pure ibuprofen and it can be used for further studies. The results of X-ray powder diffraction, IR and RAMAN spectroscopy as well as differential scanning calorimetry will be presented.

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Search for complex formation between 5-fluorouracil and β-casein in aqueous solutions by Diffusion NMR

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Oncological diseases are one of the causes of numerous deaths worldwide. Antimetabolite 5-fluorouracil (5-FU) is one of the medicinal antitumor drugs used in the treatment of a wide variety of malignancies. 5-FU, as a typical representative of pyrimidine bases, is characterized by a mobile tautomeric equilibrium of structural isomers. But in terms of therapeutic effect, only a certain type of 5-FU tautomer has an effective reactivity in the reproduction and mutagenesis of cellular DNA. The therapeutic effect of 5-FU can be increased by encapsulating it into certain molecules that act as a carrier and/or shell. In our study, beta-casein protein acts as such a natural container for creating a stable, non-toxic complex with 5-FU.

The purpose of this work is to establish signs of the formation of complexes between 5-FU and β-casein and to determine the features of protein mobility in aqueous solutions. Diffusion experiments were carried out by pulsed-field gradient NMR on the spectrometer Bruker AVANCE III.

Comparison of the spectrally resolved diffusion attenuations for 5-FU and beta-casein molecules obtained on 1H nuclei allows us to conclude that there are no signs of complex formation between the samples, regardless of their molecular ratio in aqueous solutions. Also, the results of the study on the translational mobility of 5-FU molecules on ^{19}F nuclei indicate that the 5-FU molecules are in a free state in the aqueous solution of beta-casein (Fig. 1). During the study, signs of the formation of a supramolecular structure by protein molecules in the form of a three-dimensional gel network, similar to the gel-like form formed in concentrated solutions of α- and κ-caseins, were established (Fig. 2).

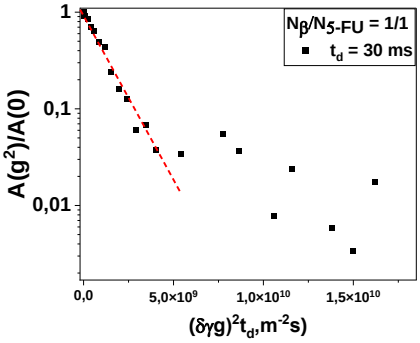

Fig. 1. Diffusion attenuation of spin echo signal of an aqueous solution of β-casein and 5-FU obtained on ^{19}F nuclei

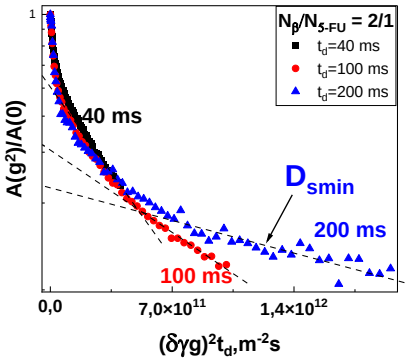

Fig. 2. Diffusion attenuations of spin echo signal of an aqueous solution of β-casein and 5-FU

The findings are direct practical relevance with the help of which we can achieve an improvement in the effects of cancer drugs and better study the nature of proteins with an internally disordered structure.

NMR measurements were performed at the Federal Centre of Shared Facilities at Kazan Federal University.

Application of high-resolution NMR spectroscopy to study the mechanisms of interaction of noble metal nanoparticles with amino acids

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Metal nanoparticles (NPs) are actively used for medical purposes. For example, gold NPs are used as contrast agents in computed tomography [1]. At the moment, there is an increased interest in the functionalization of the surface of metallic NP by various biomolecules, including amino acids, since this allows for the reduction of the toxicity of NP in living structures [2]. However, to date, there needs to be more studies devoted to studying the interaction of amino acids with the NPs of noble metals.

The purpose of this study was, using various methods of high-resolution NMR spectroscopy, to establish the parameters of the intermolecular interaction between the amino acid L-tyrosine and the NPs of two types of noble metals: gold (Au) and platinum (Pt). The samples for the NMR study were selected because the spectrophotometry method demonstrated the interaction of these NPs with L-tyrosine.

Three samples were prepared for the study:

1) The pure amino acid L-tyrosine at a concentration of 10^{-2} mol/l;

2) Two samples in which 40 µl of a solution with Au / Pt nanoparticles was added to 120 µl of an aqueous solution of tyrosine.

The study used several high-resolution NMR spectroscopy methods: 2D-NOESY, DOSY, and relaxation experiment. The first two experiments were performed on a Bruker 500 MHz NMR spectrometer, and relaxation times T1 and T2 were measured on both Bruker and Varian 400 MHz.

The results of the 2D-NOESY experiment were used to calculate the qualitative changes in the internuclear distances that occur in the tyrosine molecule in the presence of metal NPs. For this purpose, the methods described in the articles [3] and [4] were used. Both types of NPs increase the distance r3 between the proton *a* and the CH group in the tyrosine molecule (Fig. 1). The addition of gold NPs leads to a decrease in the distance r1, while the distance r2 increases.

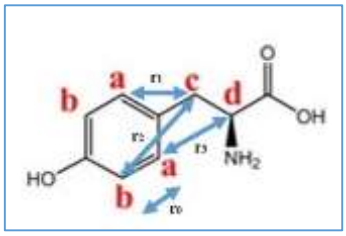

Fig. 1. L-tyrosine

The DOSY experiment demonstrated that the tyrosine molecule's diffusion coefficient does not change significantly when a solution with metal NPs is added.

The relaxation experiment showed that T1 of the tyrosine molecule's aromatic protons *a* and *b* decreases when a solution with gold NPs is added. At the same time, adding this type of NP leads to an increase in the relaxation time of the CH_2 group.

A different situation is observed with the relaxation time T2. Both types of NPs contribute to a decrease in the relaxation time of the CH_2 group relative to pure tyrosine. With the addition of gold NPs, the T2 time of aromatic protons *a* and *b* increases.

The relaxation data obtained on both NMR spectrometers correlate well for a sample with gold NPs. The study results show that the translational mobility of tyrosine molecules in solution does not change significantly when a solution with noble metal NPs is added. However, as the relaxation data show, the NPs affect the rotational mobility of the molecule, and the gold

NPs contribute to this to a greater extent. It was found that adding a solution with noble metal NPs also causes changes in the internuclear distances between protons, and in the case of gold NPs, these changes are more extensive.

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New Aspects of Structural and Molecular Organisation of Oil Resins of Different Genesis from Nuclear Magnetic Relaxation Data

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The global trend of light oil decline and rising prices for these feedstocks is forcing a reassessment of government policy and the overall course of research and production of high-viscosity and heavy oils. The Russian Federation and, in particular, the Republic of Tatarstan have large reserves of high-viscosity oils and natural bitumen, which include significant amounts of paraffins and resins. Development of high-viscosity oil and natural bitumen fields is becoming extremely important nowadays, especially in regions with traditional oil production, including the Volga-Urals oil and gas bearing province. According to the widely recognised classification, oil with paraffin content from 1.5% to 6% and higher belongs to the categories of paraffin and high-paraffin oils [1]. High concentration of paraffins, especially high molecular weight paraffins, affects the colloidal structure of oil.

In spite of widespread models of aggregates of resins, asphaltenes and paraffins proposed by different researchers and numerous information on chemical properties of resins, paraffins and asphaltenes, there is still no unified idea about the molecular structure of these components of oil.

At present, the existing disagreements [2] between theory and experimental results are mainly due to the methods of oil analysis. Chemical methods for analysing the composition of petroleum products are complex and time-consuming, as they require the separation of components, which can disrupt the integrity of the object under study and cause doubts in the data obtained.

As a result of the study of the main components of oil by nuclear magnetic resonance (NMR) method it was established that there is a characteristic feature ─ temperature hysteresis ─ of the crystallising component (paraffin), which is fixed in benzene resins, but is not detected in alcohol-benzene resins regardless of whether they are obtained sequentially or independently. It is demonstrated that in asphaltenes and paraffins isolated chemically from oil at least 10 per cent of the component, which has no signs of a solid body, is registered, and therefore it makes sense to consider it as an impurity. Having carried out an experimental study of the main components of oil, we further considered multicomponent systems and calculated regression coefficients that allow us to calculate the mass content of paraffins, resins and asphaltenes using nuclear magnetic resonance data. The research was performed under Contract No. 0009/2023/604 dated 27 January 2023.

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Structural studies of oligopeptide inhibitor of SrtA by high-resolution NMR spectroscopy

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Sortase are enzymes involved in the attachment of surface proteins to the cell wall. The mechanism of action of *Staphylococcus aureus* Sortase A (SrtA) is based on specific recognition of the LPXTG sequence (where X is any amino acid residue) at the C-terminus of the surface protein, cleavage of this site between threonine and glycine residues, subsequent transfer of the N-terminal transmembrane domain to the amino group of the pentaglycine linker and thus anchoring of proteins with this motif on the cell surface. Sortase A is involved in both early and late stages of bacterial infection because it attaches adhesins and immune evasion proteins to the cell wall. For this reason, this enzyme is a good target for combating bacterial infections [1]. The results of in vivo and in vitro (IC50 = 10.61 μM) studies of an oligopeptide with LPRDA sequence showed effective inhibition of the enzymatic activity of Sortase A through competitive binding to its active site [2].

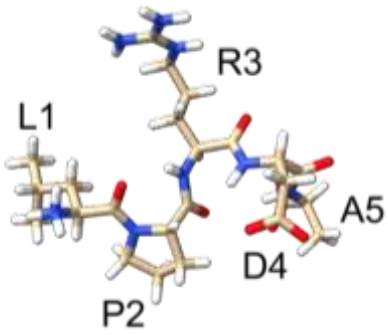

Fig. 1. Solution structure of LPRDA peptide

Here we report solution structure of LPRDA solved by high-resolution NMR spectroscopy (Fig. 1). NMR assignment was done by analyzing 1D ^{1}H and ^{13}C; 2D ^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC NMR spectra.
Obtained structure could be used for further optimization of the inhibitor to improve its selectivity and rate of inactivation of sortase.

This work was supported by the government assignment for FRC Kazan Scientific Center of RAS.

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Search for the optimal gel-forming agent for the study of erythrocytes by NMR

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Many different techniques [1] have been used to immobilize cells in an NMR tube for whole cell measurements. The most popular immobilization methods for in vivo NMR studies involve the use of gels. The gels are mixed with cells and then allowed to set to a suitable geometry. The smaller the size of the gel mesh, the better the molecules are retained in it. The approach is easy to use and offers favorable properties to maintain 3D cell cultures, and will thus help to bridge the gap between in vitro and in vivo environments in drug discovery [2].

The most attractive biocompatible gel systems can be aqueous solutions of agar-agar, as well as aqueous solutions of gelatin. Using the NMR method with a pulsed magnetic field gradient, we obtained the coefficients of self-diffusion of polymer molecules in several "phases": free molecules and molecules involved in gelation. The characteristic dimensions of the gel network formed by both agar-agar molecules and gelatin in aqueous solutions have been established. NMR measurements were carried out on a Bruker Avance 400 MHz spectrometer equipped with a pulsed magnetic field gradient unit with a maximum gradient of 28 T/m. We used a standard stimulated echo (STE) pulse train to record the diffusion attenuation of spin echo signals. NMR measurements were performed at the Federal Centre of Shared Facilities at Kazan Federal University.

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NMR study of the interaction of hyaluronic acid molecules with proteins in aqueous solutions

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Hyaluronic acid (HA) has found wide application in the field of medicine: from polymer skeletons of endoprostheses of joints to biorevitalizing agents for skin burns [1]. HA molecules are an integral component of both the extracellular and pericellular matrix [2]. As a result of the interaction of HA with membrane proteins, the functions of the cell membrane can change [3]. To date, hyaluronic acid and its complexes with proteins remains an urgent subject of research.

The purpose of this study is to establish additional effects of the interaction of HA with proteins on the example of its complex with bovine serum albumin (BSA) and egg lysozyme in aqueous solutions. According to the characteristics of translational mobility obtained by NMR, the features of the interaction of HA with these proteins are demonstrated. All NMR measurements were performed at 298 K on a 400 MHz Bruker Avance-III TM spectrometer equipped with a gradient system that allowed for a maximum gradient of 28 T/m.

The characteristics of translational mobility of HA demonstrate noticeable effects of the presence of BSA protein in the system. Thus, the addition of BSA to the aqueous solution of NA initiated an additional mechanism, as a result of which all the molecules of NA formed a gel structure. In addition, the recorded decrease in the self-diffusion coefficient of BSA molecules as a result of interaction with HA can be interpreted as a result of the formation of short-lived BSA-HA complexes. Unlike BSA, lysozyme, even at very low concentrations, actively interacts with HA and actually acts as an enzyme that hydrolyzes the glycoside bond of the polysaccharide.

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Magnetic properties of $LiCu_3O_3$ studied with ESR

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$LiCu_3O_3$ is a cuprate with mixed valence of copper – the system consists of monovalent Cu^+ and divalent Cu^{2+} ions in a ratio 1:2. Crystal structure of $LiCu_3O_3$ is an alternating square array of Li^+, Cu^+, Cu^{2+}, O^{2-}ions whose planes are perpendicular to the C_4 axis. Nodes of each fourth copper plane are occupied by non-magnetic Cu^+ ions, while the nodes of other three planes are occupied by magnetic Cu^{2+} ions and non-magnetic Li^+ ions. Li^+ and Cu^{2+} cations occupy the same structural positions [1, 2]. The random distribution of these ions causes the increasing frustration. Magnetic structure of $LiCu_3O_3$ was not studied properly before.

In this work we discuss the first results of NMR, magnetometry and ESR studies of $LiCu_3O_3$. ^6Li NMR experiments showed that at temperature below 120 K a magnetic ordering occurs. Magnetization measurements also identified an anomaly at T = 120 K. The magnetic resonance of $LiCu_3O_3$ was detected by ESR techniques. At $T > 30\ K$ the resonance frequency is proportional to the external magnetic field. And at $T < 30\ K$ resonance frequency at H = 0 becomes different from zero. Fig. 1a shows a field-frequency diagram *f(H)* of $LiCu_3O_3$ at T = 4.2 K for $H \parallel C_4$. At $T = 4.2\ K$ the value of frequency gap is $f \approx 25\ GHz$. Solid green line in Fig. 1a demonstrates approximation of *f(H)* dependence in frames of helicoidal magnetic structure.

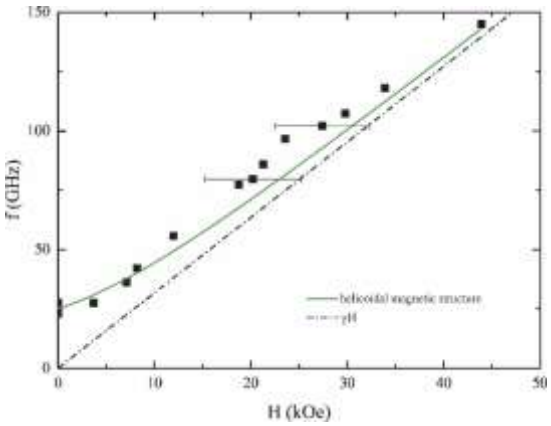

Fig. 1a. Field dependence of resonance frequency (black squares) at $T = 4.2\ K$, $H||C_4$. The dashed line shows a paramagnetic resonance spectra. The solid line represents the dependence of ESR frequency on external magnetic field calculated in frames of helicoidal magnetic structure

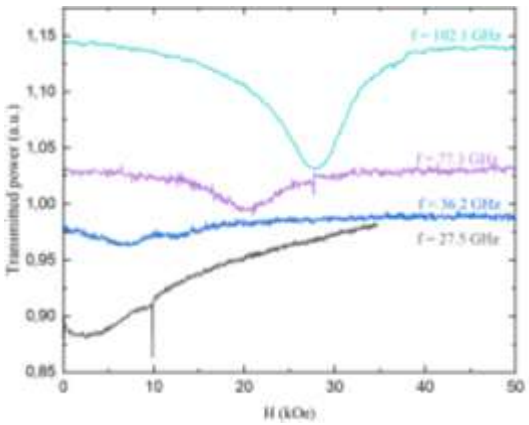

Fig. 1b. Examples of absorption lines at $T = 4.2\ K$, $H \parallel C_4$. The squares in Fig. 1a are corresponding resonance frequencies, error bars are half-width of lines at half-height

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Comparative study of Topological insulator $Bi_{1.06}Sn_{0.04}Sb_{0.9}Te_2S$ transport properties using DC and microwave measurements

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Topological insulators (TI) are materials that have a bulk band gap like an ordinary insulator, but more importantly, they have conducting states on their surface. The surface charge carriers of TI are Dirac fermions with linear dispersion law, hence those carriers are massless and have high mobility. These peculiar properties make TI promising materials for practical quantum electronics and spintronics devices. To implement TI on practice it is necessary to study their transport properties.

Transport properties of conducting samples has been extensively studied by DC transport measurement method. It is simple and comprehensible method that allows to register temperature and magnetic field dependencies of resistivity $R(T, H)$. However sometimes DC measurement method is insufficient and requires additional research for studying current carrier scattering processes. For example, using high-frequency measurements allows us to obtain information about scattering time τ. Non-resonant microwave absorption is a powerful technique that enables contactless measurements of transport properties of thin films.

In this work data obtained by measurements of DC resistance and non-resonant microwave absorption (MWA) for topological insulator $Bi_{1.06}Sn_{0.04}Sb_{0.9}Te_2S$ (BSSTS) are analyzed. BSSTS is high-quality topological insulator with bulk energy gap $\Delta E \approx 150$ meV. At low temperatures ($T < 100$ K) surface conducting states contribute predominantly to sample conductivity [1]. Therefore, we focused our study on low temperatures and obtained magnetic field dependence of resistance $R(H)$ and the absorption derivative dP/dH (H) for our sample at 4.2 K. MWA data was obtained using ESR-spectrometer Elexsys E580 (Bruker).

It was established [2] that $dP/dH \sim d\rho/dH$; hence magnetic field dependence of MWA can be interpreted as a direct measurement of the magnetoresistance. To compare obtained MWA and *R(H)* data it was necessary to integrate dP/dH (H) dependence. It should be expected that in large fields, where $\omega_c \gg \omega_0$ ($\omega_c = eB/m^*$ is a cyclotron frequency, e is electron charge, m^* is its effective mass, $B \approx H$ is magnetic field induction, ω_0 is the spectrometer frequency) the course of the curves $P(H)$ and $R(H)$ will be the same. The analysis of the experimental data showed that the above dependences coincide with each other in the fields $H >$700 Oe ($\omega_0 = \omega_c$ at $H \approx 200$ Oe). In lower fields the curves diverge. From a qualitative point of view, *P(H)* data exhibit all characteristic features of TI magnetoresistance, including considerable difference between cases of parallel and perpendicular magnetic field.

Since the ESR technique is very sensitive, such approach opens a powerful opportunity to study the magnetoresistance of different materials in a contactless way.

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Structure, magnetic properties and spin Hall effects in $Pt_{1-x}Mn_x$/Py heterostructures

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Field-free magnetization switching is an important problem in spintronics focused at magnetoresistive random-access memory (MRAM) technologies. There are various ways to implement field-free magnetization switching in thin-film structures with perpendicular magnetic anisotropy (PMA), one of which involve the exchange bias – a phenomenon occurring at the FM/AFM interface, where FM designates ferromagnetic metal, and AFM – antiferromagnetic metal. Using antiferromagnets that contain heavy normal metal in the composition, it becomes possible to implement field-free switching using a spin Hall effect.
Structural and magnetic properties of two-layer FM/AFM heterostructures were investigated. Here, the Mn_xPt_{1-x} intermetallic compound was used as an antiferromagnet, and ferromagnetic layer was made of permalloy ($Ni_{81}Fe_{19}$ or Py). It was found that the synthesized epitaxial and polycrystalline heterostructures crystallized in tetragonal $L1_0$-phase. Magnetocrystalline anisotropy in the plane of epitaxially grown on MgO substrates Py layers was found.

Traditionally, spin Hall effects are investigated by the spin-torque ferromagnetic resonance (ST-FMR) method using coplanar wave-guide. In our work, inverse spin Hall effect (ISHE) was studied with the cavity-based FMR method in the X-band (~ 9.4 GHz). A broadening of the resonance lines of AF/F heterostructures was found in comparison with single F-layers. For the first time, spin-pumping-induced ISHE voltage signal generated in the Mn_xPt_{1-x}/Py heterostructure was registered at Kazan Federal University. Based on the experimental data, Hall angle values for antiferromagnets containing various amounts of heavy normal metal were estimated.

Structural features of kaolinite from the weathering crust according to EPR data

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Kaolinite is one of the most common clay minerals. In nature, most often it formed during the processes of chemical weathering or hydrothermal changes in rocks. Kaolinite has an important and various industrial significance, and it is necessary to take into account its morphological and structural-crystalline features. Currently, the assessment of the structural and morphological parameters of kaolinite carried out using various methods. In this work, the degree of perfection of the kaolinite crystal structure was assessed by several parameters obtained by X-ray diffraction analysis of the clay fraction (indices HI, AGFI, IK; CSR size; dimethyl sulfoxide (DMSO) intercalation [1, 2] and other techniques), scanning electron microscopy, and also the method of electron paramagnetic resonance (EPR), which is the most important for determining the structural features of minerals.

The work is devoted to a detailed study of kaolinite from weathering crust along the rocks of the crystalline basement of the Volga-Ural region based on the study of geological materials from the drilling of prospecting, exploratory and deep wells. Kaolinite, together with chlorite, illite, and illite-smectite, are the main minerals in the clay component of the weathering crust, the percentage of which varies depending on the zone of the weathering profile. It has been established that in most of the studied wells, kaolinite prevails among clay minerals and is the end product of the weathering process, its percentage increases in the upper zones of the weathering profile.

The data obtained show that the degree of crystalline perfection of kaolinite improves from bottom to top along the weathering profile; this reflected in the increase in the values of the HI and AGFI indices, and the decrease in IK. The reaction rate upon intercalation with DMSO also depends on the degree of "crystallinity" and morphology of the studied kaolinites. The EPR data also confirm that kaolinite with the best structural and morphological parameters will be characteristic of the upper zones of the weathering profile.

The EPR spectra of kaolinite characterized by the presence of two groups of signals associated with local defects in the structure. Narrow lines in the region of g≈2.0 (signal A), which correspond to electron-hole centers and appear during isomorphic substitutions of cations in the octahedral layers. Most likely, these are (O^--Mg^{2+}) complexes replacing ($O^{2-}Al^{3+}$) [3, 4]. Signal B in the g≈4.3 region, which has the form of a triplet, binds to Fe^{3+} ions [5]. In this case, the outer (lateral) lines of the triplet B – Fe(II) – correspond to the substitutions $Fe^{3+} \rightarrow Si^{4+}$ on the side surfaces of the mineral particles, while the central line – Fe(I) – refers to Fe^{3+} in tetrahedral positions inside the crystallites and on the basal surfaces [3].

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Generation and detection of spin current in iridate/manganite heterostructures

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We present a result on experimental studies of the spin current generation by a microwave spin pumping at GHz frequencies under conditions of the ferromagnetic resonance (FMR) in an epitaxial iridate/manganite heterostructure $SrIrO_3/La_{0.7}Sr_{0.3}MnO_3$. At FMR the microwave magnetic field component interacts with a magnetization of the $La_{0.7}Sr_{0.3}MnO_3$ film forcing a spin current j_s to flow perpendicular of the $SrIrO_3/La_{0.7}Sr_{0.3}MnO_3$ interface. The j_s. value is determined by a spin mixing conductance $g^{\uparrow\downarrow}$,which has a real part ($\mathrm{Re}g^{\uparrow\downarrow}$) and an imagery part ($\mathrm{Im}g^{\uparrow\downarrow}$), and by a precession amplitude of the magnetic moment *m*, caused by the microwave field:

$$j_S = \frac{h}{4\pi}\left(\mathrm{Re}g^{\uparrow\downarrow} m\frac{dm}{dt} + \mathrm{Im}g^{\uparrow\downarrow}\frac{dm}{dt}\right). \quad (1)$$

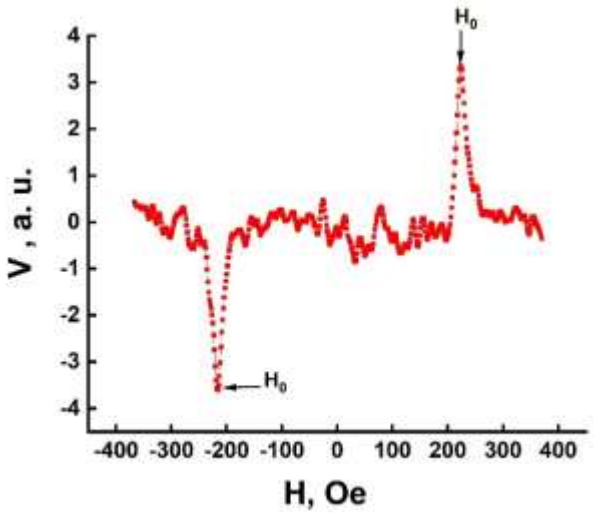

Fig. 1. Magnetic field dependence of voltage response, caused by spin current of $SrIrO_3/La_{0.7}Sr_{0.3}MnO_3$ heterostructure at 30 mW spin pumping, f= 2.3 GHz, T=300 K

Because of the inverse spin-Hall effect, a charge current j_Q appears, which is characterized by the parameter – a spin-Hall angle θ_{SH}:

$$\overrightarrow{j_Q} = \theta_{SH}\frac{2e}{\hbar}\left[\vec{n} \times \overrightarrow{j_S}\right]. \quad (2)$$

Fig. 1 shows, that a changing direction of the magnetic field H the response signal changes its sign in accordance to (2), as the direction of the unit vector ***n*** is changed. The spin magnetoresistance, which allows us to evaluate θ_{SH} that characterizes the efficiency of the spin current conversion to the charge current will be discussed as well. The relation of the spin current to the charge current was evaluated from magnetic field angle dependencies of the spin magnetoresistance. It is important to note, that key feature of the 5d transition metal oxide $SrIrO_3$ is that it exhibits besides an electron-electron interaction also a very strong spin-orbital interaction.

This work was supported by the grant of Russian Science Foundation, project no. №23-79-00010.

Electron Spin Resonance in $EuSn_2As_2$ Crystal Near the Magnetic Ordering Temperature

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In recent years, magnetic topological insulators attract a lot of attention of researchers due to the possibility of their application in spintronics. The interaction between magnetic moments and surface states can lead to many exotic effects, including the anomalous quantum Hall effect and the spin valve effect. $EuSn_2As_2$ is one of the representatives of this family of materials. Overall, the electronic and magnetic properties of the $EuSn_2As_2$ compound are well studied. However, some features of its magnetic structure remain unclear and continue to be discussed.

The $EuSn_2As_2$ compound is one of the recently discovered promising magnetic topological insulators. It crystallizes in a Bi_2Te_3 type structure with rhombohedral (R-3m) symmetry and consists of SnAs bilayers interconnected by hexagonal crystalline Eu layers via the van der Waals bond.

The purpose of this work is to study the process of transition of the $EuSn_2As_2$ crystal to the magnetically ordered state near the ordering temperature of europium magnetic moments (T_m~24K). In this paper, temperature dependencies of magnetic susceptibility and parameters of electron spin resonance spectra (ESR) measured at applied magnetic field with both perpendicular and parallel to *c*-axis orientations were investigated and analyzed to establish peculiarities of the $EuSn_2As_2$ magnetic state. The presence of two types of ESR signals, which are presumably associated with different types of magnetic ordering in the normal and defective areas of the crystal, was revealed.

This research was supported by Russian Science Foundation, Grant No. 21-72-20153.

Approaches to determining the glass transition temperature of polymers by computer simulation

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At present, artificial polymers and polymeric materials are extremely important in human life. It is impossible to overestimate the role of polymers and products made from them in all branches of modern industry. Polybutadiene is a synthetic elastic polymer with high wear resistance. The share of polybutadiene rubber accounts for about a quarter of the total world consumption of synthetic rubbers. It is mainly used in the manufacture of tires and is also used as an additive to improve the toughness of plastics.

One of the key parameters when using polymeric materials is the glass transition temperature, which is determined by the chemical composition and structure of polymer chains. Depending on the temperature, polymers can be in a glassy, highly elastic or viscous state. This parameter is not a strictly defined value, since the transition to the glassy state occurs in a fairly wide temperature range. The difficulty in determining the glass transition temperature can be explained by the fact that polymer structures contain not only amorphous regions, but also crystalline ones. In addition, for the same structure, the properties may depend on the distribution of the repeating link. Computer modeling can help in studying the relationship between bulk properties and intermolecular interactions and thus bring us closer to understanding the glass transition phenomenon.

In this paper, various approaches to determining the glass transition temperature of polymers are studied. Using computer simulation, monodisperse amorphous cis-1,4-polybutadiene was studied. Several methods were used to estimate the glass transition temperature: bilinear and hyperbolic approximations; determination using the Tate equation; also the glass transition temperature was estimated from the dependences of the thermal expansion coefficient and total energy on temperature. Using these methods, the glass transition temperature was estimated in the range from 10 K to 800 K and pressure up to 100 MPa. The obtained values are in good agreement with the experimental data.

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Ab initio investigation of heterostructures based on ferroelectric and metal with Rashba splitting

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It is desirable that the materials used in spintronic devices and for the detection of Majorana fermions in solids should have a large and ideal spin-orbit splitting of the Rashba type. Recently, it has been proposed to combine ordered surface doping with interface engineering, i.e. to grow alloy monolayers on an insulating polar surface [1]. The Rashba effect describes the spin-orbit splitting that occurs at surfaces and interfaces as a result of inversion symmetry breaking [2].

In this work, we studied film heterostructures with various combinations of components, for which the presence of a spin–orbit splitting of the Rashba type was assumed [2,3]. In these heterostructures, due to the electron density gradient at the interfaces, a current vortex arises associated with the electron spins. The structural and electronic properties of these systems were studied. An electronic calculation of DFT+*U* was made taking into account the spin-orbit coupling. All calculations were carried out using the VASP program [4] built into the MedeA program [5].

An enumeration of heterostructures based on several ferroelectrics and various heavy metals was made. For each of these heterostructures, the band structures were calculated taking into account the spin-orbit interaction, and on their basis the values of the Rashba parameter α_R characterizing the spin-orbit splitting were obtained [6]. It was investigated how interfacial contact layers, spacing parameters, thickness, interface polarity and ferroelectric polarization affect the values of the Rashba parameter.

The results of this study can be used to develop functional materials for spintronics based on the properties of these compounds.

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Unravelling Magnetic Properties in $LiGdF_4$ via EPR-Spectra Simulation

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The magnetic properties of rare-earth tetra-fluorides, exemplified by $LiGdF_4$, offer a fascinating arena for studying complex competing interactions. These materials are known for their diverse behaviours arising from the delicate balance between competing exchange interactions, dipolar couplings, and single-ion anisotropy. Specifically, $LiGdF_4$ remains disordered down to at least 0.3K [1]. In this study, we delve into the precise modeling of these magnetic interactions using Electron Paramagnetic Resonance (EPR) spectra simulations.

Our investigation begins with considering $LiGd_xY_{(1-x)}F_4$ samples with varying Gd concentrations (x=0.005, 0.05). Magnetisation measurements provide valuable insights into the anisotropic Curie-Weiss temperature, showcasing the complexity involved in accurately determining microscopic spin-Hamiltonian parameters. Electron spin resonance spectroscopy reveals detailed EPR spectra with fine structures attributed to S=7/2 Gd^{3+} ions. Intriguingly, our analysis uncovers additional weak absorption lines, which can be attributed to the coupled pairs of Gd ions.

Our approach is rooted in the meticulous modeling of EPR spectra. Through exact diagonalisation of the spin-Hamiltonian, both for individual spins and coupled pairs, we perform comprehensive simulations. Leveraging the local symmetry of Gd^{3+} ions, we deploy Stevens operators to characterise anisotropy effects. Our modeling process intricately involves sub-level energy calculations, transition frequency determinations, and matrix element evaluations.

We have successfully determined single-ion anisotropy parameters and g-factors from single-ion spectra simulations and the allowed interval for the AFM exchange constant for the nearest-neighbour spin pairs J_{NN} from a series of EPR-spectra simulations analogous to those mentioned above, for two S=7/2 Gd^{3+} ions with the spin-Hamiltonian including Heisenberg exchange and dipolar coupling, as well as the single-ion contribution and magnetic field. This procedure leads to a satisfactory agreement between experiment and simulation for all distinguishable components in the presence of a significantly more pronounced single-ion spectral background.

In summary, our work not only sheds light on the magnetic properties of $LiGdF_4$ but also demonstrates the power of simulation techniques in deciphering the behaviour of quantum systems.

The work was supported by Russia Science Foundation Grant 22-12-00259, results are published [2].

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Magnetocaloric properties of the $LiGdF_4$ single crystal

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Double fluorides $LiREF_4$ (RE = Gd-Yb) have gained attention as model objects in physics of dipolar magnetism. These fluorides share scheelite type, $I4_1/a$ crystal symmetry; primitive cell contains two magnetically equivalent rare-earth RE^{3+} ions at sites with the S_4 point symmetry that compose two sublattices [1]. The most isotropic material in this fluoride family is $LiGdF_4$ since Gd^{3+} ions in the *s*-state have the spin-only angular momentum $S = 7/2$. This material was recently recognized as an excellent refrigerant material for the low-temperature magnetic cooling, but there is an apparent lack of knowledge on its basic magnetic properties. In particular, no magnetic ordering was observed so far down to temperatures of 0.3–0.4 K [2]. The delayed magnetic ordering can presumably originate from a fine balance of dipolar and exchange interactions that has been found recently [3].

We report the detailed study of the magnetocaloric effect (MCE) in a dipolar-Heisenberg magnet $LiGdF_4$ using magnetization measurements performed on a single crystal sample. Entropy variation on isothermal demagnetization from the magnetic field up to 3 T is determined in the temperature range of 2–10 K for two principal directions of the applied field (parallel and perpendicular to the tetragonal *c*-axis of the crystal). The MCE is found to be highly anisotropic, with the cooling efficiency being up to twice higher at $\mathbf{H} \parallel c$. The results are nicely interpreted in the frame of a conventional molecular field approach taking into account considerable anisotropy of the paramagnetic Curie-Weiss temperature. These results are compared to earlier studies of MCE in powder samples of $LiGdF_4$ [2] as well as with analogous data for other well known magnetocaloric materials. Our findings may open new possibilities to enhance the efficiency of magnetic refrigeration in the liquid helium-4 temperature range.

The work (sample growth and data processing) was supported by Russian Science Foundation, Grant No 22-12-00259 and by Basic research program of HSE University. Magnetometry studies were supported by Kazan Federal University Strategic Academic Leadership Program (PRIORITY-2030).

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Ab initio magnetic properties simulation of nanoparticles $LiTbF_4$, $LiDyF_4$, DyF_3, TbF_3

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Nanoparticles based on rare earth fluorides were actively investigated due to variety of possible applications in medicine [1] and biotechnology [2]. In this regard, it becomes desirable to know the volume distribution of the magnetic moment in rare earth fluoride nanoparticles. Examination of this feature in experiments is a difficult task, therefore, the use of computer modeling methods is a preferable method.

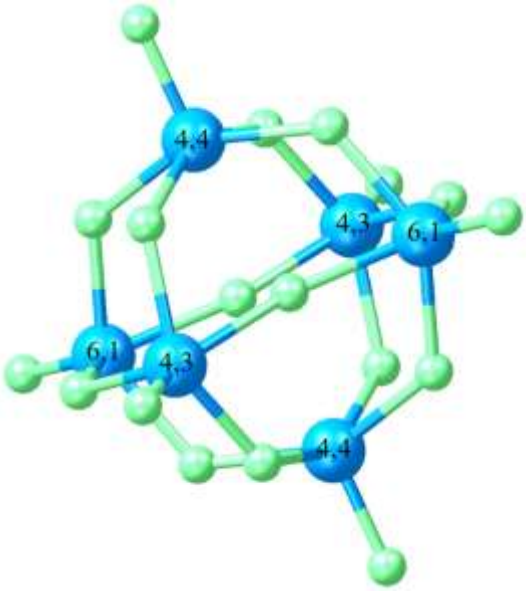

Fig. 1. Optimized DyF_3 nanoparticle with a size of 8Å, 26 atoms; numbers are the values of the magnetic moment for atoms

In this work, using DFT calculations within the Medea software package, nanoparticles of dipole magnets $LiTbF_4$, $LiDyF_4$, DyF_3, TbF_3 with dimensions of 8,10,12,15 Å have been simulated. Structural optimization was carried out for the obtained models. Using the VASP 6 module, the magnetic moments of the structures were calculated and the distribution of ions over the surface was analyzed.

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High-frequency dielectric anomaly in a quasy-2D square kagomé lattice nabokoite family compounds

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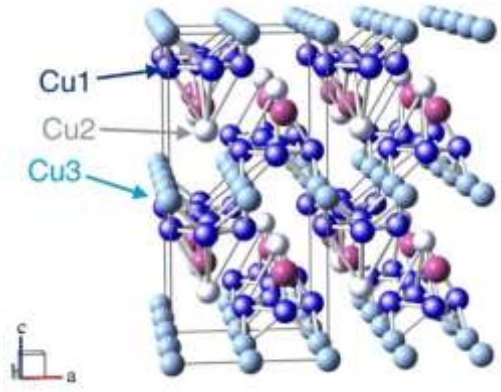

Fig. 1. General view of the structure of the nabokoite family compounds. Blue, white, and cyan balls indicate 3 non-equivalent positions of copper ions; pink balls indicate the positions of alkaline ions

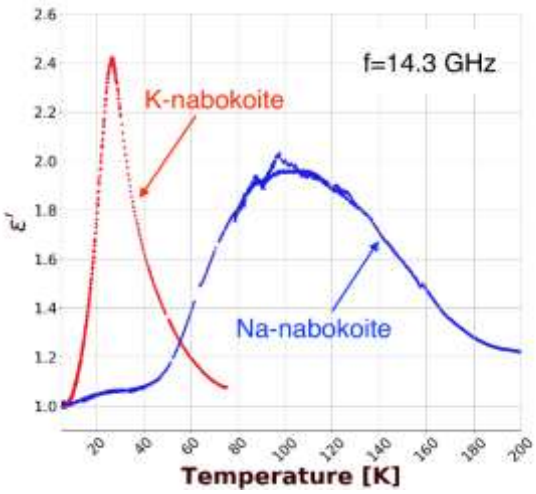

Fig. 2. Temperature dependence of the real part of the dielectric permittivity of potassium (red) and sodium (blue) compounds of the nabokoite family

Nabokoite family compounds $ACu_7(TeO_4)(SO_4)_5Cl$ (A=K, Na, Cs, Rb) are among the few systems in which a frustrated magnetic subsystem of the square kagomé lattice (SKL) type is formed [1,2]. These compounds have a layered structure (Fig. 1). Quasi-two-dimensional layers are formed by copper ions in Cu1 and Cu3 positions, while ions in Cu2 position 'decorates' SKL layers. Curie-Weiss temperature for nabokoites is 100-200 K, but traces of magnetic order are observed for some of these compounds only below 4.5 K [2], indicating broad temperature range for spin-liquid physics. Earlier studies of K-nabokoite [1] revealed dielectric anomaly at 24 K. The change in dielectric properties can be related to a rearrangement of the crystal structure of the sample leading to a change of exchange bonds and, finally, to the magnetic ordering.

We have studied ultra-high-frequency (9-14 GHz) dielectric properties of the nabokoite family compounds in the temperature range 1.7-300 K. Nabokoite sample was placed in microwave cavity, variation of the cavity eigen-frequency and Q-factor with temperature allowed to determine ε' and ε'' temperature dependences. We have observed dielectric anomalies (both in real and imaginary parts of dielectric permittivity) for K- and Na-nabokoites

at ≈25 and ≈105 K, correspondingly (Fig.2). No dielectric anomaly of comparable amplitude was observed for Rb- and Cs-nabokoites over the studied temperature range.

The work was supported by Russia Science Foundation Grants 22-12-00259 (ultra-high-frequency measurements) and 23-23-00205 (samples preparation).

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Synthesis and magnetic properties of oxides $La_2Zr_2O_7:Nd^{3+}$ and $SrY_2O_4:Sm^{3+}$

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Pyrochlore oxides are the subject of extensive research because of their amazing magnetic properties caused by geometric frustration that appears due to the location of magnetic ions in the lattice [1]. Pyrochlore oxides of the type $R_2Zr_2O_7$ (R-rare earth ion) have a face-centered cubic structure, with the space group$Fd\overline{3}m$ (No. 227) [2]. Strontium oxides $SrY_2O_4:R^{3+}$ are also geometrically frustrated magnet, the crystal structure is orthorhombic with the space group P_{nam} [3]. The sample $(La_{1-x}Nd_x)_2Zr_2O_7$ (x=2%) synthesized by a solid state reaction method. A single crystal of SrY_2O_4 doped with Sm^{3+} ions (2 %) was grown by the optical floating zone technique. Chemical composition control and crystallinity confirmation were carried out using X-ray diffraction analysis on Bruker D8 Advance Cu Ka, λ=1.5418 Å.

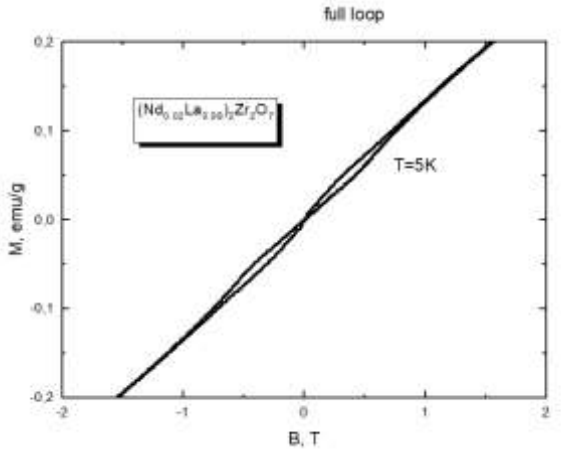

Fig.1. External magnetic field dependence of the magnetization (M) $(La_{0.98}Nd_{0.02})_2Zr_2O_7$ at a temperature of 5 K

In this work, the temperature (5 –305 K) and magnetic field (0 – 9 T) dependences of the magnetization of the samples were measured using by vibration sample magnetometer *PPMS*® system. The modelling of the energy spectrum and magnetization in the model of exchange charges in the full basis of the electronic configuration Nd^{3+} $4f^3$ is carried out. Experimental data and simulations agree both qualitatively and quantitatively for the powder sample $(La_{0.98}Nd_{0.02})_2Zr_2O_7$. In this paper, For the first time, an anomalous behaviour of the Nd^{3+} magnetic moment was observed in a micro powder $(La_{0.98}Nd_{0.02})_2Zr_2O_7$. A butterfly-shaped hysteresis was detected at a temperature of 5 K (insert in Fig. 1). The EPR spectra were measured and analyzed, it's temperature dependence was constructed. Further theoretical study of this effect is required.

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Table of contents

T A B L E O F C O N T E N T S

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Digital typesetting
E.I. Boltenkova, A.V. Bogaychuk

Cover design
D.A. Tayurskii

Supported by:

MINISTRY OF SCIENCE AND HIGHER EDUCATION OF THE RUSSIAN FEDERATION

Kazan Federal UNIVERSITY

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