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

ACTUAL PROBLEMS OF MAGNETIC RESONANCE AND ITS APPLICATION

XXII International Youth Scientific School

ACTUAL PROBLEMS OF MAGNETIC RESONANCE AND ITS APPLICATION
KAZAN

Euro-Asian Symposium «Trends in Magnetism»: EASTMAG-2022
Kazan, Russia, August 22-26, 2022

Program and Proceedings

Kazan
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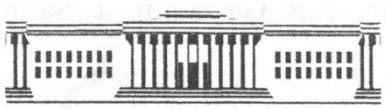

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ISBN 978-5-00130-624-5

This collection contains the reports of young scientists submitted to the XXII 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
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ISBN 978-5-00130-624-5

Program

Wednesday, August 24

10:00 – 10:15 **G.A. Bochkin**, "MQ NMR dynamics in an inhomogeneous spin chain"

10:15 – 10:30 **I.D. Lazarev**, "Skew Wigner-Yanase information and its extensions in MQ NMR spectroscopy"

10:30 – 10:45 **S.A. Lopatina**, "Spin and isospin properties of two-dimensional semiconductor structures"

10:45 – 11:00 **G.A. Nikolaev**, "Anomalous spin resonance around even fillings in a strongly correlated 2D electron system"

11:00 – 11:30 **Coffee break**

11:30 – 11:45 **M. Smirnov**, "Application of high-resolution ^{1}H NMR for the research of various types of vegetable oils"

11:45 – 12:00 **M.V. Stepushkin**, "Influence of a change in the domain structure on the Hall effect in CoPt thin films"

12:00 – 12:15 **N. Snegirev**, "Singularity of a hyperfine structure in Mössbauer spectra under combined magnetic dipole and electric quadrupole interaction"

12:15 – 12:30 **A.Yu. Germov**, "Hyperfine fields in ferromagnetic nanoparticles according to NMR data in a local field"

12:30 – 12:45 **Yu.N. Koemets**, "Effect of strain rate on magnetic transformation of L-Pbf medical steel 316L"

12:45 – 13:00 **A.A. Seryapina**, "Search for metabolic markers of essential arterial hypertension in rats"

13:00 – 14:00 **Lunch**

14:00 – 14:15 **Yu. Slesareva**, "Transient phenomena in multi-pulse protocols in solid-state ^{1}H NMR in Cu- and Ni-oxamidato complexes"

14:15 – 14:30 **D.V. Shurtakova**, "Calculated and experimental the EPR spectra parameters of impurity centers in tricalcium phosphate"

14:45 – 15:00 **K.R. Mirsalimova**, "Crowding-agents influence on BSA translational diffusion by pulsed field gradient NMR"

15:15 – 15:30 **A.S. Parfishina**, "Van Vleck paramagnets – new features in comparison of $LiTmF_4$ and $Li(Tm_{0.02}Y_{0.98})F_4$: NMR study"

15:45 – 16:00 **R.F. Likerov**, "The CW EPR and pulsed EPR studies of the $^{51}V^{4+}$ ions in $Sc_2{}^{28}SiO_5$"

16:00 – 16:30 **Coffee break**

16:30 – 16:45 **D.V. Popov**, "ESR measurements of ludwigite $Mn_{1.17}Co_{1.83}BO_5$"

16:45 – 17:00 **G.Iu. Andreev**, "Investigation of magnetization and magnetostriction in lithium – ytterbium tetrafluoride"

17:00 – 17:15 **D.E. Zheleznyakova**, “Magnetic Fluctuation Effect in Microwave Absorption of the $EuFe_2As_2$ Crystals Near the Magnetic Ordering Temperature”

17:15 – 17:30 **T.N. Enderova**, “High-frequency Nonresonant Microwave Absorption Study of Transport Properties of the $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$ Topological Insulator”

17:30 – 17:45 **A.M. Garaeva**, “Study of magnetic properties for micro- and nanoscale DyF_3 powders”

17:45 – 18:00 **A.H. Kadikova**, “Synthesis and magnetic properties of thin film systems Fe_3Al and Fe_3Al/Pt”

18:00 – 18:15 **Chisom P. Ezeamaku-Humphrey**, “Magnetic Resonance Imaging and Kids: Clinical Applications and Challenges”

MQ NMR dynamics in an inhomogeneous spin chain

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We consider multiple quantum (MQ) dynamics of a spin-1/2 chain with arbitrary DDI constants (they can, for example, be all different) in the approximation of nearest neighbor interactions. In an MQ NMR experiment, the system is subjected to a sequence of resonant RF pulses, and we assume that the evolution is described by the average Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N-1} D_{i,i+1}\left(I_i^+ I_{i+1}^+ + I_i^- I_{i+1}^-\right), \tag{1}$$

where N is the number of spins in the chain, $D_{i,i+1}$ is the dipolar coupling constant between spins i and $i+1$, I_i^+ and I_i^- are, respectively, the raising and lowering operators acting on spin i. We assume that the system is initially in the thermal equilibrium state.

The Jordan-Wigner transformation allows us to transform our spin system into a system of non-interacting fermions. It also allows us to show that the MQ NMR spectrum consists of MQ coherences of order 0 and ±2 only.

We obtain the following expression for the intensity of MQ coherences of order ±2:

$$J_{\pm 2}(t) = \frac{1}{2N}\sum_k \sin^2(2\mu_k t), \tag{2}$$

where N is the chain length, t is the duration of the RF pulse sequence, and μ_k are the single-fermion energies, the eigenvalues of the matrix ½D, where D is:

$$D = \begin{pmatrix} 0 & D_{1,2} & 0 & \dots & 0 \\ D_{1,2} & 0 & D_{2,3} & \dots & 0 \\ 0 & D_{2,3} & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & D_{N-1,N} \\ 0 & 0 & 0 & D_{N-1,N} & 0 \end{pmatrix} \tag{3}$$

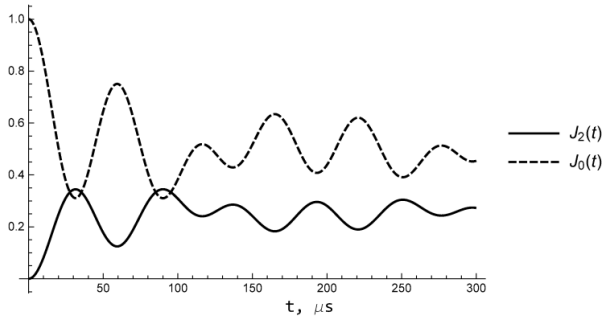

Fig.1. Theoretical evolution of MQ coherences of order 0 and ±2 in a chain where $D_{3k+1,3k+2} = 2\pi\cdot 6096$ s^{-1}, $D_{3k+2,3k+3} = 2\pi\cdot 4444$ s^{-1}, $D_{3k,3k+1} = 2\pi\cdot 3339$ s^{-1}

The intensity of order-0 MQ coherence $J_0(t)$ can then be obtained from the formula

$$J_0(t) + J_2(t) + J_{-2}(t) = 1 \tag{4}$$

As an example, we calculate the evolution of MQ coherences for a chain where three nearest-neighbor DDI constants cyclically repeat, that is, $D_{3k+1,3k+2} = 2\pi\cdot 6096$ s^{-1}, $D_{3k+2,3k+3} = 2\pi\cdot 4444$ s^{-1}, $D_{3k,3k+1} = 2\pi\cdot 3339$ s^{-1}, and chain length N=400 (see Fig. 1) and a chain with two alternating DDI constants (such chains can be found, for example, in hambergite crystals).

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Skew Wigner-Yanase information and its extensions in MQ NMR spectroscopy

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Wigner and Yanase introduced [1] the notion of skew information to quantify the information content of quantum states in the presence of conserved quantities. Later, Luo demonstrated [2] that the statistical idea underlying the skew information is the Fisher information in the theory of statistical estimation and introduce skew information as a new uncertainty relation. Since uncertainty relation is a core issue in quantum mechanics and quantum information theory, many extensions and generalizations of the quantity (like Wigner-Yanase-Dyson information) have been developed. Moreover, skew information as well as the Fisher information allows [4] the development of powerful methods for the investigation of entanglement, including many-particle entanglement.

Now we review various skew information notions and develop [5, 6] experimental methods for measuring them within MQ NMR. In particular, we demonstrate [6] that the Wigner–Yanase information in a spin system (s = 1/2) with the dipole–dipole interactions (DDI) in the MQ NMR experiment at the system temperature T equals the double second moment of the MQ NMR spectrum obtained at the temperature 2T. Using the properties of the skew information, we investigate many-spin entanglement within the MQ NMR spectroscopy. We perform a comparison of an estimation of the entangled cluster size obtained with Fisher information and Wigner–Yanase information. We use a nonspherical nanopore filled with a gas of spin-carrying atoms (for example, xenon) or molecules [5, 7] and a zigzag chain [8] in a strong external magnetic field as models for a comparison of the dependencies of numbers of the entangled spins on the temperature.

We acknowledge funding from the Ministry of Science and Higher Education of the Russian Federation (Grant No. 075-15-2020-779)

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Spin and isospin properties of two-dimensional semiconductor structures

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Modern trends in condensed matter physics widely include research of spin properties of heterostructures based on AlAs. This material is an interesting target because it has large effective mass. Due to that fact, there is a domination of electron-electron interaction over kinetic energy which leads to a higher significance of many-particle effects. These research rely not only on fundamental, but also on practical interest from the point of producing isospin-based logic elements, so called "valleytronics"[1] (from valley + electronics) in analogy with spintronics. The underlying reason for this similarity can be connected with SU(2) symmetry group, which exists for both spin and valley degrees of freedom.

In this work relative valley population and spin and isospin ferromagnetic phase transition in the AlAs-based heterostructures is investigated in the Quantum Hall Effect (QHE) regime. Experiments were held 0.5 K provided by He-3 cryostat and in magnetic fields up to 15 T. Due to g-factor anisotropy in X and Y valleys, the single particle spin splitting was different for certain orientation of the in-plane component of magnetic field in direction [010]. So, that we could probe electron spin resonance (ESR) from each valley separately, allowing us to estimate their relative population. Analysis of measured data allowed us to estimate relative valley occupancy. Energy spectrum and valley occupancy can be modified by applying tilted magnetic field [2] or applying mechanical strain [3, 4]. Experiment is implemented using the method of ESR detection based on high sensitivity of longitudinal magnetoresistance of two-dimentional electron system due to microwave irradiation absorption [5]. This research has uncovered a spin and isospin ferromagnetic transition in the QHE regime near filling factors $\nu = 2, 3$.

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Anomalous spin resonance around even fillings in a strongly correlated 2D electron system

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The electron spin resonance (ESR) was studied in a two-dimensional strongly correlated electron system confined at ZnO/MgZnO heterojunction in the regime of the quantum Hall effect (QHE). By gradually tilting the external magnetic field with respect to the sample surface we were able to induce ferromagnetic phase transition near the exactly even filling factors of QHE [1]. The change of spin properties in the electron system, associated with the phase transition, was studied using ESR. The detection of the spin resonance was based on the extreme sensitivity of the longitudinal resistance of the 2D channel to the microwave radiation absorption [2]. Thus, ESR is observed as a peak in the longitudinal resistance at a fixed frequency when the magnetic field is swept.

At odd filling factors, as expected, ferromagnetic ground state is realized and we observed ESR with usual characteristics. For instance, at odd fillings the absorption of electromagnetic radiation induces the resonant heating of the 2D electron system that causes the rise of the sample resistance. But the physical picture becomes much more interesting at even filling factors. At zero tilt angle, the ground state of the system is believed to be paramagnetic, so ESR should not be observed. Yet, we see ESR under these conditions and, surprisingly, the ESR is detected as a resonant dip in the magnetoresistance as if the electron system is cooled due to the microwave absorption. Such anomalous behavior contradicts previous experimental observations made on electron systems with rather small strength of e-e interactions.

Gradual increase of the tilt angle allowed us to capture the evolution of the key ESR characteristics as the system continuously approached the ferromagnetic phase transition. Surprisingly, the electron spin resonance retained its “heating” behavior in the ferromagnetic phase at even fillings.

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Application of high-resolution ^{1}H NMR for the research of various types of vegetable oils

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Vegetable oils are an important component in the human diet. A significant problem is to determine the quality of oils consumed in food. Some types of vegetable oils are vulnerable to counterfeits, because the production volumes of these types of oils are very limited [1]. The NMR spectroscopy method has good prospects for application in the food industry, since it does not require special sample preparation, and is also a non-destructive method [2].

The aim of this work was, using high-resolution ^{1}H NMR spectroscopy, to determine the percentage of essential fatty acids of three different types of vegetable oil: sesame, sunflower and olive. It was also necessary to investigate the possibility of using NMR relaxometry to detect differences between samples.

High-resolution NMR spectra were obtained on a Varian 400 MHz high-resolution NMR spectrometer with a constant magnetic field B = 9 T. To measure the relaxation times T_1 and T_2, the inversion-recovery and CPMG sequences were used, respectively.

^{1}H NMR high resolution spectra of vegetable oil samples were obtained. The relative integral intensity of the signals in the spectrum was calculated using the MagicPlot program. To calculate the percentage of fatty acids in the samples, the method proposed in the article [3] was used. The content of essential fatty acids was calculated, the results are presented in Table 1. The obtained values were compared with literature data [4].

Oil type	Linolenic acid, %	Linoleic acid, %	Mono-unsat. FA, %	Sat. FA, %
Sesame	0,7	43,4	39,3	16,6
Sunflower	0,8	45,3	32,9	21
Olive	1,5	41,4	35,6	21,5

Table 1. Percentage of essential fatty acids in vegetable oil samples

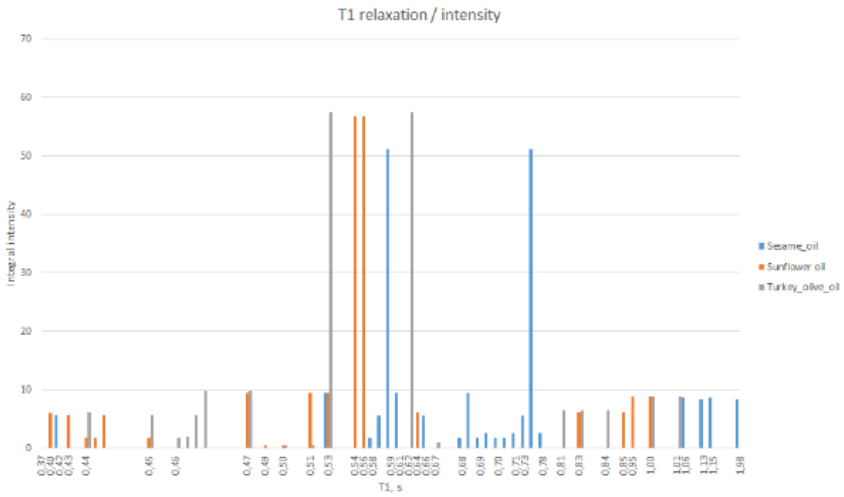

Fig.1. Dependence of proton relaxation times T1 on the integral intensity of the signal of three vegetable oil samples

The high-resolution NMR method makes it possible, firstly, to measure the relaxation times of all nonequivalent protons in a sample, and secondly, to estimate the fraction of nonequivalent protons with relaxation times related to certain time ranges. Figure 1 shows the dependence of the measured relaxation times T_1 of vegetable oil samples on the relative intensity of the corresponding signal in the relaxation spectrum.

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Influence of a change in the domain structure on the Hall effect in CoPt thin films

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Ferromagnetic/heavy metal films, in which skyrmions can be formed, are a promising material for creating memory elements and spintronic devices. When used in electronic devices, one of the most effective ways to detect skyrmions can be the Hall effect. To measure it, a Hall cross structure is formed on the film, and the smaller the size of the cross, the greater will be the contribution of a single skyrmion. Ideally, when the cross is comparable in size to the skyrmion. However, as the size decreases, the influence of the film boundaries increases, which can affect the mobility of the skyrmions or the accuracy of measuring the Hall effect.

To study the effect of a change in the domain structure on the Hall effect, samples containing two Hall crosses 5x5 μm in size were fabricated from the 8 nm thick film containing 10 Co and Pt bilayers (thicknesses of 0.3 and 0.5 nm, respectively). Further, one of the crosses was left unchanged, and the second was cut with the needle of an atomic force microscope (AFM), which reduced the size of the working area to 0.5x0.5 μm. A comparison of the Hall magnetization reversal curves showed that the cuts do not make a significant contribution to the film parameters.

The film magnetization reversal and its effect on the Hall effect were studied using AFM. The sample was initially demagnetized, after which the working area of the cross was successively magnetized by the AFM magnetic needle. The probe moved along a line close to the surface, which locally magnetized the area near this line. During this, a change in the Hall voltage was recorded. Next, the magnetic force microscopy (MFM) image of the domain structure of the working area was scanned; the line was shifted, and the process was repeated — Figs. 1, 2. The processed line is shown in white, the cuts are green. Fig. 3 shows the change in the Hall effect for all passes. As expected, as the magnetized region expands, the change in the Hall voltage increases. There is an anomalous segment where the Hall effect first decreases, but then increases again. Comparison with magnetic images explains this effect. It is due to the spatial inhomogeneity of the magnetic fields generated by the AFM probe.

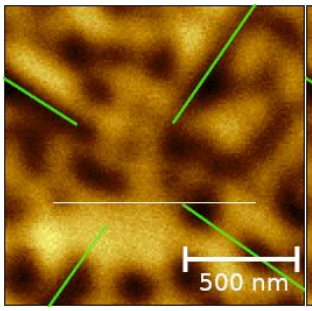

Fig. 1. MFM image on the 18th pass

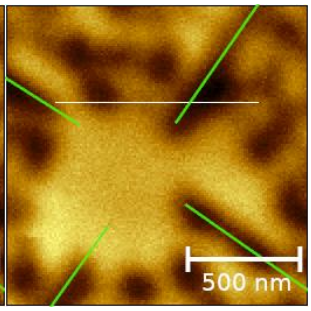

Fig. 2. MFM image on the 50th pass

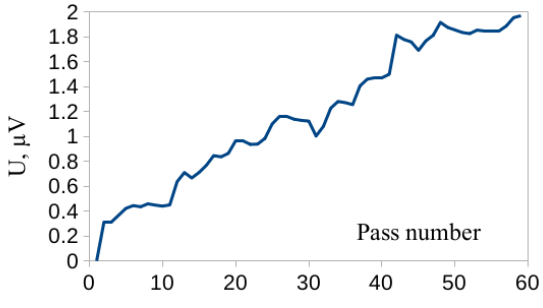

Fig. 3. Hall effect with successive magnetization reversal

Singularity of a hyperfine structure in Mössbauer spectra under combined magnetic dipole and electric quadrupole interaction

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It is known that at Mössbauer resonance, energy transitions occur between the excited and ground sublevels of ^{57}Fe nuclei. In a magnetic field, the nuclear sublevels of the ground state of the ^{57}Fe nucleus (spin I_g = 1/2) and the excited state (spin I_e = 3/2) split into two (m_g = ± 1/2) and four (m_e = ± 1/2, ± 3/2) sublevels, respectively (m_i is the magnetic quantum number) [1]. According to the selection rules (Δm = 0, ± 1), six transitions are possible. In this case, the spectra consist of six lines that form the so-called magnetic sextet (fig. 1, a) [1].

However, in many crystals, in addition to the magnetic field, the Mössbauer nuclei can be affected by electric crystal fields, which lead to an additional shift in the nuclear levels of the excited state. Then, to describe the Mössbauer spectra, it is necessary to take into account the combined magnetic dipole and electric quadrupole interactions.

In this case, when the direction of the main axis of the electric field gradient (EFG) is orthogonal relative to the direction of the iron magnetic moment, the appearance of mixed states of the ^{57}Fe nucleus leads to an increase in the number of lines in the spectrum from 6 to 8 (fig. 1, b) [1].

In this work, a theoretical model has been developed to describe nuclear resonance transitions in iron atoms in the approximation of a combined magnetic dipole and electric quadrupole hyperfine interaction. On the example of $FeBO_3$ single crystals, the features of the formation of a hyperfine structure in the Mössbauer spectra in the temperature range of magnetic phase transitions will be discussed. The report will also highlight the importance of considering the effective thickness of the absorber used. We expect that the developed technique and the results obtained will be of wide interest. The main results discussed in the report can be found in the publication [1].

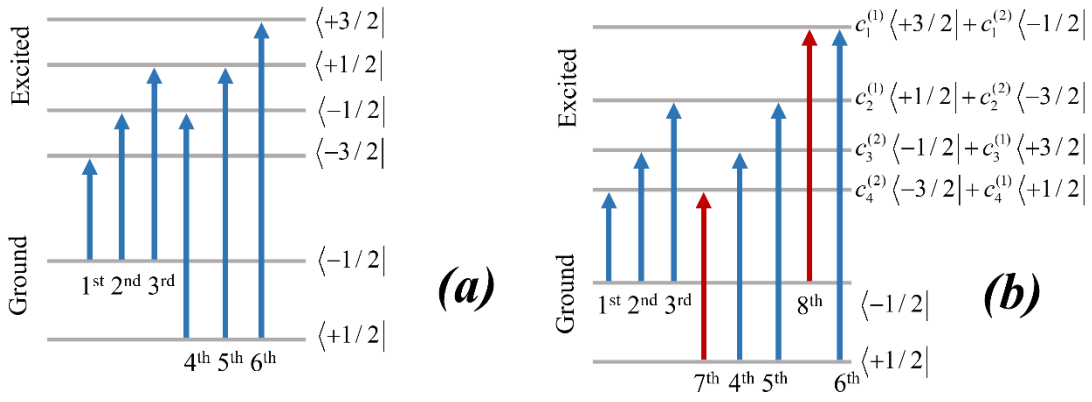

Fig. 1. Diagram of nuclear transitions between the ground and excited states of ^{57}Fe. (a) Only magnetic splitting of nuclear sublevels is present; (b) A combined magnetic dipole and electric quadrupole interaction when the direction of the magnetic hyperfine field is orthogonal to the main axis of EFG

This work was funded by the Russian Foundation for Basic Research, project # 19-29-12016\21-мк.

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Hyperfine fields in ferromagnetic nanoparticles according to NMR data in a local field

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Substantial progress in the area of nanotechnology requires special quality of magnetic nanoparticles. Conventional methods of analysis are not always efficient to the study of nanoparticles. The main methods for investigating nanoparticles are magnetization measurements and electron microscopy. Other conventional methods are found to be inefficient or expensive due to very small particle sizes. Local nuclear resonance methods allow us to solve several problems including phase analysis [1,2,3], analysis of the atomic environment, observation of ordered structures [4], observation a single-domain [5] or superparamagnetic state.

It is well known that the unique properties of nanoparticles are often connected with high specific surface. However, ferromagnetic nanoparticles have peculiarities connected with volume of particles rather than surface. For example, such phenomena as domain walls, single domain state, superparamagnetism depend on size of ferromagnetic cluster, type of atoms, impurities, distance between particles, temperature and external magnetic field.

We used the local field ^{57}Fe,^{59}Co,^{61}Ni NMR in order to study size effects in Fe,Co,Ni nanoparticles, correspondingly. A nanoscale effect has been found. It consists in observation of two lines in NMR spectra corresponding to multidomain and single-domain state. Experimental results of ^{57}Fe NMR of Fe@Fe_2O_3 nanoparticles demonstrate the change of demagnetizing field depending on the average particle size.

Also, the problem of observation of domain walls using NMR has been thoroughly analyzed. We have demonstrated and confirmed that domain walls cannot give an additional line in the local field NMR spectrum, but can create additional pedestal of domain line.

Effect of different type of shell is also investigated on nanoparticles of Ni, Ni@NiO, Ni@C. We have shown that type and width of the «non-magnetic» shell affect only on the distance between particles and their configuration and do not change NMR spectra. For the samples of nickel nanoparticles in a carbon, oxide shell and without it, if the sizes of the nanoparticles are comparable, of the interface plays insignificant role in the observed size effect.

This study was carried out within the state program «Function» № 122021000035-6.

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Effect of strain rate on magnetic transformation of L-Pbf medical steel 316L

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Medical chromium-nickel austenitic steel 316L is used for both veterinary and human medical implants. The development of additive manufacturing technologies (AM) allow using new design solutions for manufacturing of implants. Austenitic steel 316L is considered to be a stable austenitic steel, which is a single-phase paramagnetic FCC austenitic state in the range of all exploitative temperatures. As a general rule, samples manufactured by additive laser technology may have the austenitic state without of residual delta-ferrite phase. Two types of martensite phases can form in the stainless steel 316L. The first one is paramagnetic ε-martensite with HCP crystal lattice, while the other one is ferromagnetic α′-martensite with cubic crystal lattice. The martensitic α′- phase forms during deformation and embrittles steels.

This report presents the results of the investigation of the magnetic properties during deformation processes in samples of 316L medical stainless steel manufactured by laser 3D printing.

Samples of austenitic steel 316L manufactured by laser powder melting (L-PSP) were deformed at room temperature at different compression rates with a testing machine Instron 1342 ($8\cdot10^{-4}$ c^{-1}; $3\cdot10^{-3}$ c^{-1}; $1\cdot10^{-2}$ c^{-1}; $2\cdot10^{-2}$ c^{-1}). Magnetic measurements of deformed samples were performed using a LakeShore 7407 vibrating sample magnetometer at the Institute of Metal Physics. Magnetic field was up to 9 kOe.

The ferromagnetic delta ferrite phase was found in the unreformed L-PBF sample (Fig 1). The coercive force increased sharply after deformation, which was associated with the formation of the ferromagnetic phase of deformation α′-martensite.

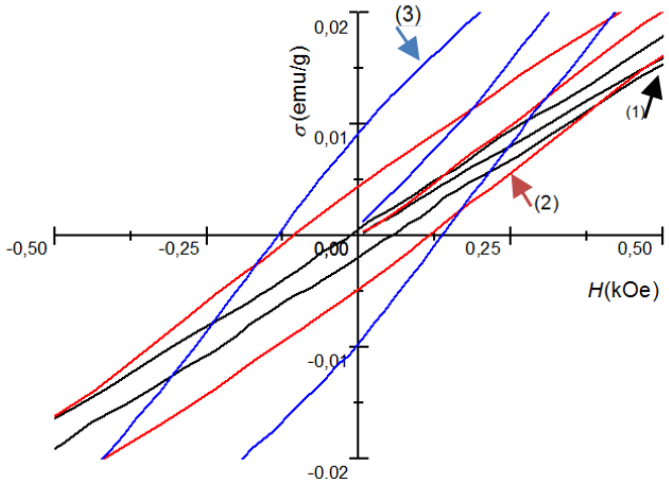

Fig. 1. Results of the magnetic property studied for L-PBF sample (1) before deformation, $8\cdot10^{-4}$ c^{-1} after deformation with rates $8\cdot10^{-4}$ c^{-1} and (3) - with rates $2\cdot10^{-2}$ c^{-1}

The received results are discussed compared with the literature data.

Support by RSF (project No. 22-29-01514) is acknowledged.

Search for metabolic markers of essential arterial hypertension in rats

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Metabolomics, along with proteomics, genomics, and transcriptomics, provides an essential information on molecular mechanisms involved in normal and pathological cellular processes. Thus, metabolomics may contribute to the portrait of various diseases, facilitating therapeutic decision making. It is potentially of an assistance in studying and diagnosing complex, multi-factorial diseases, such as arterial hypertension. Blood pressure is regulated through a number of neuronal and hormonal mechanisms, and when choosing antihypertensive therapy, doctor should be able to define individual's particular characteristics as accurate as possible. Metabolic profiling of pathological conditions is developing rapidly in last few years. Researchers tested a range of detection techniques, and by now, combination of NMR spectroscopy with mass spectrometry is proved to be the most effective and precise method [1].

In our study, techniques of NMR spectroscopy and mass spectrometry were applied to assess metabolic profile of blood serum in hypertensive and normotensive rats, in order to find out if there are prospective biomarkers for hypertensive disease. We used ISIAH rat strain, which is a recognized model of essential arterial hypertension, reflecting both genetic and environmental effects on blood pressure (ISIAH stands for "inherited stress-induced arterial hypertension"). As for normotensive control, WAG rat strain was used.

We analyzed 20 serum samples of 3-month-old ISIAH and WAG male rats (10 animals in each group). Identified were 57 low-molecular metabolites. In order to determine which metabolites explained the most variance, multidimensional analysis (PCA) was performed on the data obtained. PCA identified two principal components explaining in the total 48% of variance between experimental data.

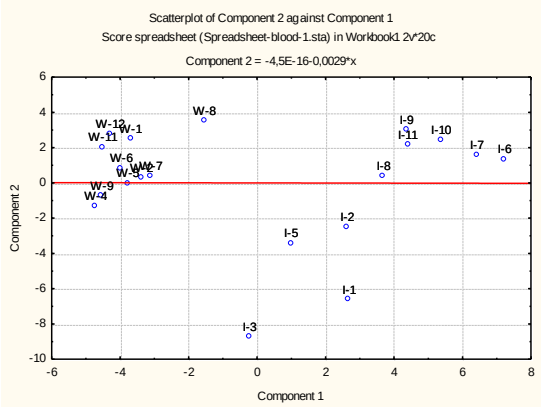

Fig. 1. PCA results for ISIAH (I-X) and WAG (W-X) groups

Distribution of ISIAH and WAG groups in the coordinates of these components demonstrated that first component contributed the most into difference between two strains of rats (Fig. 1). The axis of this component had significant positive loadings from glucose, tryptophan and 2-hydroxyisobutyrate, and negative ones – from methionine sulfoxide and isobutyrate. These findings indicate physiological mechanisms presumably involved in the pathogenesis of hypertension in ISIAH rats: glucose metabolism, gut microbial changes and oxidative stress.

This study was supported by Russian Science Foundation (project No 22-25-20025).
Authors also are thankful to the Laboratory of proteomics and metabolomics of International Tomography Center (SB RAS, Novosibirsk).

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Transient phenomena in multi-pulse protocols in solid-state ^{1}H NMR in Cu- and Ni--oxamidato complexes

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Metal−oxamidato complexes are considered as structural units for new materials for spintronics and quantum computing applications. Carr-Purcell pulse protocol is usually applied to increase the coherence time in presence of the spectral diffusion [1]. Here we present the results of ^{1}H NMR study of Cu(II)-oxamidato complex in comparison with its diamagnetic Ni(II)-containing analog. The presence of magnetic ions creates the inhomogeneous broadening and accelerates the relaxation processes. Given these conditions, we cannot consider the pulse sequences as ones consisting of 90- and 180-degree pulses for all of the resonating nuclei. An improved Carr-Purcell pulse protocol suggested in [2] was applied for the elimination of unwanted echoes. The experiments have shown the presence of a transient phenomenon that should be taken into account when developing the quantum computing protocols.

The reported study was supported by Russian Science Foundation, Research Project № 21-72-10178 (Yu.S.) and № 22-43-04424 (R.Z. and Yu.K.). E.V. would like to thank the financial support from the government assignment for FRC Kazan Scientific Center of RAS.

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Calculated and experimental the EPR spectra parameters of impurity centers in tricalcium phosphate

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Tricalcium phosphate (TCP) is actively used in medical preparations for the restoration and remodeling of bone and dental tissue. There are varieties of β-TCP (chemical formula (β-$Ca_3(PO_4)_2$) and α-TCP (chemical formula (α-$Ca_3(PO_4)_2$) [1]. For biomedical applications, it is necessary to know the exact composition and structure of materials. A good method for studying calcium phosphates is the Electron Paramagnetic Resonance (EPR) method. However, the interpretation of complex spectra causes questions. It is not always definitely to determine to which center one or another resonance line belongs. To confirm the assumptions about impurity centers and their parameters, quantum mechanical calculations of the EPR structure and parameters can be made.

The aim of this work is to obtain information about impurity centers in TCP from the EPR spectra. For this purpose, the description of the EPR spectra of TCP and comparison of the obtained parameters with the calculated ones was made.

The samples of TCP are a powder were obtained at the Baikov Institute of Metallurgy and Materials Science by the wet (precipitation) technique from solutions of nitrates and ammonium hydrogen phosphate. Therefore, the nitrogen center could get into "pure" phosphates.

EPR spectra were obtained on the spectrometer Elexsys-580/680 in the X- and W-bands at room temperature. EPR signals were detected in all samples after the irradiation. To describe EPR spectra we used «MatlabR2010a» with a special module “Easyspin”. Quantum Espresso software was used for quantum mechanical calculations. Calculations were performed for TCP with the replacement of the PO_4 group by the NO_3 group. In this case, it is necessary to compensate for the charge by removing the neighboring calcium ion [2].

Figure 1 shows the EPR spectrum of TCP described with parameters g_x=1.9981, g_y=1.9981, g_z=2.0028, A_x=90 MHz, A_y=100 MHz, A_z=190 MHz. Also, the distribution of parameters of hyperfine splitting of 15-20% was added to the model, which may be associated with the distribution of powders by size.

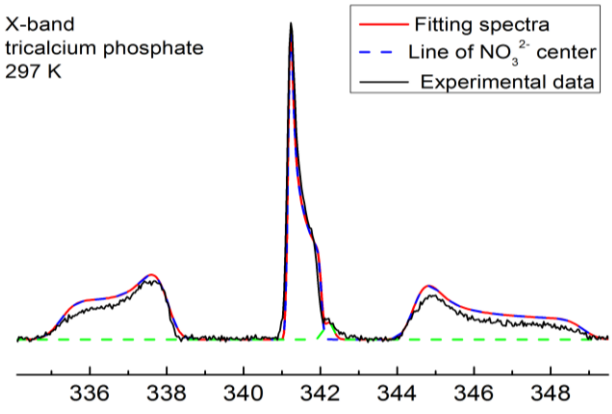

Fig.1. TCP EPR spectra with the fitting in the X- bands

For the nitrogen complex NO_3^{2-} in TCP, g-factors were calculated for four different variants. Each variant differs in surrounding symmetry. The obtained values for different variants differ within less than 0.1%. The values obtained are equal to g_x=1.9972± 0.0005, g_y=1.9976±0.0002, g_z=2.0028±0.0001.

The values obtained from the fitting of the spectrum and from quantum mechanical calculations practically coincide. This makes it possible to confirm the presence of nitrogen impurities in TCP. It can also be argued that quantum mechanical calculations give good agreement with experiment and can later be used to decipher complex spectra.

The reported study was funded by RFBR according to the research project № 20-32-90159

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Crowding-agents influence on BSA translational diffusion by pulsed field gradient NMR

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Bovine serum albumin (BSA) plays a crucial role in the physiologically active compounds transport in living organism. Information on the diffusive transport of proteins in a viscous microenvironment and their interaction consideration are of great importance for protein functioning. The volume of macromolecules in cellular and extracellular makes up 5-40% of the total available volume (macromolecular crowding). One of the most common ways to create macromolecular crowding conditions in vitro is the use of synthetic compounds and proteins as the crowding agents. Crowding agents are commonly affect biomolecules via the effect of excluded volume explained by the impermeability of the biopolymers.

In this work the effect of two crowding agents (glycerol and polyethylene glycol 300) on the self-diffusion coefficient of BSA was shown. The diffusion experiments were carried on the NMR spectrometer Bruker Avance (600 MHz) with the maximum gradient field of 0.55 T m^{-1}. The data analysis allows us to estimate the self-diffusion coefficient of BSA in the wide concentration range of crowding-agents.

It was shown that the glycerol does not deviate the BSA dynamics from the Stokes-Einstein postulates (Fig 1a). This means that the effect of glycerol on the change of the self-diffusion coefficient is due viscosity increasing. The self-diffusion coefficient of BSA in the presence of PEG 300 in solution is strongly deviates from Stokes-Einstein prediction (Fig 1b). This behavior can be caused by excluded volume effects and intermolecular interactions in solution.

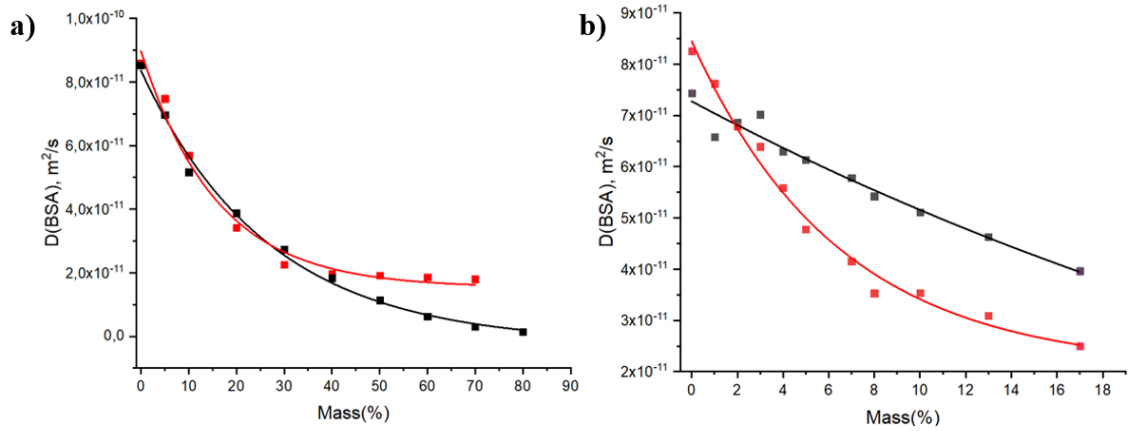

Fig. 1. Change in the self-diffusion coefficient of BSA in the presence of: a) glycerol b) PEG 300

This work was supported by the Russian Foundation for Basic Research [Grant N 20-04-00157].

Van Vleck paramagnets – new features in comparison of $LiTmF_4$ and $Li(Tm_{0.02}Y_{0.98})F_4$: NMR study

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Both of the $Li(Tm_{0.02}Y_{0.98})F_4$ and $LiTmF_4$ are Van Vleck paramagnets (VVP). They have a singlet ground state and the nearest excited doublet state of the ground multiplet in a paramagnetic rare-earth ion [1]. Van Vleck paramagnets could be researched by NMR method due to a gigantic induced magnetic field at the rare-earth nucleus as a consequence of strong hyperfine interaction. We reported the study of ^{169}Tm nucleus in diluted single crystal VVP $Li(Tm_{0.02}Y_{0.98})F_4$ in comparison with our the newest obtained data of $LiTmF_4$.

Van Vleck paramagnets $LiTm_{0.02}Y_{0.98}F_4$ and $LiTmF_4$ both have a tetragonal structure of scheelite ($CaWO_4$) with a space group C_{4h}^6 [2]. NMR studying of VVP single crystals were carried out by pulse home-built spectrometer. Magnetic field range was 0–0.8 T, working frequencies were 14.15 MHz, 8.43 MHz and 8.16 MHz, temperature range was 2–4.2 K.

As a result of a series of experiments, an anisotropy of the spin-spin relaxation rate (T_2^{-1}) close to the direction [001] were measured and calculated for both VVP single crystals $Li(Tm_{0.02}Y_{0.98}F_4)$ and $LiTmF_4$. Angular dependence of a spin-lattice relaxation rate (T_1^{-1}) were measured for a diluted VVP $Li(Tm_{0.02}Y_{0.98}F_4)$. The inhomogeneous linewidth was obtained for the $Li(Tm_{0.02}Y_{0.98}F_4)$ and compared with a results for concentrated VVP $LiTmF_4$.

Temperature dependencies of T_1^{-1} and T_2^{-1} were measured for the $Li(Tm_{0.02}Y_{0.98}F_4)$. Energy interval between the singlet ground state and first excited doublet state was obtained from approximation of experimental results and reached 25.9±0.2 cm^{-1} in approach of two-phonon Aminov-Orbach relaxation process. It is markedly different from previously known value for the concentrated $LiTmF_4$ which was 31 cm^{-1} [3]. According to this result, we assumed different roots of correlation time in cases of diluted $Li(Tm_{0.02}Y_{0.98}F_4)$ and concentrated Van Vleck paramagnets $LiTmF_4$.

The reported study was funded by Russian Science Foundation, project №22-22-00257.

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The CW EPR and pulsed EPR studies of the $^{51}V^{4+}$ ions in $Sc_2{}^{28}SiO_5$

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Orthosilicate monocrystals Sc_2SiO_5 and Y_2SiO_5 and with different dopants rare earth and iron groups are widely used in numerous applications. For example, yttrium and scandium orthosilicates with 4f- and 3d- dopant ions (Nd^{3+}, Yb^{3+}, Cr^{3+}) are used in various lasers and related applications. In recent years more attention was drawn towards these materials since it is possible to use them for quantum computing applications, one of which is quantum memory devices [1,2]. In order to use orthosilicates with 4f- and 3d- dopant ions, it is necessary to measure key properties such as spin – lattice relaxation times and phase memory lifetimes. In addition to that, it is useful to measure orientation dependencies ESR spectra in the monocrystals in order to obtain g-factors and hyperfine constants.

In this work we present the results of the CW EPR and pulsed EPR experiments for $^{51}V^{4+}$:$Sc_2{}^{28}SiO_5$ (0.005 %at.). The CW EPR method was used to obtain the angular dependencies of the ESR spectra in different crystallographic planes in X- and Q- bands. The CW EPR spectra also allowed to identify the valence state of the vanadium ions in the crystal as 4+. From the approximation of the experimental results the g-factor values and hyperfine constants were found.

The temperature dependencies of the relaxation times were measured using the pulsed EPR which are shown on Fig. 1, with fitting line and its components shown by dashed lines. It was found that T_1^{-1} is approximated by the sum of the direct process and Aminov – Orbach process with decent accuracy $T_1^{-1} = A \cdot T + B \cdot exp\left(-\frac{\Delta}{k \cdot T}\right)$, where A= 20.6 s^{-1} K^{-1} B = $1.09 \cdot 10^6$ s^{-1}; Δ = 98K .

The phase memory lifetimes were measured by Hann two-pulse method at various temperatures and the results are shown on Fig. 2.

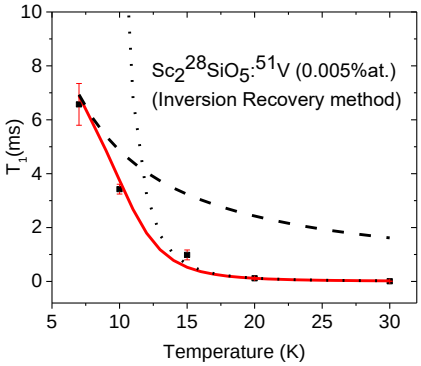

Fig. 1. Temperature dependence of the spin – lattice relaxation times T_1 for $^{51}V^{4+}$: $Sc_2{}^{28}SiO_5$ (0.005 %at.)

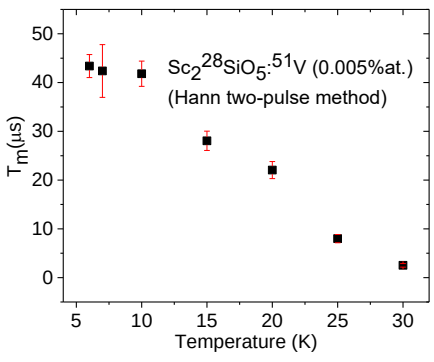

Fig. 2. Temperature dependence of the phase memory lifetimes T_m for $^{51}V^{4+}$: $Sc_2{}^{28}SiO_5$ (0.005 %at.)

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ESR measurements of ludwigite $Mn_{1.17}Co_{1.83}BO_5$

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Oxyborates with structural formula $(M^{2+})_2(M^{3+})BO_5$, with (M^{2+}) and (M^{3+}) being metallic ions of corresponding valence, are named ludwigites. Metallic ions in this type of a compound create zigzag walls in crystal structure with four non-equivalent positions for them, therefore producing unusual magnetic properties, such as random magnetic ions distribution, mixed valence, strong electronic correlations, uncommon charge ordering, etc. In bimagnetic ludwigites one can easily observe evolution of said properties in dependence of relative concentrations of magnetic ions [1,2]. That makes bimagnetic ludwigites particularly interesting.

The aim of this work is investigation of magnetic properties of $Mn_{1.17}Co_{1.83}BO_5$ ludwigite via ESR spectra analysis. EPR spectra were measured using a Bruker spectrometer. Figure 1 shows obtained ESR spectra. The measurements were performed at temperature range from 5 to 340K. With these measurements several points of interest were obtained at temperatures 50K, 130K and 250K. It is possible, that these points mark different phase and structural transitions.

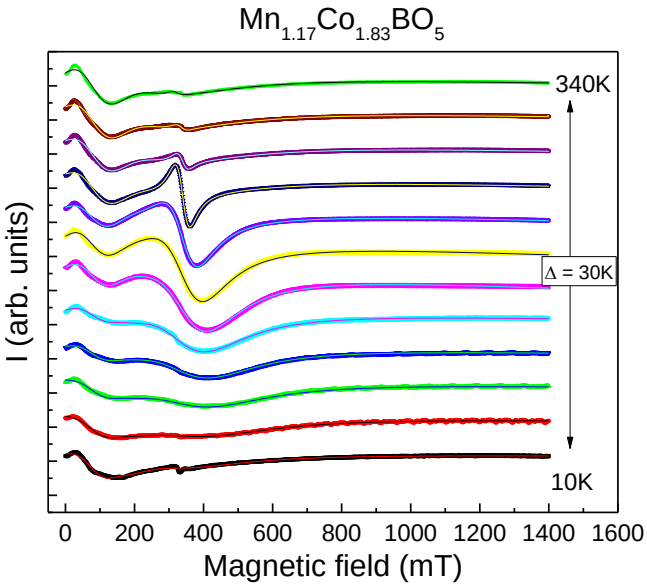

Fig. 1. ESR spectra for Mn1.17Co1.83BO5

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Investigation of magnetization and magnetostriction in lithium – ytterbium tetrafluoride

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Lithium – rare earth tetrafluorides (or, double fluorides) $LiRF_4$ (R is a rare-earth element) are model objects of the physics of dipolar magnetism. Scheelite type $I4_1/a$ crystal symmetry presents a slightly-distorted diamond-like arrangement of rare earth ions, which is suitable for study of order-by-disorder magnetic phenomena. $LiYbF_4$ is XY-dipolar antiferromagnet, $T_N = 0.130$ K, magnetic moments are ordering in (001) plane [1, 2, 3].

Single crystals were grown using Bridgeman-Stockbarger method, powder sample was synthesized by sintering powders of LiF and YbF_3 in proportions from to the phase diagram [4]. Static magnetostriction measurements were performed on a home-made capacitive dilatometer [5] at high fields (up to 9 T) and low temperatures (down to 2 K). Magnetization was measured by vibration sample magnetometer *VSM* at *PPMS* system. Theoretical analysis makes use of Yb^{3+} ion Hamiltonian, diagonalized in the full space of the energy states of $4f^{13}$ electronic configuration [6].

Experimental data and simulations agree both qualitatively and quantitatively for the powder sample as well as for the single crystal samples. Also, our theoretical approach explains $LiYbF_4$ single crystal inverse susceptibility experimental data from [3] better than the original calculations.

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Magnetic Fluctuation Effect in Microwave Absorption of the $EuFe_2As_2$ Crystals Near the Magnetic Ordering Temperature

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The superconductivity formation mechanism in high-temperature superconductors is not finally established till now. There is an assumption that the Cooper pair formation is mediated by magnetic fluctuations. Therefore, materials in which superconductivity and magnetism coexist are of interest for research. The parent compound for creating some superconductors is $EuFe_2As_2$. It is not superconducting at ambient pressure, but superconductivity is emerged with applying an external pressure or by replacing Eu by Na, K, Rb or As by P or Fe by Co [1].

We have studied the transition of $EuFe_2As_2$ crystals to a magnetically ordered state. The influence of magnetic fluctuations near the ordering temperature of Eu magnetic moments (T_c = 19 K) on the microwave absorption (MWA) and magnetic susceptibility of the sample was investigated.

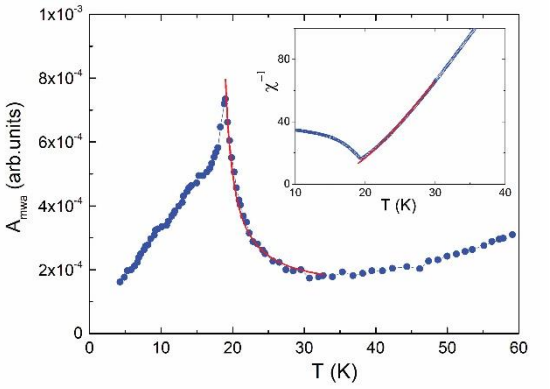

Fig. 1. Temperature dependence of the MWA amplitude in the EuFe2As2 crystal (points). The solid line is the fitting with eq. (1). Insert is the temperature dependence of the inverse magnetic susceptibility close to the magnetic ordering temperature and its fitting with eq.3 (solid line)

The result of measuring MWA with a change in temperature is shown in Figure 1. An absorption maximum is observed at the Eu magnetic ordering temperature T_c = 19 K. To model the obtained dependence, we used the equation:

$$A_{mwa} = a + b \cdot T^{\frac{1}{2}} + A_{cr}(T) \qquad (1)$$

$$A_{cr}(T) \sim A_0 \left(\frac{T-T_c}{T_c}\right)^{-zv} \qquad (2)$$

On the right side of equation (1), the first and second terms are associated with scattering by defects and phonons, and the third term reflects the contribution of critical fluctuations of the order parameter. Near the transition point, it can be written in the form (2). Here z is the dynamic critical exponent, ν is the critical exponent of the correlation length. The fitting yielded the value $z\nu$ = 0.8.

To separate these parameters, we used data of the inverse magnetic susceptibility (insert in Fig.1). It is known that $\nu \approx 1/2\ \gamma$, where γ is the critical exponent of magnetization. Fitting with expression

$$\chi^{-1}(T) = \chi_0^{-1}\left(\frac{T-T_c}{T_c}\right)^{\gamma} \qquad (3)$$

allows us to get the value γ = 1.25. Thus, the value z = 1.28. Such z value shows that the magnetic fluctuations occur in weakly linked planes.

The work was supported by the Russian Science Foundation, project no. 21-72-20153.

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High-frequency Nonresonant Microwave Absorption Study of Transport Properties of the $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$ Topological Insulator

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Topological insulators (TI) are attractive quantum materials for research due to their non-trivial electromagnetic properties [1]. The surface charge carriers of TI are Dirac fermions with high mobility, whose momentum is aligned perpendicular to its spin and they are protected by time-reversal symmentry against non-magnetic impurities and defects. Such properties make TI promising materials for practical quantum electronics and spintronics devices. In this work we studied effects of weak antilocalization on carrier scattering processes in $Bi_{1.08}Sn_{0.02}Sb_{0.9}Te_2S$(BSSTS) 3D TI using high-frequency nonresonant microwave absorption (NMA) together with classic four-probe DC resistance measurements. Power absorption in resonator is proportional to ohmic resistance which allows us to compare data obtained by those two methods [2]. BSSTS is one of the best 3D TI by its transport characteristics. Single crystals were synthesized in the Zavoisky Physical-Technical Institute. Thin flakes were cleaved off to use in experiments.

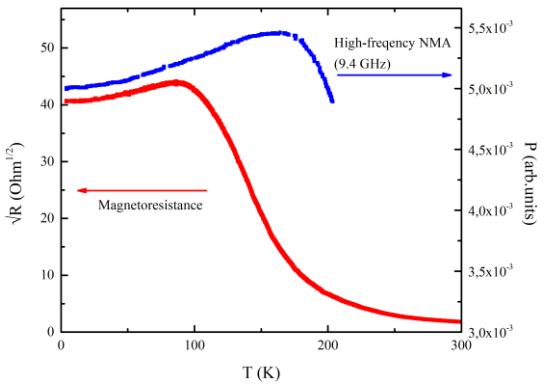

Fig.1. Temperature dependences of resistance and NMA amplitude of BSSTS thin flakes

Comparison of temperature dependences obtained by DC resistance and NMA amplitude measurements (Fig. 1) reveals that high-frequency method is more sensitive to surface conduction state of TI. At low temperatures ($T < 100$ K) BSSTS resistance behavior is determined by metallic contribution of topological surface states, while in case of NMA amplitude this contribution remains dominant up to T=170 K. This allows us to make a conclusion that scattering time is larger than measurement frequency [3]. It implies that scattering events are rare and gives indirect evidence of weak antilocalization effect.

Weak antilocalization effects are most prominent at low temperatures and easily observed in magnetoresistance measurements [4]. Therefore, we obtained magnetic field dependences of resistance and NMA amplitude of BSSTS at 1.5 K and 4.2 K. Results exhibit clear evidence of weak antilocalization contribution to TI conductivity. Analysis of the results allowed us to estimate that phase coherence lengths l_ϕ at those temperatures are close to 400 nm which is relatively high in comparison with similar bismuth chalcogenide compounds.

The high-frequency method of nonresonant microwave absorption has proved to be a reliable method for studying the transport characteristics of topological insulators. Further application of this method will allow us to obtain additional information about the processes of scattering of current carriers in the studied compound.

The work was supported by the Russian Science Foundation, project no. 21-72-20153.

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Study of magnetic properties for micro- and nanoscale DyF_3 powders

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The DyF_3 compound has unique properties, which makes it possible to use it as a high-field contrast agent for MRI [1] and additives to Nd-Fe-B magnets to increase the coercive force [2]. Dysprosium fluoride is a ferromagnet with an easy magnetization axis along the [010] axis of the crystal lattice; the space symmetry group is Pnma (orthorhombic); the Curie temperature is 2.55 K along the [010] axis for a single crystal [3].

DyF_3 powders with characteristic sizes of 30 nm x 16 nm, 50 nm x 30 nm, 70 nm x 40 nm, 220 nm x 150 nm were obtained by hydrothermal synthesis via chloride reaction [4], powder size of 7 μm x 5 μm – by crushing a single crystal. Chemical composition control and crystallinity confirmation were carried out using X-ray diffraction analysis on Bruker D8 Advance Cu Ka, λ=1.5418 Å. The shape and characteristic size of the particles in the powders were determined from photographs obtained using transmission electron microscopy on a HitachiHT Exalens microscope.

In this work, the temperature (1,8 – 300 K) and magnetic field (0 – 7 T) dependences of the magnetization of the samples were measured using the magnetic properties measurement system (Quantum Design), St. Petersburg State University. The modeling of the energy spectrum and magnetization in the model of exchange charges in the full basis of the electronic configuration Dy^{3+} $4f^9$ in DyF_3 is carried out. The temperature of the phase transition to the ferromagnetic state was determined for all samples by the temperature dependences of magnetization. There is a shift in the Curie temperature with a decrease in the particle size in the powder. The critical exponent of the correlation length for a dipole ferromagnet was determined experimentally. Magnetic moments are oriented mainly along the axis of easy magnetization. The saturation value of the magnetic moment in strong magnetic fields changes with decreasing particle size. It is shown that the change in magnetization is caused by surface effects and clustering.

The work was carried out at the expense of funds, subsidies, allocated to the Kazan Federal University for the implementation of the state task in the field of scientific activity (project number 0671-2020-0051).

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Synthesis and magnetic properties of thin film systems Fe_3Al and Fe_3Al/Pt

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Magnetoresistive random access memory (MRAM) is one of the most significant directions of spintronic device development. The main advantage of this type of memory is its non-volatility, i.e. the ability to store the recorded information when disconnected from the power supply. MRAM is based on heterostructures with layers of ferromagnetic (F) and normal (N) metals. The resistivity of a three-layer F/N/F heterostructure, for example, depends on the magnetization arrangement of the two F-layers (giant magnetoresistance effect). Therefore, the "0" and "1" states of the simplest MRAM cell differ in the resistance values. The information which is stored requires the magnetization of one of the F-layers to be switched between the two opposite directions. A promising phenomenon for rapid magnetization direction switching is the spin Hall effect. This effect occurs in F/N-type heterostructures, where N is heavy normal metal with large spin-orbit coupling.

In this paper, we present results of the synthesis and magnetic properties studies of the ferromagnetic alloy thin films of Fe_3Al and of the F/N heterostructure based on it, where platinum is used as a heavy normal metal. The Fe_3Al thin films were grown by molecular beam coprecipitation in an ultrahigh vacuum chamber manufactured by SPECS (Germany). Evaporation rates of iron and aluminum from two high-temperature cells were set at their temperatures and the deposition rate of each element was calibrated using a quartz sensor. The substrates were the single crystal plates of MgO compound with orientation (001) with a roughness of less than 0.5 nm (epi-ready grade).

A 30 nm thick Fe_3Al film served as a sample for the study of magnetic properties. A 15 nm thick platinum layer was deposited on half of the sample area. To prevent oxidation, the area of the samples was covered with a 3-nm thick aluminum capping layer. The low-energy electron and X-ray diffraction data shows that the Fe_3Al film is single-crystalline with the $[110]_{Fe3Al}||[100]_{MgO}$ epitaxy character. According to atomic force microscopy, the Fe_3Al film is not continuous but has an island morphology.

Magnetic properties were studied at room temperature by the vibration sample magnetometry of the PPMS-9 system by Quantum Design (USA). Magnetic hysteresis loops were studied under the magnetic field applied either in the film plane or along the film normal. It is shown that Fe_3Al film is ferromagnetic. Saturation magnetization of the Fe_3Al/Pt heterostructure exceeds that of the Fe_3Al film by ~ 6% indicating the induced magnetism of the Pt-layer. The differences were found in the ferromagnetic resonance spectra (FMR) of these two samples. Thus, the FMR line of Fe_3Al/Pt heterostructure has a greater width than the line of single thin film of Fe_3Al. In our opinion, the increase of the line width is associated with the losses arising from the generation of charge currents in the platinum layer under conditions of so-called "spin pumping" due to the inverse spin Hall effect. Peculiar FMR lineshape transformation observed under sample rotation within 10 degrees from the normal are observed that we assign presumably to the resonance specific for a ferromagnetic film with an island morphology.

Magnetic Resonance Imaging and Kids: Clinical Applications and Challenges

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Most diseases in kids need diagnostic methods, with the first line of action being X-rays and CT scans. In recent times, MRI is becoming highly necessitated because of the absence of radiation in the procedure. The MRI creates more detailed images in organs with high perfusion and water content than any other imaging technique.MRI also has higher sensitivity in detecting tumours and metastases than scintigraphy and CT scans, especially in neurology.

Studies have shown that despite its beauty, MRI also has limitations. One of them is that it can't be used on patients with metallic implants (braces, tooth implants, percutaneous bone pins, etc.) because it generates vast artefacts on the images. Also, the metals can be harmful to kids being under the influence of the strong magnetic fields of the MRI scanner – about 60,000 times stronger than the earth's magnetic field. Secondly, the high cost of MRI is one that, most times, patients or parents can't afford, especially if repeated imaging is required.

However, this paradigm shift in pediatric radiology is also met with other challenges. In this review, we discussed some of the problems that arise in pediatric MRI apart from its high cost and limitations in patients with implants. Magnetic fields, the imaging environment and even noise produced by the strong magnets in the scanners have been found to have adverse effects on kids.

The noise and extended stay under the scanner create emotional distress during children's MR imaging. Cries and motion disrupt the procedure and, most times, are restarted, making the process longer.

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Signed for use: 02.09.2022.
Format: 60×84 1/8. Typeface: «Times New Roman».
Conventional printing plates: 1,9.
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