Poster session
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Poster abstract	Remarks
1. Study of the corrosion resistance by adding Si, Nb elements to TiZrCN compounds	

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Carbon nitride series of Ti, Zr, Nb, Si samples were used. The reason for choosing these elements is that they are very suitable as coating materials for electronics in future space exploration because their radiation corrosion coefficients are very small. Our goal is to study the structural properties of these samples after irradiation with gamma, neutrons and heavy ions. Here we need XRD method, neutron diffraction method, SEM and TEM analysis. After chemical corrosion of these samples, XRD analyzes were performed. NaCl, which is the strongest corrosion medium, was used for corrosion. Gamma irradiation of samples is now ready. Our next goal is to study the structure of samples after Gamma irradiation by XRD and Neutron diffraction method. At the same time, we are currently carrying out irradiation with Xe+26 heavy ions in the laboratory of nuclear reactions. We also plan to study the mechanism of defect formation using the positron spectroscopy method.

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2. Pressure induced phase transition in ferroelectric $Nd_2Ti_2O_7$

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In this study, the X-ray diffraction patterns of NTO were examined under pressures ranging from 1 atm to 32 GPa. The results showed that the broadening and shifting of diffraction peaks in the range of 22^0 to 31^0 can be attributed to pressure-induced lattice strain and the Scherrer effect on the crystal structure. The XRD peak at 23.5^0 is observed to be greatly affected by this phenomenon up to a pressure of 19.2 GPa. A microstrain effect was also observed in the low angle region, which can be explained by an increase in the number of defects present in the material. The gradual decrease in peak intensity and disappearance of peaks at low angles can be attributed to pressure-induced phase transitions. The Rietveld structure refinement confirmed that at ambient conditions, the crystal is ferroelectric and adopts the P21 (ferroelectric) monoclinic structure. The high pressure diffraction peaks were modeled with different structures, with the Pna21 orthorhombic phase being the best fit and the Reitveld refinement for high pressure phase confirmed that, the mentioned models are not fit exactly for transition, except Pna21 orthorhombic phase. The Raman spectrum from 1 atm to 32 GPa also confirm our results. The fingerprint region for NTO was determined to be 5^0 to 16^0 (2θ) which is in agreement with the $P2_1$ space group at low pressures. The study also shows that high pressure structure models are mostly related to the shifting of rare-earth ions and partly from the rotation and deformation of TiO_6 octahedrons.

The results of this study provide new insights into the behavior of NTO under high pressure. The pressure-induced lattice strain and microstrain effects observed in the XRD patterns suggest that the material may be highly sensitive to external pressure. Additionally, the observation of new peaks and phase transitions at high pressures suggests that NTO may have potential for use in high-pressure applications. However, further studies are needed to fully understand the implications of these findings for the practical use.

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3. New preprocessing and reconstruction algorithms for neutron tomography data

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Computed tomography methods based on various physical principles (X-rays, neutrons, electromagnetic field, etc.) have become widely used in such fields as medicine, physics, geology, archeology and many others. Due to the unique properties of the interaction of neutrons with matter, neutron tomography takes an important position in modern materials science [1].

However, there are some possibilities for improving this method. It is necessary to enhance the quality of the images, reduce computational resources for reconstruction, and speed up experiments. One of the solutions is the use of new mathematical algorithms for data preprocessing and reconstruction. The most promising in this field are algorithms based on convolutional neural networks and deep machine learning [2-3].

This report demonstrates several convolutional neural networks for neutron tomography tasks. A comparative analysis of efficiency with existing algorithms was carried out.

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4. Pressure-induced phase transition in a nanostructured zinc ferrite

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The study of ferrites of spinel type is of great importance due to the wide variety of their structural and magnetic properties, which are of interest from the point of view of fundamental and applied research. In particular, canted states of an antiferromagnet, ferrimagnet, and spin glass can be realized in these compounds [1].

Significant saturation magnetization, relatively high electrical resistance, low electrical losses and good chemical stability make spinel-type ferrites are important for a wide range of technological applications as transformer cores, rod antennas, storage devices [2,3]. Moreover, such ferrites can be useful in biomedicine: as an effective heating agent for the treatment of cancer tissues through magnetic hyperthermia, as biomarkers for MRI diagnostics and magnetic drug delivery systems [3].

A wide range of magnetic properties of spinel ferrites is determined by the features of the distribution of iron ions between different crystallographic positions in crystal structures of the spinel type [2]. One of the important parts of the prospective research of spinel-type ferrites is the synthesis of complex ferrites with a controlled redistribution of iron ions between positions A and B, leading to a change in the magnetic properties of ferrites [3]. In addition, understanding of the relationship between the structural properties and the magnetic order of spinel ferrites can be given by high pressure exposure.

In the present work, ferrite with the spinel structure Zn0.34Fe2.53O4 was chosen for X-ray and neutron diffraction studies at high pressure and in a wide temperature range. Experiments on neutron diffraction in a wide temperature range were carried out on a DN-12 diffractometer with a pulse high-flux reactor IBR-2 [FLNP, JINR]. X-ray diffraction data were obtained on a specialized Xeuss 3.0 diffractometer (Xenocs SAS, France) using a high-pressure cell with diamond anvils.

The distribution of magnetic moments of iron ions in crystallographic positions A and B is studied. The calculated lattice parameters, interatomic distances and angles, and magnetic moments as functions of temperature and pressure are presented. A phase transition from the initial phase with a cubic structure (Fd-3m) to a high-pressure phase with an orthorhombic structure (Pnam) in Zn0.34Fe2.53O4 ferrite at a pressure above 18 GPa has been discovered. The structural mechanisms of the phase transition in ferrites with a spinel structure are discussed.

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5. Studying of the processes the formation of luminescent nanoparticles in glass ceramics

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Glasses with high optical transparency are excellent carrier materials for capturing luminescent nanoparticles. Ions of rare earth elements are sources of effective luminescence, and nanoparticles doped with these ions are characterized by high quantum yield, fine-tuning of optical properties and reduced concentration quenching of luminescence [1]. When choosing optical materials, much attention is paid to the phenomenon of up-conversion. Up – conversion materials can absorb several photons in the infrared region of the spectrum, followed by luminescence in the visible region [2]. The optimal class of materials for up-conversion, from the point of view of physicochemical properties, are rare-earth ions for multiphoton transformations. The efficiency of up-conversion luminescence of rare-earth ions depends both on the type of rare earth ion and on the matrix into which it is introduced during synthesis. Fluorides, oxides, halides and other materials with low photon energy are used as matrices [3].

We have studied luminescent composite glass ceramics with up – conversion, which was obtained by doping into a glass matrix of the composition $2.2SiO_2$–$1.3GeO_2$–$6.9PbO$–$7.6PbF_2$–$2.0CdF_2$ with oxides of rare earth elements Ho_2O_3 and Tm_2O_3 in a wide molar range were chosen as the initial glass matrix. The structural features of nanoparticles formation in heat-treated oxyfluoride glasses have been studied by methods of small-angle X-ray scattering and X-ray diffraction. The method of small-angle X-ray scattering made it possible to calculate the fractal dimension and morphology of nanostructures in the system. X-ray diffraction data of oxifluoride glasses were obtained to determine the crystalline state of formation of PbF_2:Tm-Ho nanoparticles. Crystallized PbF_2 nanoparticles are the host system for rare earth ions Tm^{3+} and Ho^{3+}, whose entry into the cubic crystal lattice of PbF_2 and provide the formation of conditions for up-conversion luminescence.

In conclusion, it was found that nanoparticles, presumably PbF_2:Tm-Ho with sizes of 16-20 nm are formed and an increase in the average size of the fluctuations in the density of glass is observed from 71 to 92 nm. With an increase in the concentration of Fe_2O_3 and Tm_2O_3 oxides, an increase in both the average sizes of nanoparticles and the sizes of local areas of density fluctuations was found. The obtained structural information will be useful for analyzing the optical properties of nanostructured fluorescent glass ceramics with increased transformation.

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6. BIOHLIT - Information system for radiobiological research

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The report presents the conception and current status of developing the BIOHLIT information system that ensures storing and analyzing data based on algorithms of computer view, machine and deep learning for radiobiological studies at LRB JINR. This interdisciplinary project is performed by groups from MLIT and LRB as a joint work. The main idea is to develop a convenient framework for data analysis that helps to atomize work processes when morphofunctional alters of laboratory animals CNS after irradiation are observed. There are two steps: behavioral research and morphological analysis. The problems of the first step include detection issues and manual calculation some animal acts. Algorithms of computer view solve this problem. The problems of automating the morphological analysis of histological slides are solved in frames of the project by implementing algorithms based on the neural network approach and computer vision methods.

7. The structural evolution of the P2-type $Na_{2/3}[Fe_{1/3}Mn_{2/3}]O_2$ cathode material during electrochemical cycling

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Developing efficient cathode materials is very important task for the wide distribution of the sodium-ion batteries (SIB). Among various SIB cathode materials, P2-type layered manganese oxides Na_xMnO_2, x ~ 2/3 have received much attention. Manganese is low-cost, earth abundant and environmentally friendly element. However, rapid capacity decay upon repeated cycling restricts Na_xMnO_2 materials practical application. It is believed that the reasons of the capacity decreasing are irreversible structural change during Na^+ deintercalation/intercalation process and Jahn–Teller distortion due to the presence of Mn^{3+} in the material. The elemental doping/substitution can effectively improve the phase transition and cycling stability of the Mn-based layered materials [1].

$Na_{2/3}MnO_2$ (NMO) and $Na_{2/3}[Fe_{1/3}Mn_{2/3}]O_2$ (NFMO) powders with P2-type structure (space group $P6_3$/mmc) were synthesized by solid-state calcination [2,3]. The evolution of structural phase transitions during the charge-discharge of the $Na_{2/3}[Fe_{1/3}Mn_{2/3}]O_2$ cathode material after repeated electrochemical cycling against sodium has been studied by *in situ/operando* X-ray diffraction. Initially, $Na_{2/3}[Fe_{1/3}Mn_{2/3}]O_2$ has a hexagonal structure, referred to in the literature as P2, with cell parameters a = 2.9112(2) Å, b = 11.332(2) Å. After the complete sodium intercalation (1.5 V), orthorhombic distortions appear in the structure (space group Cmcm), denoted in the literature as P'2. At the beginning of the charge process, the P'2 phase is transformed into the hexagonal phase P2 through another intermediate phase P"2, the structure of which is to be clarified in additional experiments. The hexagonal P2 phase exists up to a voltage of 4.15 V, when it abruptly transforms into the hexagonal OP4 phase (space group P-6m2). During the discharge, the sequences of the transitions is following OP4 → P2 → P"2→ P'2. After repeated cycling, the sodium deintercalation/intercalation process occurs without the formation of the OP4 phase, which does not appear in diffraction patterns already after 50 charge-discharge cycles.

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8. Effect of doping with transition elements on the crystal and magnetic structure of half-Heusler compounds $MnNi_{0.9}M_{0.1}Sb$ (M = Ti, V, Cr, Fe, Co, Zn)

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Half-Heisler magnetic intermetallic compounds of transition metals exhibit interesting physical properties such as magnetoresistance, ferromagnetic and antiferromagnetic magnetic states, and superconductivity. It is observed the shape memory effect and superelasticity with opportunity to control there phenomena by means magnetic field. It makes these compounds promising materials to apply for creation permanent magnets, elements of electronic devices and cooling technology.

In our work we present the results of investigation the crystal and magnetic structure of half-Heusler intemetallic compounds MnNiSb and $MnNi_{0.9}M_{0.1}Sb$ (M = Ti, V, Cr, Fe, Co, Zn) by means of neutron diffraction in the temperature range 10–300 K and by X-ray diffraction in the pressure range 0–30 GPa at room temperature.

It has been found that the initial cubic structure $F\bar{4}3m$ and ferromagnetic phase remain in the investigated temperature range. New reflections correspond to the antiferromagnetic phase have not been found. Partial substitution of another transition element for nickel leads to a decrease in the magnetic moment of the Mn ions. Under high pressure, the cubic structure $F\bar{4}3m$ remains stable for all compounds under study.

9. Development of lithium-ion batteries with increased specific energy and power

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In this work, the adaptation of neutron scattering methods for studying the microstructure of electrode materials of lithium-ion batteries in order to improve their characteristics with respect to specific energy is continued. Using small-angle thermal neutron scattering data, the effect of conductive carbon additives (graphene and graphene oxide) on the porous structure of positive electrodes (cathodes) based on the following promising materials is considered: lithium-iron oxide ($LiFePO_4$), lithium titanate ($Li_4Ti_5O_{12}$) and lithium-nickel-manganese-cobalt oxide ($LiNiMnCoO_2$). To separate the scattering at closed and open pores, the electrodes were wetted with a typical liquid electrolyte with a deuterated liquid base (DMC), which led to compensation of scattering at open pores. It is established that the considered electrically conductive carbon additives change the porosity of the electrode to varying degrees and affect the wettability of materials both due to different degrees of penetration into the pores of the source material and due to the effect on the initial matrix. A generally universal effect on the scattering of polymer binder (PVDF) has also been found.

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10. Neutron tomography of rocks and cement materials: Advanced data treatment

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Neutron tomography has been actively developing in recent decades [1]. Its application extends to a variety of scientific research [2]: cement materials, plants, batteries, meteorites, archaeology, rocks, etc. In FLNP JINR, there is a neutron radiography and tomography facility placed on beamline 14 of the high-flux, pulsed reactor IBR-2 [3]. Structural studies of a large variety of materials, including highly anisotropic mica-rich rocks and cement materials for radioactive waste disposal, have been performed at this facility since 2016. The obtained structural information in such experiments represents a 3D phase distribution initially encoded as a 3D distribution of neutron attenuation coefficient. For each measured sample, more than 16 Gb dataset of images is collected. In our work, we developed new approaches to analysis of such amount of data, including image segmentation, texture and particle analysis. In particular, we have shown the correlation of a non-uniform distribution of phases in biotite gneisses with its seismic and magnetic properties, the relation of structural features in dikes to magma movement, the influence of graphite inclusions in cements on their Young's modulus.

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11. Influence of superconductivity on helimagnetism in Nb/Dy and Nb/Ho superlattices

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Nowadays studying of proximity effects at the interface between two media are in focus of view [1-5]. In particular hybrid heterostructures comprising superconducting (S) and ferromagnetic (F) layers are currently attracting great attention due to a diverse set of proximity effects. Manifestations of the influence of ferromagnetism on the superconducting properties of S/F heterostructures include phase changes of the superconducting wave function ("π-phase superconductivity") and spin-triplet Cooper pairing. Converse proximity effects in which superconductivity influences ferromagnetism have received less attention. These magnetic proximity effects (MPEs) are expected in systems where the F and S transition temperatures, T_F and T_C, are comparable, including for instance cuprate high-T_C superconductors and ferromagnetic manganates. Promising systems for study of MPEs are S/F heterostructures comprised of niobium and rare-earth (RE) materials. First of all high transparency of S/F interface is reported for such RE/Nb systems as Gd/Nb which simplifies penetration of superconducting correlations in F system [3,4]. Second, the REs are characterized by weak ferromagnetism, which equalize energies of both interactions and make MPEs easier. Last, but not least many REs such as Dy and Ho are known rare-earth ferromagnets with helimagnetic non-collinear structure allowing for generation of long-range triplet superconductivity. Taking into account all these considerations, RE/Nb structures potentially interesting for search of magnetic proximity effects.

To study the effect of superconductivity on helicoidal magnetic ordering systems Nb(5nm)/[Dy(2,4,6nm)/Nb(25nm)]x12//Al_2O_3, Nb(5nm)/[Ho(2,4,6nm)/Nb(25nm)]x12//Al_2O_3 were prepared, with thickness of the magnetic layers, both less and more than the period of the magnetic helicoid d_h~3÷4 nm. Attestation of the structures was carried out. The reflection of X-rays was measured, showing a high repeatability of Dy/Nb and Ho/Nb bilayers over the depth of the structure, the presence of interlayer roughness at the level of $\sigma \approx 10$ Å. Thus, preliminary data demonstrate the homogeneity of these systems at the level of Nb/Gd structures. For these structures, the position of the diffraction peaks recorded from the Dy and Ho layers showed that the helicoid axis is directed perpendicular to the plane of the structure. The results of atomic force microscopy showed the presence of inhomogeneities in the plane of the structure with a characteristic size of 98 nm.

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