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Poster abstract	Remarks
1. The effects of high pressure on the crystal structure and vibration spectra of layered perovskite-like $Nd_2Ti_2O_7$	

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Abstract

The structural and vibrational properties of the layered perovskite-like Nd_2Ti_2O7 compound were investigated using X-ray diffraction and Raman spectroscopy at pressures up to 30 GPa. The results revealed a gradual structural phase transition from the initial monoclinic $P2_1$ phase to the monoclinic P2 phase at approximately 19 GPa. This pressure-induced phase transition was accompanied by anomalies in unit cell compression and pressure behavior in vibrational modes [1]. Group theory predicted 132 Raman-active modes for the monoclinic crystal structure of $P2_1$ symmetry, and an increase in observed mode wavenumbers was observed at pressures below the phase transition pressure. Anomalies in the pressure behavior of certain vibrational modes near the transition pressure were related to changes in pressure coefficients [2]. Some vibrational modes disappeared, while new ones appeared after the phase transition, indicating a distortion of the TiO_6 octahedra [3]. The anomalies or changes in pressure behavior close to certain pressures suggested the continuous character of the phase transition. The study also observed anomalies in the pressure behavior of lattice parameters at approximately 19 GPa, indicating a structural phase transformation. The lattice compression was found to be anisotropic, with the c-axis in the monoclinic phases being the most compressible. The average compressibility of the "c" parameter was about three times larger than those of the "a" and "b" parameters. After the structural phase transition, strong compression anisotropy remained. Additionally, a sharp increase in the monoclinic angle β in the vicinity of the transition pressure was observed.

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2. Precision Laser Inclinometer as a unit of the future network for visualization of the earth's surface.

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The Precision Laser Inclinometer[1] (PLI) is a novel compact technology that provides a portable alternative to common seismometers, while enabling more precise sensing of ground movements.

To visualize the Earth's surface, one PLI is not sufficient; it is necessary to use multiple devices combined into a PLI's network. Currently, software development is underway to meet the needs of the PLI's network. This report describes the key aspects and issues associated with this work.

The further plans for the development visualization of Earth's surface movement will be overviewed.

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3. Nanoscale structure of electrode coatings for lithium-ion batteries with carbon additives according to small-angle scattering

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Rechargeable chemical current sources occupy an important place in the development of renewable energy sources and electric vehicles. As part of the development of energy-intensive and efficient rechargeable energy storage devices, an urgent task is to improve the lithium-ion batteries that are used today.

The effect of conductive carbon additives (graphene and electrochemical graphene oxide) on the porous structure of positive electrode coatings based on lithium-iron-phosphate (LFP), lithium-titanate (LTO) and lithium-nickel-manganese-cobalt oxide (NMC) has been studied by the method of small-angle neutron scattering. To separate the scattering at closed pores from the scattering at open pores, the electrodes were wetted with a deuterated electrolyte, which made it possible to compensate for the scattering at open pores. It has been found that electrically conductive carbon additives change the porosity of electrode materials to varying degrees and affect their wettability both due to the different influence of the degree of penetration into the pores of the initial matrix, and due to the effect on the matrix and changes in its morphology. It is found that in the size range of $100 < D < 1000$ Å, carbon additives noticeably change the porosity of the initial electrode material. These changes correlate with the wettability of the material with liquid electrolyte. The use of contrast variation made it possible to qualitatively evaluate the effectiveness of embedding carbon additives in the electrode coating. Structuring of the binder polymer (PVDF) was also detected: Tangles with a characteristic radius of inertia of 32 Å are observed in all electrode coatings. The greatest relative changes due to additives were observed in the NMC-based system, which correlates with its lower initial porosity compared to other materials. In this case, along with the change in porosity due to the embedding of additives, tangles of the binder polymer make a significant contribution to scattering.

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4. Analysis and verification of 3-D structures of heat shock proteins associated with type 2 diabetes mellitus based on MD-modeling methods

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Abstract

A topical issue is to study the causes of such an acute social problem as diabetes mellitus. The solution to this problem can be the use of molecular dynamics simulation to determine the effect of amino acid substitutions on the interaction of proteins with each other.

The paper is devoted to mastering the technique of computer molecular dynamics simulation with multi-purpose program codes AMBER, DL_POLY, CHARMM and visualization software VMD for the analysis of original and modified 3-D structure of heat shock proteins.

In this paper, based on molecular dynamics calculations, a comparative analysis of 3-D structures of native and mutational forms of the HspB6 protein was carried out. The features of the structural organization of native and mutant proteins were studied, a comparative analysis of the equilibrium configurations of proteins was carried out by overlapping (superposition), and the effect of amino acid (mutational) substitution on the initial structure was revealed.

A clear statement of tasks in the field of molecular dynamic (MD) modeling in this direction, in our opinion, could serve as modeling and determination of 3-D structures and conformations of small heat shock proteins HspB6 (Fig. 1). At the same time, modifications and stability of HspB6, the ability to interact with the partner protein HspB1 can be the key tasks of MD modeling on the important issue of type 2 diabetes mellitus. In this paper, based on MD calculations, a comparative analysis of the 3-D structures of the native and mutational forms of the HspB1 protein was carried out.

In the literature, the mutant form of HspB1 protein is associated, correlated with various diseases such as Alzheimer's, ALS (amyotrophic lateral sclerosis) and diabetic neuropathy (a type of diabetes mellitus DM-2). For example, in the above-mentioned protein, with mutational changes (substitutions of amino acid residues), the glutamate, HspB6GLU, located in a position homologous to the amino acid residue, is replaced by cysteine, HspB6CYS. Thus, the "cysteine" mutant form of HspB6 is caused by GLU/CYS substitution. Further, this mutant form of HspB6 will be designated as HspB6 Glu116Cys and will be the purpose of our calculations using the MD modeling method. In this work, the crystalline form of the HspB6 protein (ID: 4JUS) was selected from the PDB (Protein Data Bank) database, then the steps of minimizing energy and heating the sample for the native and mutation forms of the protein were carried out at room temperatures. The features of the structural organization of proteins of native and mutant types are investigated, a comparative analysis of the equilibrium configurations (states) of proteins by superposition is carried out, the effect of mutational (amino acid) substitution on the original structure is revealed.

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5. High pressure effect on crystal, magnetic structure and vibrational spectra of van der Waals material

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Van der Waals compounds are currently one of the most interesting objects of research in the field of condensed matter physics due to the recently discovered magnetic properties in their two-dimensional forms [1]. The structural features lead to a significant sensitivity of the physical properties in these compounds to external influences, which can cause many unusual phenomena: charge, orbital and spin ordering, superconductivity, various phase transitions, also important for the development of a wide range of spintronic devices [2]. The magnetic properties of van der Waals quasi-two-dimensional magnets are determined by a delicate balance of magnetic interactions within one layer of magnetic ions and correlations between neighboring layers. This balance can be easily altered by applying high pressure [3].

High pressure investigation is a direct method of controlled change in magnetic interactions due to variations in interatomic distances and angles. Investigations at high pressures provides a unique opportunity to study the relationship between changes in structural parameters and magnetic properties, which is necessary to understand the nature and mechanisms of physical phenomena observed in the van der Waals materials.

This work is devoted to the investigation of the crystal, magnetic structure and vibrational properties of $CrBr_3$ in wide temperature and pressure ranges using neutron diffraction at DN-6 diffractometer of the IBR-2 reactor (FLNP, JINR, Dubna, Russia) with the combination of X-ray diffraction and Raman spectroscopy. The observed negative thermal volume expansion in $CrBr_3$ below T_C = 37 K at ambient pressure, associated with spin-lattice coupling, is detected also at high pressures. The Curie temperature of $CrBr_3$ reduced rapidly with a pressure coefficient dT_C/dP = −4.1(4) K/GPa, implying instability of the initial FM order. Accordingly, the effect of high pressure leads to the suppression of magnetic ordering, and the transition from the initial FM state is expected at P~8.4 GPa to either AFM or PM. Our results also demonstrate an isostructural phase transition in $CrBr_3$ ferromagnet in a pressure range of 2.5 - 7 GPa. This transition became apparent in the Raman spectra of about P~2.5 GPa by the appearance of an additional Raman mode and, ultimately, manifested itself in anomalies in the behavior of the lattice parameters and unit cell volume with pressure. In addition, anomalies in the behavior of vibrational mode frequencies detected at P~15 GPa may indicate another phase transformation, presumably associated with the metallization process.

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6. Structural study of catalyst materials with positron annihilation spectroscopy

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ZSM-5 is an aluminosilicate zeolite belonging to the pentasil family of zeolites. It is widely used in the petroleum industry as a heterogeneous catalyst for hydrocarbon isomerization reactions.

Bismuth vanadate is the inorganic compound with the formula $BiVO_4$. It is a bright yellow solid. It is widely studied as visible light photocatalyst. $BiVO_4$ has received much attention as a photocatalyst. In the monoclinic phase, $BiVO_4$ is an n-type photoactive semiconductor with a bandgap of 2.4 eV.

The study modified catalytic petroleum Zeolite ZSM-5 and photocatalyst $BiVO_4$ material by irradiating electron beam and ion beams from the accelerators, respectively. This process forms new faces in the material in the form of nanoparticles in controlled conditions of flux and dose. These two materials were then studied structurally using positron annihilation spectroscopy (PAS), which is a well-known method for investigating materials on the scale of a few angstroms to tens of nanometers. To obtain insight into the structural study of these materials, other nuclear spectrometer methods such as XPS, NMR, TEM, SEM and RBS can be combined with PAS.

The study of samples by PAS methods is carried out at the JINR DLNP in the positron spectroscopy sector [1-5].

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7. Vacuum system of the LINAC-200 accelerator.

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The linear accelerator Linac-200 at JINR is constructed to provide electron test beams with energy up to 200 MeV to carry out particle detector R&D, to perform studies of advanced methods of beam diagnostics, and to work as an irradiation facility for applied research. While the accelerator largely reuses refurbished parts of the MEA accelerator from NIKHEF, the accelerator vacuum system is renovated. The working vacuum level in various parts of the accelerator should be considered the level $P = 5 \leq 10^{-8}$ torr. The structural scheme of the vacuum system is based on the modular principle: each station is provided with separate pumping units constantly operating (magnetic discharge pumps), the possibility of connecting a mobile vacuum station and pumping from the atmosphere, and each station is separated from each other by manual and electropneumatic gate valves. In this report, the design and status of new vacuum system will be presented.

8. Test stand for calibration traveling wave monitors for a linear electron accelerator Linac-200

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The linear accelerator Linac-200 at JINR is a new DLNP facility, constructed to provide electron test beams to carry out particle detectors R&D, to perform studies of advanced methods of electron beam diagnostics, for applied and biological research and for student practices. During accelerator operation, it is important to monitor the current and position of the electron beam. Traveling wave monitors (TWM) are one of the beam diagnostic tools. Such monitors make it possible to track the current and position of the beam in the accelerating chamber. To study and test TWM a stand was assembled. Tests performed on this stand will improve the beam current transmission parameters. The report presents the design features of the stand and the methodology of the tests.

9. Linac-200 electron accelerator as a core for new electron test beam facility at DLNP JINR

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The linear accelerator Linac-200 at JINR is a new DLNP facility, constructed to provide electron test beams to carry out particle detectors R&D, to perform studies of advanced methods of electron beam diagnostics, for applied and biological research and for student practices. The core of the facility is a refurbished MEA accelerator from NIKHEF. The key accelerator subsystems including controls, vacuum, precise temperature regulation were completely redesigned or deeply modernized. Two test beam channels are verified in test mode: the first one with electron energy in range 5–25 MeV, and the second one with electron energy in range 40–200 MeV. The pulse current varies smoothly from 80 mA down to almost zero (single electrons in a pulse). This report presents the status, operation parameters and perspectives of the facility.

10. Research of a vacuum ceramic window made of beryllium oxide on the test stand of the LINAC-200 accelerator

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Based on the LINAC-200 accelerator, a new DLNP facility, a test stand is being developed to research various microwave nodes. It is necessary to output the microwave capacity from the klystron, for which a ceramic window made of beryllium oxide is used, which is selected due to its properties (thermal conductivity ≥230 W/m*^{0}K).
In this work, a ceramic window of a microwave system is simulated to comprehend what thermal and mechanical processes will happen when this element is used on a stand at a power of about 10 MW per pulse, a pulse duration of 4 μs, a pulse repetition rate of 10 Hz, at a microwave range frequency 2856 MHz. The CST Studio Suite program is selected for modeling, the results are presented in this report. Based on them, conclusions are drawn about the future mode of operation of the system.

11. Proximity effects at superconducting and ferromagnetic heterostructures

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Nowadays studying of proximity effects at the interface between two media are in focus of view [1-4]. 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.

The requirement, among other things, for such systems is that the thicknesses of ferromagnetic layers should be on the order of the correlation length of superconductivity in ferromagnetic ξ_F~1÷5 nm [4]. To reduce the exchange interaction, alloys of ferromagnetic materials with non-magnetic materials are used. When making structures with given parameters, the structures are heterogeneous, clusters with a diameter of ξ_{cl}=5÷10 nm are formed. Clusters interact with each other. This condition is known in the literature as super-spin glass [5]. The effect of the superconducting transition on the super-spin glass state in various types of heterostructures was investigated: V/FeV/V (Cr)/FeV/Nb, Nb/CuNi [1].

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 [2]. 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.

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12. Study of cultural heritage objects from the ancient Turkic cult-memorial complex of East Kazakhstan with non – destructive neutron methods

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Archaeological objects, objects of cultural heritage have a special value due to their uniqueness, antiquity and existence in a single copy, therefore, the most justified is the use of modern methods of non-destructive testing for their research. One of such methods of non-destructive testing, which gives sufficiently complete information about the surface and internal structure of the objects under study, are the methods of neutron radiography and tomography.

This work reports on the results of the study of metal and ceramic objects of cultural heritage (weapons and household items) found in the cult-memorial complex of Eleke Sazy, located on the territory of Tarbagatay district of East Kazakhstan region.

The features and spatial distribution of phases and the internal structure of metal objects were studied by neutron radiography and tomography at the experimental station TITAN on the 1st channel of the stationary research reactor WWR-K (Institute of Nuclear Physics, Almaty). The phase composition of the ceramic fragments was analyzed by neutron diffraction using the DN-6 diffractometer at the IBR-2 high-flux pulsed reactor of the Frank Laboratory of Neutron Physics, JINR, Dubna, Russia.

Based on the results of these studies, corrosion occurring on the surface of copper or bronze finds was determined, which is important for the development of the methodology of restoration and preservation of valuable archaeological objects.

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