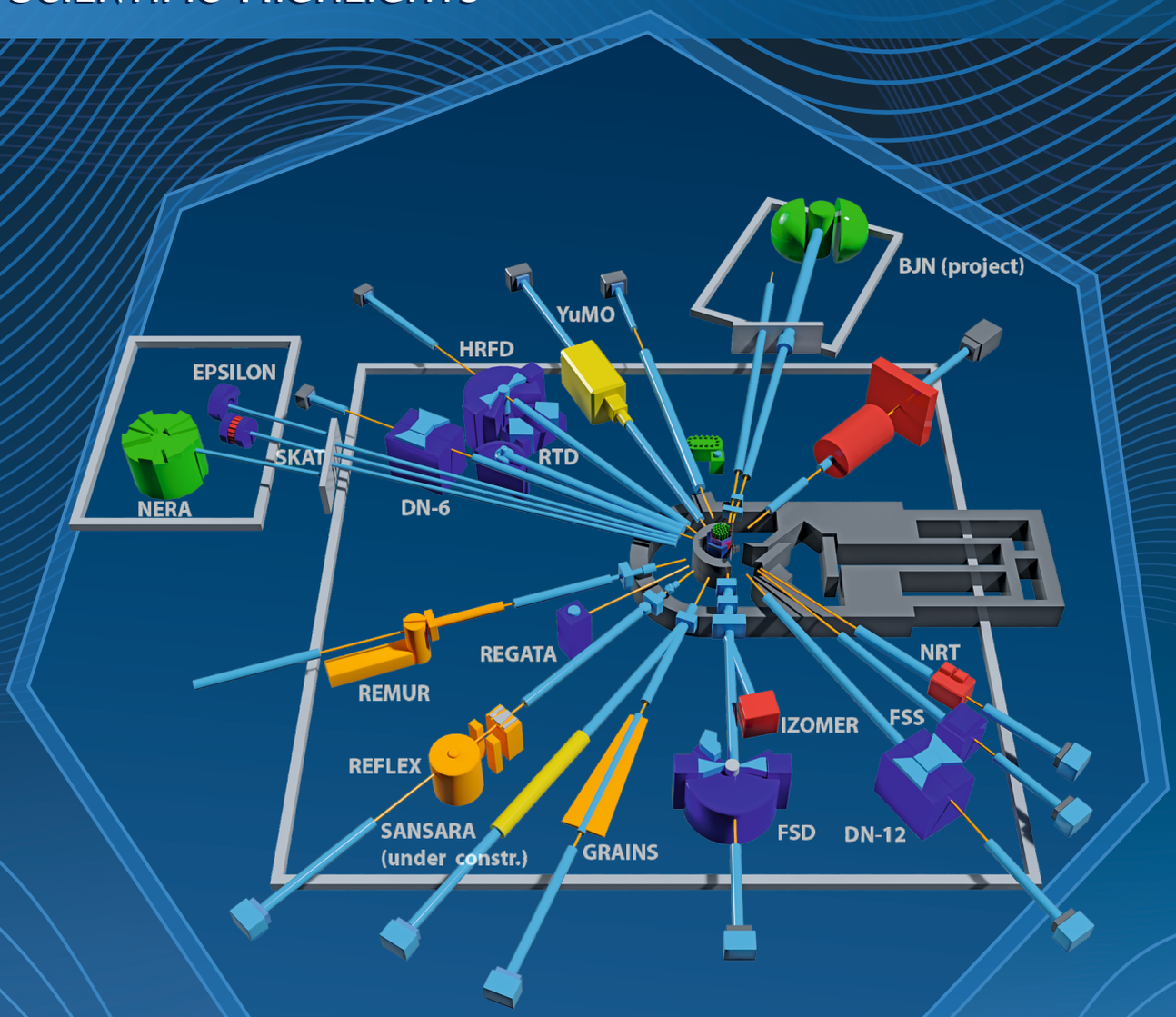
NEUTRON RESEARCH AT IBR-2 FOR MEMBER STATES

Scientific Highlights



FLNP

JOINT INSTITUTE
FOR NUCLEAR RESEARCH

The development of a large-scale scientific infrastructure has always contributed to the development of research activities in general. An example of such infrastructure is the successfully operating IBR-2 high-flux pulsed reactor, which is one of the fundamental facilities of JINR. Today, IBR-2 has 15 stations for conducting neutron research in condensed matter physics and applied nuclear physics. The reactor was put into operation in 1984; then in 2007-2010 it underwent a deep modernization, and starting from 2021, an intermediate upgrade is underway with a license extension for the next period.

The IBR-2 reactor is operated in accordance with the user policy program, which allows maintaining high research activity and ensuring high efficiency in the operation of this facility. Up to 200 experiments per year were carried out on IBR-2 before it was shut down for repairs in 2021. The user policy is largely aimed at attracting scientific groups from the JINR Member States and partners of JINR.

The purpose of this digest is to illustrate the active and effective use of IBR-2 by scientists from the JINR Member States, which is reflected in publication activity on various emerging topics and research frontiers. It presents a selection of research highlights of findings by these scientific groups over the last decade. The examples cut across the main areas of research at IBR-2, including solid-state physics, applied research, functional nanomaterials, life sciences, environmental sciences, and cultural heritage. These areas represent the cutting edge of world science and form one of the modern scientific foundations of the Frank Laboratory of Neutron Physics at JINR.

Summarizing the presented review, we can say that JINR has extremely positive experience in operating the neutron source of the 'IBR-2 type'. Undoubtedly, this research facility is a center of attraction for scientists from the JINR Member States, which is confirmed by the fairly large number and variety of works published based on the results obtained at IBR-2.

E.V. Lychagin

FLNP Director

1. Condensed matter physics

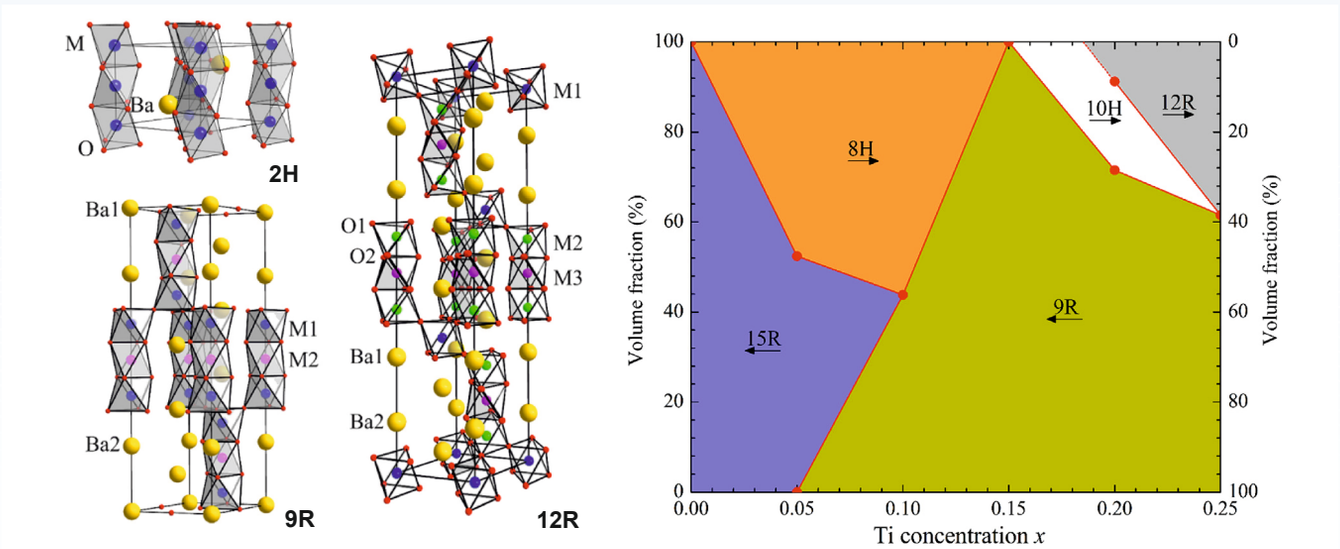
- Crystals
- Phase transitions
- Magnetism
- High pressure

Structural polymorphism and magnetism in doped barium titanates: neutron diffraction studies

Cooperation in the framework of the IBR-2 user program:
Institute of Research and Development, Duy Tan University, Da Nang, Vietnam

Scientists from Vietnam studied atomic and magnetic structures of novel multiferroic compounds comprising ferromagnetic and ferroelectric properties

Novel multiferroic materials combining magnetic and ferroelectric properties and showing significant spontaneous electric polarization and magnetization, are of current interest. In this work, the structural analysis of the $BaTi_{1-x}Fe_xO_3$ and $BaTi_{1-x}Mn_xO_3$ compounds was performed using the neutron diffraction method. Neutron diffraction experiments were made on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. At low iron concentrations and room temperature, the $BaTi_{1-x}Fe_xO_3$ compounds exhibit a polar structure with tetragonal symmetry, space group *P4mm*. When the iron concentration is x=0.07, the crystal structure of the studied compounds varies and is described by a centrosymmetric hexagonal space group P63/mmc. A series of structural phase transitions 15R ® 8H ® 9R ® 10H ® 12R were observed in the $BaTi_{1-x}Mn_xO_3$ compound upon doping with titanium. Antiferromagnetic ordering in the 15R, 9R and 8H structural phases was observed at low temperatures. The magnetic propagation vectors are q = (0 0 1/2) for the 15R and 9R phases and q = (0 0 0) for the 8H phase. The magnetic ordering temperatures and the ordered Mn magnetic moments are suppressed rapidly with the increase in the titanium concentration.



Structural models of selected possible polytypes and structural phase diagram of the of $BaTi_{1-x}Mn_xO_3$ compounds in the Ti concentration range x< 0.25 according to neutron diffraction data.

[1] Dang N.T., Kozlenko D.P., Phan T.L, Kichanov S.E., Dang N.V., Thanh T.D., Khiem L.H., Jabarov S.G., Tran T.A., Vo D.B., Savenko B.N., Structural polymorphism of Mn doped $BaTiO_3$, *J. Electron. Mater.* 45 (2016) 2477. DOI: 10.1007/s11664-016-4382-z

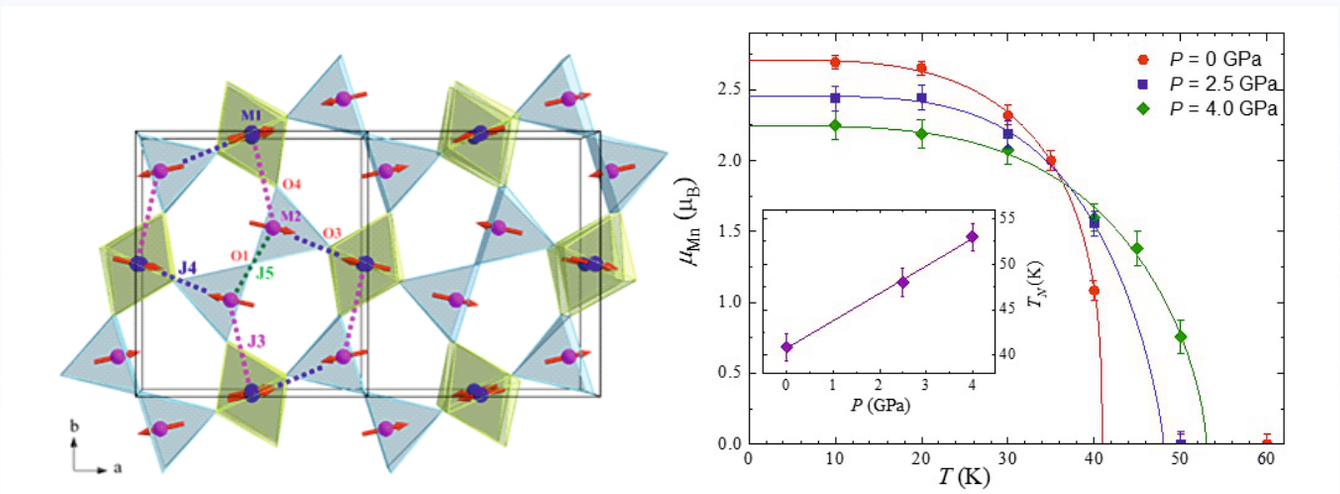
[2] Kozlenko D.P., Dang N.T., Phan T.L., Kichanov S.E., Khiem L.H., Jabarov S.G., Tran T.A., Manh T.V., Le A.T., Nguyen T.K., Savenko B.N., The structural, magnetic and vibrational properties of Ti-doped $BaMnO_3$, *J. Alloys Comp.* 695 (2017) 2539. DOI: 10.1016/j.jallcom.2016.11.159

Effect of pressure on the magnetic order of multiferroic $BiMn_2O_5$

Cooperation in the framework of the IBR-2 user program:
Institute of Research and Development, Duy Tan University, Danang, Vietnam;
Institute of Physics, ANAS, Baku, Azerbaijan

Scientists from Vietnam and Azerbaijan studied the effect of high pressure on the magnetic structure in a frustrated multiferroic

Multiferroic materials exhibiting strong coupling between electrical and magnetic orders are a great deal of current fundamental and technological interest. These materials display challenging physical phenomena such as the control of electrical polarization by the application of an external magnetic field and the manipulation of magnetization by an electric field, providing the opportunity to produce new multifunctional devices. The presence of competing interactions makes the $BiMn_2O_5$ compound highly frustrated, leading to various magnetic orders with long modulation wavelengths. The magnetic frustration makes these compounds sensitive to pressure. In this work, the crystal and magnetic structures of $BiMn_2O_5$ were investigated [1] using neutron powder diffraction at high pressure. Neutron diffraction experiments were performed on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. The results demonstrate that the long-range commensurate antiferromagnetic order with a propagation vector q = (1/2, 0, 1/2) stabilizes under high pressure. Upon compression, the Neel temperature, T_N, linearly increases. The temperature-dependent curves of the structural parameters show clear anomalies around T_N, evidencing strong magnetoelastic coupling in the compound. The magnetic ordering was shown to be affected by the displacement of the Mn^{3+} ions, which increases magnetic degeneracy. The magnetic properties of the compound were explained in terms of competing exchange interactions.



Crystal and magnetic structure of $BiMn_2O_5$ with labeled magnetic interactions. Temperature dependencies of the average ordered Mn^{3+}/Mn^{4+} magnetic moment at selected pressures and pressure dependence of the Neel temperature.

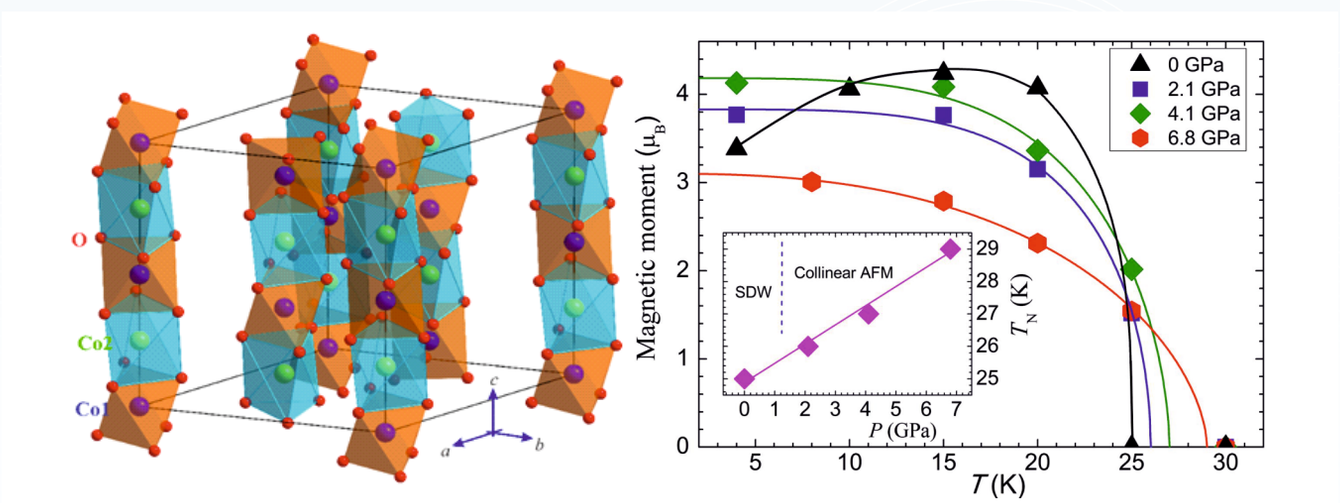
[1] Dang N.T., Kozlenko D.P., Kichanov S.E., Jabarov S.G., Mammadov A.I., Mekhtieva R.Z., Phan T.L., Smotrakov V.G., Eremkin V.V., Savenko B.N., Revealing the formation mechanism and effect of pressure on the magnetic order of multiferroic $BiMn_2O_5$ through neutron powder diffraction, *J. Electron. Mater.* 46 (2017) 3373. DOI: 10.1007/s11664-017-5351-x

Pressure induced modifications of the magnetic order in the spin-chain compound $Ca_3Co_2O_6$

Cooperation in the framework of the IBR-2 user program:
Institute of Research and Development, Duy Tan University, Danang, Vietnam

Scientists from Vietnam initiated structural studies of a spin chain magnetic system under high pressure

The low dimensional spin chain magnetic systems exhibit a rich variety of challenging physical phenomena. Among spin chain systems, an interesting model compound is $Ca_3Co_2O_6$. Due to the different crystalline electric field splittings, the Co^{3+}(I) and Co^{3+}(II) ions with the octahedral and the triangular base prism oxygen coordination have the low spin state LS (S = 0) and the high spin state HS (S = 2), respectively. A competing magnetic state results from a delicate balance of intra- and interchain magnetic interactions realized on the geometrically frustrated triangular lattice. Further important insight in exploration of particular factors responsible for a complex physical phenomenon observed in $Ca_3Co_2O_6$ and underlying structure-properties relationships can be achieved by high pressure studies. The crystal and magnetic structures of $Ca_3Co_2O_6$ were studied by neutron powder diffraction at high pressures on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. The symmetry of the long-range magnetic order in the quasi-1D spin chain compound was shown to be highly sensitive to application of high pressure. The pressure application leads to a suppresion of the spin density wave magnetic phase and stabilization of the collinear commensurate antiferromagnetic phase [1]. The role of the competing intra- and interchain magnetic interactions mediated by variation of interatomic distances was analyzed revealing a significant increase in the intrachain interactions upon compression. The pressure evolution of the Néel temperature of the pressure-induced antiferromagnetic (AFM) phase was analyzed in the framework of the mean field theory approach for the 1D Ising model showing good agreement with the experimental value.



The rhombohedral crystal structure of $Ca_3Co_2O_6$. Temperature dependencies of the ordered Co magnetic moment at selected pressures according to neutron diffraction data and pressure dependence of the Néel temperature, T_N, of $Ca_3Co_2O_6$.

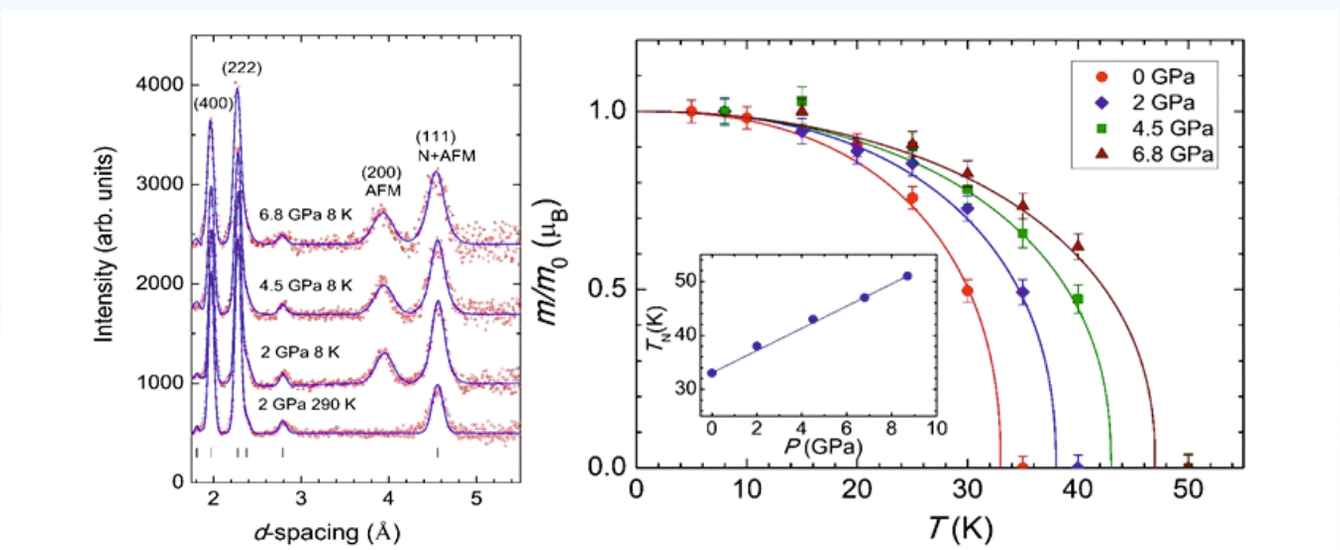
[1] Kozlenko D.P., Dang N.T., Golosova N.O., Kichanov S.E., Lukin E.V., Lampen Kelley P.J., Clements E.M., Glazyrin K.V., Jabarov S.H., Phan T.L., Savenko B.N., Srikanth H., Phan M.H., Pressure-induced modifications of the magnetic order in the spin-chain compound $Ca_3Co_2O_6$, *Phys. Rev. B* 98 (2018) 134435. DOI: 10.1103/physrevb.98.134435

High pressure effects on the crystal and magnetic structures of Co_3O_4

Cooperation in the framework of the IBR-2 user program:
Institute of Electrochemistry and Energy Systems, BAS, Sofia, Bulgaria;
Institute of Physical Chemistry, BAS, Sofia, Bulgaria;
University of Chemical Technology and Metallurgy, Sofia, Bulgaria

Scientists from Bulgaria initiated structural studies of a spinel cobalt oxide under high pressure to clarify the appearance of possible unconventional spiral and spin liquid states

The spinel cobalt oxide Co_3O_4 has attracted a special attention as a promising system with a geometrical frustration for a search of unconventional spiral and spin liquid states mediated by thermal fluctuations. The competing magnetic interactions in the Co_3O_4 compound can be varied by application of high external pressure via reduction of relevant bond distances and angles. The neutron powder diffraction measurements were performed on the DN-6 diffractometer at the IBR-2 reactor of FLNP JINR. The results [1] revealed the formation of the complex phase separated magnetic states, involving long range antiferromagnetic (AFM) ordered and magnetically disordered phases in Co_3O_4 at ambient pressure. Application of high pressure leads to suppression of the short-range disordered phase and a remarkable (~1.5 times) increase in the Néel temperature of the AFM phase. This effect is caused by a pronounced distance dependence of the nearest neighbor superexchange interactions. The next nearest neighbor superexchange interactions are found to play important role in the formation of the magnetic properties of Co_3O_4 in the studied pressure range.



Neutron diffraction patterns of Co_3O_4 at selected pressures and temperatures. Temperature dependences of the cobalt ordered magnetic moments at selected pressures, and the Néel temperature, T_N, of Co_3O_4 as a function of pressure.

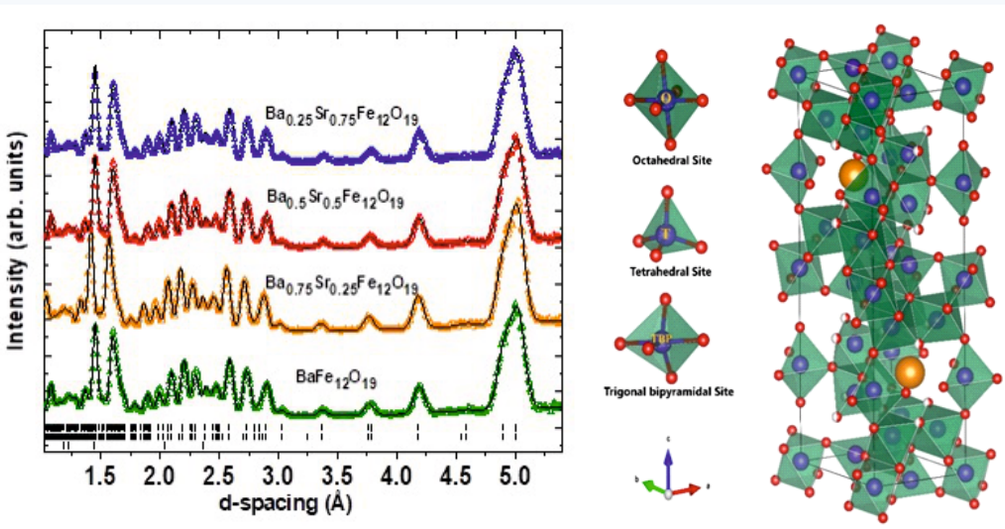
[1] Golosova N.O., Kozlenko D.P., Nicheva D., Petkova T., Kichanov S.E., Lukin E.V., Avdeev G., Petkov P., Savenko B.N., High pressure effects on the crystal and magnetic structures of Co_3O_4, *J. Magn. Magn. Mater.* 508 (2020) 166874. DOI: 10.1016/j.jmmm.2020.166874

The structural and magnetic properties of the complex iron oxides: neutron diffraction studies

Cooperation in the framework of the IBR-2 user program:
Faculty of Science, Fayoum University, El Fayoum, Egypt;
Reactor and Neutron Physics Department, Nuclear Research Center, Egypt

Scientists from Egypt studied atomic and magnetic structures of complex iron oxides with substituted ions regulating their physical properties

In the last few decades, barium hexaferrites have been widely studied due to their important role in several applications, such as permanent magnets in motors and sensors, as well as MRI systems and other devices. Furthermore, the physical properties of these materials can be modified and controlled through the substitution of various ions at different crystal lattice sites. Our research was aimed at elucidating the structure-property relationships for $Ba_{1-x}Sr_xFe_{12}O_{19}$ hexaferrite for different values of *x* using neutron diffraction. Neutron powder diffraction measurements were made on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. The crystal structure is described by the hexagonal symmetry of the *P63/mmc* space group. The magnetic structure forms due to Fe^{3+} cations, which locate at five nonequivalent crystallographic sites with tetrahedral, octahedral, and trigonal bipyramidal coordination. The observed growth in the magnetization of the $Ba_{1-x}Sr_xFe_{12}O_{19}$ samples with increasing x is due to a competition between Sr^{2+} and Ba^{2+} cations occupying the octahedral sites and a migration of Fe^{3+} ions from octahedral to tetrahedral sites in order to adjust the substituted Sr^{2+} cations.



Neutron diffraction patterns of $Ba_{1-x}Sr_xFe_{12}O_{19}$ (x = 0, 0.25, 0.5, 0.75) processed by the Rietveld method. The schematic representation of the obtained crystal structure of hexaferrites $Ba_{1-x}Sr_xFe_{12}O_{19}$ with different oxygen-related structural units.

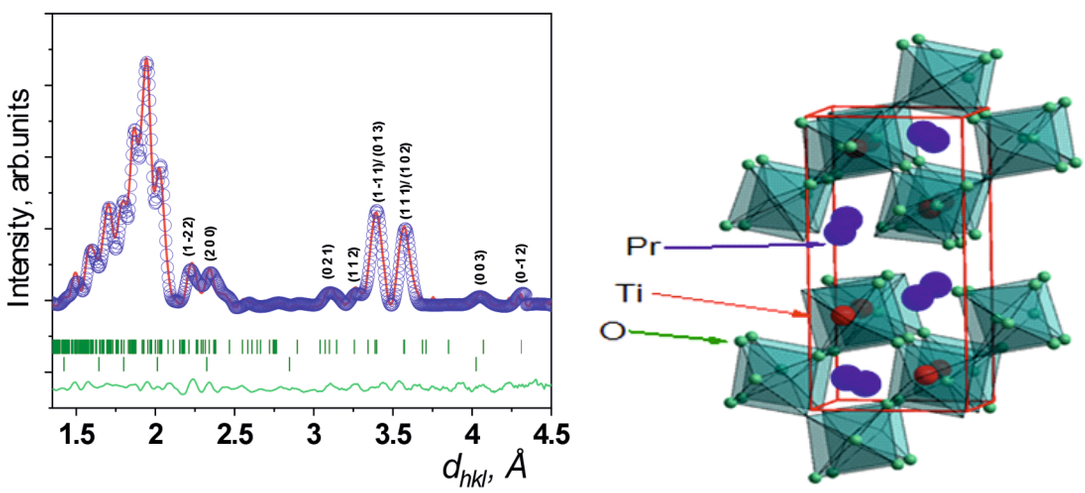
[1] El-Sayed S., Hashhash A., Refai H.S., Rutkauskas A.V., Baleidy W.S., Lis O. N., Hassen A., The detailed studies of the structural and magnetic properties of hexaferrites $Ba_{1-x}Sr_xFe_{12}O_{19}$ for $0.0 \leq x \leq 0.75$, *J. Mater. Sci. Mater. Electron.* 32 (2021) 10977. DOI: 10.1007/s10854-021-05757-1

The effects of high pressure on the crystal structure of layered perovskite-like compounds

Cooperation in the framework of the IBR-2 user program:
Institute of Physics, Ministry of Science and Education of the Republic of Azerbaijan, Baku, Azerbaijan

Scientists from Azerbaijan studied the effect of high pressure on layered perovskite-like compounds with advanced piezoelectric properties

The layered perovskite-like (PL) materials with the general formula $A_2B_2O_7$ is of current interest due to their advanced piezoelectric properties and various applications in nowadays technologies. The spontaneous polarization in the PL materials is determined by displacements of the rare-earth ions perpendicular to the *a*-axis, as well as the rotations of TiO_6 octahedra around the *b* crystallographic axis. Neutron diffraction experiments on the DN-6 diffractometer at the IBR-2 reactor of FLNP JINR were performed to reveal the crystal structure of a series of layered $Ln_2Ti_2O_7$ (Ln= La, Nd, Pr) compounds. To get insight into the high-pressure effect on structural properties of the PL compounds, detailed studies combining X-ray and neutron diffraction were made. Upon pressure, a phase transition in the PL layered compounds occurred. Based on the diffraction data, as well as previous theoretical calculations, the structural model with monoclinic *P21/m* space group was chosen [1, 2]. It was assumed that the structural modification at pressure application is related to the symmetrization of the arrangement and geometry of the Ti-O6 octahedra [1, 2]. These structural changes lead to the phase transition from the initial ferroelectric to the paraelectric state in the PL compound upon compression.



Neutron diffraction patterns of $Pr_2Ti_2O_7$ at ambient conditions, which were processed by the Rietveld method, and a schematic presentation of the monoclinic crystal structure of $Pr_2Ti_2O_7$.

[1] Asadov A.G., Kozlenko D.P., Mammadov A., Mehdiyeva R., Kichanov S.E., Lukin E.V., Lis O.N., Rutkauskas A.V., A structural phase transition in $La_2Ti_2O_7$ at high pressure, *Physica B* 655 (2023) 414753. DOI: 10.1016/j.physb.2023.414753

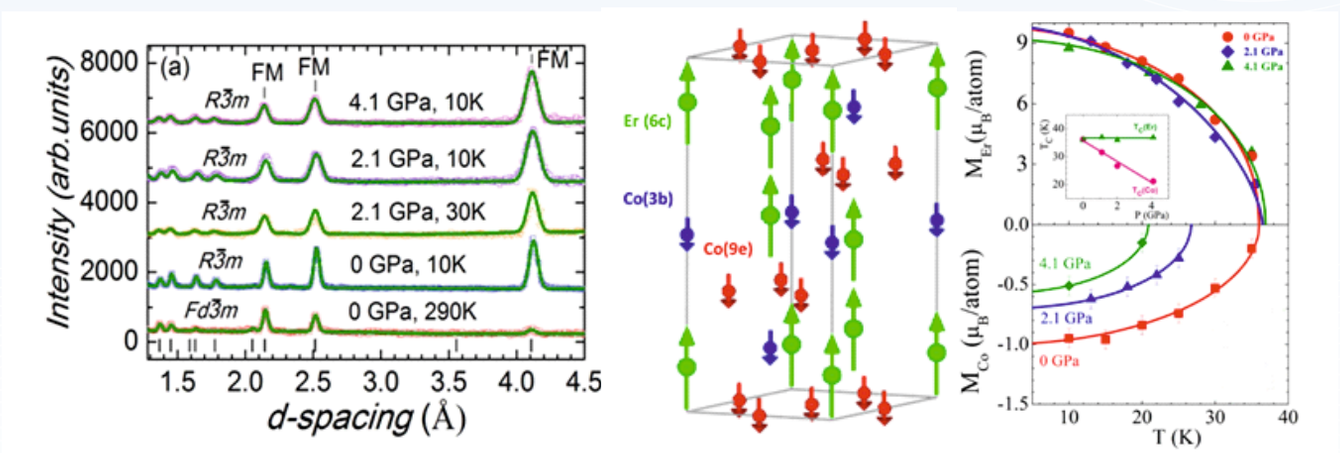
[2] Asadov A.G., Mammadov A., Kozlenko D.P., Mehdiyeva R., Kichanov S.E., Lukin E.V., Lis O.N., The effects of high pressure on the crystal structure and vibration spectra of layered perovskite-like $Nd_2Ti_2O_7$, *Solid State Ionics* 406 (2024) 166447. DOI: 10.1016/j.ssi.2023.116447

Magnetic phenomena in RCo_2 intermetallides: high pressure research

Cooperation in the framework of the IBR-2 user program:
Babes-Bolyai University, Cluj-Napoca, Romania;
Romanian Academy, Cluj-Napoca Branch, Cluj-Napoca, Romania

Scientists from Romania initiated the studies of high pressure effect on the magnetic structure in an interesting class of strongly correlated electron systems

Intermetallic rare-earth and cobalt compounds demonstrate a wide range of interesting physical properties determined by the correlation between the magnetization of R and Co sublattices and which can be controlled by manipulating the magnetic field [1]. This correlation is often explained by the concept of the itinerant electron metamagnetism, which suggests a spontaneous magnetization of cobalt due to the influence of the rare earth. Systematic neutron diffraction studies of the atomic and magnetic structures of RCo_2 compounds [1-4] with variations in thermodynamic parameters such as temperature in the range of 10–300 K and pressure in the range of 0–5 GPa were performed on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. In the experimental and supporting theoretical studies, a sequential collapse of cobalt sublattice magnetization in the background of nearly unchanged Er sublattice magnetization was revealed for $ErCo_2$ [4]. Combined studies showed the applicability of the traditional itinerant electron metamagnetism concept and evidenced more complex nature of magnetism in $ErCo_2$ [4] and related RCo_2 intermetallic systems.



Neutron diffraction patterns of $ErCo_2$ compound measured at selected pressures and temperatures and processed by the Rietveld method. The crystal structure and ferrimagnetic arrangement of Er and Co moments and temperature dependences of erbium and cobalt magnetic moments at different pressures are shown.

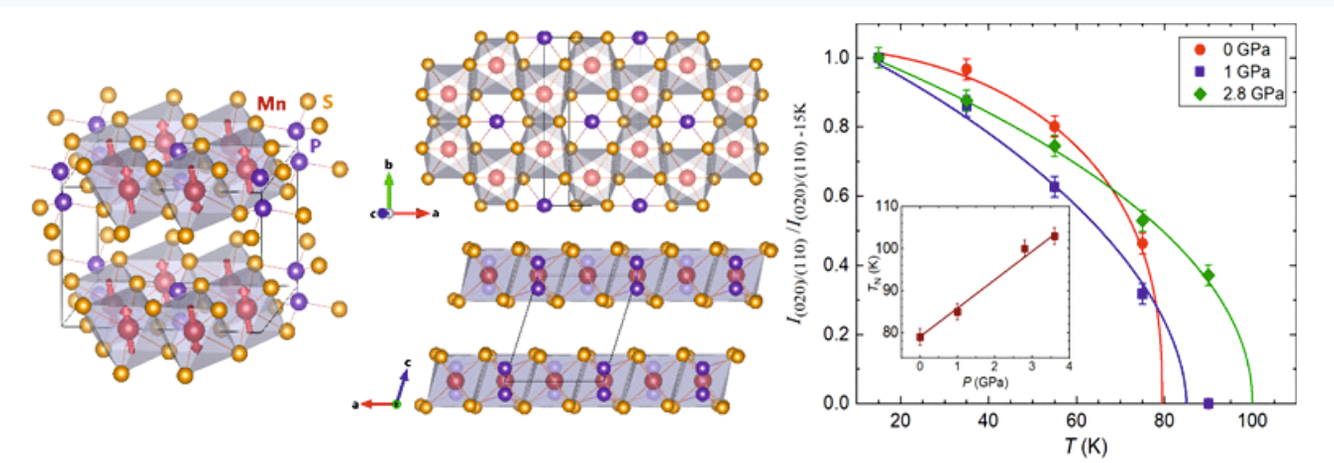
[1] Burzo E., Vlaic P., Kozlenko D.P., Pressure effects on the magnetic behavior of cobalt in rare-earth compounds, *Rom. J. Phys*. 60 (2015) 200. https://rjp.nipne.ro/2015_60_1-2/RomJPhys.60.p200.pdf
[2] Burzo E., Vlaic P., Kozlenko D.P., Kichanov S.E., Dang N.T., Lukin E.V., Savenko B.N., Magnetic properties of $TbCo_2$ compound at high pressure, *J. Alloys Comp.* 551 (2013) 702. DOI: 10.1016/j.jallcom.2012.10.178
[3] Burzo E., Vlaic P., Kozlenko D.P., Kichanov S.E., Dang N.T., Rutkauskas A.V., Savenko B.N., Magnetic properties, electronic structures and pressure effects of $Ho_xY_{1-x}Co_2$ compounds, *J. Alloys Comp.* 584 (2014) 393. DOI: 10.1016/j.jallcom.2013.09.076
[4] Burzo E., Vlaic P., Kozlenko D.P., Kichanov S.E., Rutkauskas A.V., Savenko B.N., Sequential collapse in $ErCo_2$: beyond the limits of itinerant electron metamagnetism, *Sci. Rep.* 5 (2015) 8620. DOI: 10.1038/srep08620

High-pressure effect on structural, magnetic and vibrational properties of van-der-Waals magnets

Cooperation in the framework of the IBR-2 user program:
Institute of Research and Development, Duy Tan University, Da Nang, Vietnam

Scientists from Vietnam studied the structural and magnetic states of a quasi-two-dimensional layered material from a class of promising van der Waals magnets

High pressure provides a unique opportunity for controlled changes in the structural and magnetic properties of compounds under the external influences (pressure, temperature), and opens up prospects for the creation of new materials with unique properties. In addition, with changes in temperature and pressure, various physical phenomena are discovered in many compounds. Neutron diffraction allowed to get new insight into the high-pressure behavior of the structural and magnetic states of a quasi-2D layered van der Waals material, $MnPS_3$. Unique experiments were performed on the DN-6 and DN-12 instruments of the IBR-2 reactor of FLNP JINR to study the effect of high pressure on the crystal and magnetic structures of promising van-der-Waals magnets in a wide temperature and pressure ranges [1,2]. The long-range antiferromagnetic order appears in $MnPS_3$ at ambient pressure below the Néel temperature, T_N≈79(2) K, with the oriented magnetic moments nearly perpendicular to the vdW planes [1]. It was obtained that the antiferromagnetic magnetic state remains stable in $MnPS_3$ at high pressures with a noticeable increase in TN. A different response of the magnetic interactions in MnPS3 were demonstrated in comparison with $FePS_3$ [2], which is caused mainly by different signs of the interplane magnetic interaction exchange constant at ambient pressure, which remains positive in the case of MnPS3, and changes from negative to positive under pressure in $FePS_3$.



The crystal and magnetic structure of $MnPS_3$, and temperature dependence of the magnetic contribution to the integrated intensity of the (020)/(110) peaks at selected pressures according to neutron diffraction data.

[1] Kozlenko D.P., Lis O.N., Dang N.T., Coak M., Park J.-G., Lukin E.V., Kichanov S.E., Golosova N.O., Zel I.Yu., Savenko B.N., High-pressure effects on structural, magnetic, and vibrational properties of van der Waals antiferromagnet $MnPS_3$, *Phys. Rev. Materials* 8 (2024) 024402. DOI: 10.1103/PhysRevMaterials.8.024402

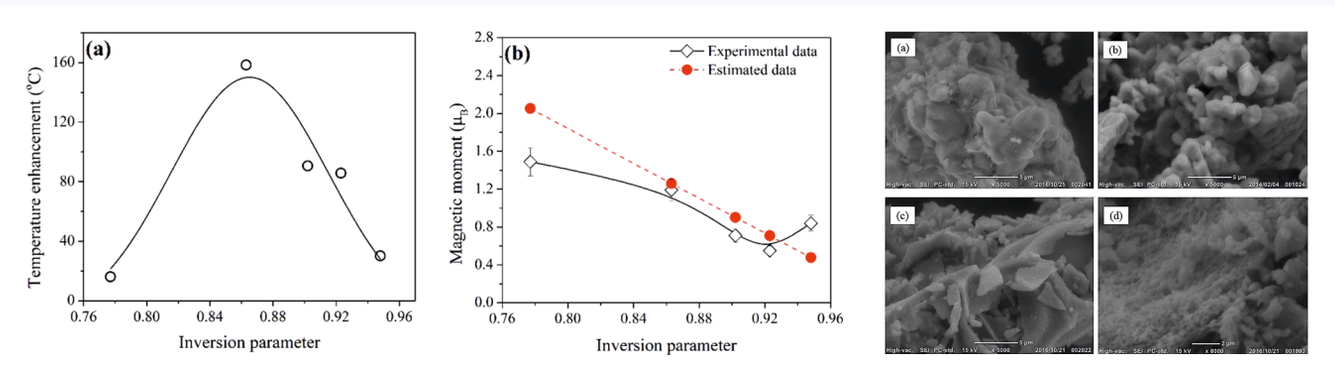
[2] Coak M.J., Jarvis D.M., Hamidov H., Wildes A.R., M. Paddison J.A., Liu C., Haines C.R.S., Dang N.T., Kichanov S.E., Savenko B.N., Lee S., Kratochvílová M., Klotz S., Hansen T.C., Kozlenko D.P., Park J.-G., Saxena S.S., Emergent magnetic phases in pressure-tuned van der Waals antiferromagnet $FePS_3$, *Phys. Rev. X* 11 (2021) 011024. DOI: 10.1103/PhysRevX.11.011024

Structural and magnetic properties of chemically synthesized ferrite magnetic materials

Cooperation in the framework of the IBR-2 user program:
National University of Mongolia, Ulaanbaatar, Mongolia;
Institute of Physics and Technology, Mongolian Academy of Science, Ulaanbaatar, Mongolia

Scientists from Mongolia investigated the structural and magnetic properties of synthesized ferrite magnetic materials for medical and biological applications

In recent years, interest in ferrite magnetic nanomaterials has considerably grown, mainly due to their highly promising medical and biological applications. Some magnetic materials such as fine ferrite powders having high heat generation ability in AC magnetic fields were considered for application in thermal coagulation (hyperthermia) therapy of cancer tumors. During hyperthermia, when the magnetic nanoparticles are heated up to 41–45 °C, the tumor is destroyed without harming surrounding healthy tissues. Using HRFD diffractometer at the IBR-2 reactor of FLNP JINR, ferrites $Cu_xMg_{1-x}Fe_2O_4$ were investigated as a class of heat generating magnetic nanomaterials. The results showed that the copper is one of the convenient substitutions for the magnesium ferrite, which enhances the heat generation ability and does not cause significant defects in crystal and magnetic structures [1]. In addition, for the $MgFe_2O_4$ magnetic material, a strong influence of the parameters of chemical synthesis on the crystal structure (e.g. inversion parameter), magnetic properties, heat-generating ability and morphology, was revealed [2]. For the series of $MgAl_xFe_{2-x}O_4$ ferrites with the different content of the Al substitution, it was found the that $MgAl_{0.2}Fe_{1.8}O_4$ sample produced by the solid-phase reaction method exhibits the lowest crystallite size and lattice volume and strongest bond strength, and, therefore, the highest heat generation ability [3].



Investigation of $MgFe_2O_4$ ferrite series using neutron powder diffraction, SEM and B-H analysis.

[1] Uyanga E., Sangaa D., Hirazawa H., Tsogbadrakh N., Jargalan N., Bobrikov I.A., Balagurov A.M., Structural investigation of chemically synthesized ferrite magnetic nanomaterials, *J. Mol. Struct.* 1160 (2018) 447. DOI: 10.1016/j.molstruc.2018.01.010

[2] Uyanga E., Hirazawa H., Sakai T., Bobrikov I.A., Balagurov A.M., Jargalan N., Sangaa D., Correlation between synthesis and physical properties of magnesium ferrite, *J. Sol-Gel Sci. Technology* 95 (2020) 223. DOI: 10.1007/s10971-020-05247-6

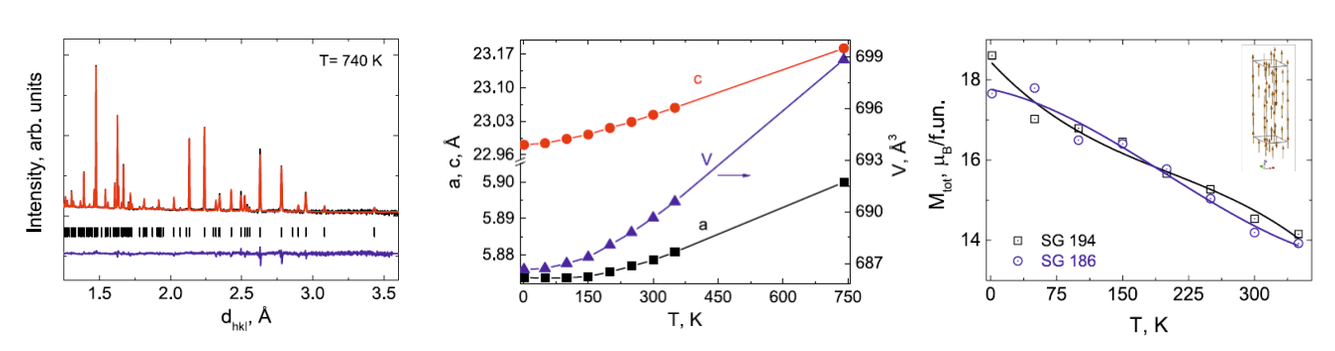
[3] Khishigdemberel I., Uyanga E., Hirazawa H., Enkhmend B., Bobrikov I.A., Sangaa D., Kiseleva T., Structural, infrared and magnetic properties of $MgAl_1Fe_{2-x}O_4$ compounds: Effect of the preparation methods and Al substitution, *Solid State Sci.* 109 (2020) 106400. DOI: 10.1016/j.solidstatesciences.2020.106400

Investigation of structural and magnetic properties of hexaferrites

Cooperation in the framework of the IBR-2 user program:
SSPA “Scientific and Practical Materials Research Centre of NAS of Belarus”, Minsk, Belarus

Scientists from Belarus used neutron diffraction to clarify the origin of ferroelectric properties in hexaferrites

Strontium ferrites of M-type and their solid solutions exhibit unique functional properties including large magneto-crystalline anisotropy, high values of the Curie temperature, very low electrical conductivity and relatively large magnetization. Hexaferrite systems are suitable for use in microwave and millimeter wave devices as permanent magnets, in high-density magnetic recording media, in magneto-optics and as gyromagnetic materials. The influence of temperature factor to crystal structure together with magnetic and electric properties of strontium hexaferrite partially substituted with diamagnetic indium ions were investigated. Ferroelectric properties were observed in the $SrFe_{11.9}In_{0.1}O_{19}$ compound that contradicts to the conventional opinion, which considers its crystal structure in the framework of the centrosymmetric space group *P63=mmc* (No. 194). For determining features of the crystal structure, which are responsible for ferroelectric properties of strontium hexaferrite, neutron diffraction measurements on the HRFD diffractometer at the IBR-2 reactor of FLNP JINR were done in temperature range from 1.5 to 740 K.



Neutron diffraction pattern from $SrFe_{11.9}In_{0.1}O_{19}$. Temperature dependencies of structural parameters a, c and volume V of the unit cell and total magnetic moments assuming different models.

[1] Turchenko V., Kostishyn V.G., Trukhanov S., Damay F., Porcher F., Balasoiu M., Lupu N., Bozzo B., Fina I., Trukhanov A., Waliszewski J., Recko K., Polosan S., Crystal and magnetic structures, magnetic and ferroelectric properties of strontium ferrite partially substituted with In ions, *J. Alloys Comp.* 821 (2020) 153412. DOI: 10.1016/j.jallcom.2019.153412

[2] Turchenko V.A., Trukhanov S.V., Kostishin V.G., Damay F., Porcher F., Klygach D.S., Vakhitov M.G., Lyakhov D., Michels D., Bozzo B., Fina I., Almessiere M.A., Slimani Y., Baykal A., Zhou D., Trukhanov A.V., Features of structure, magnetic state and electrodynamic performance of $SrFe_{12-x}In_xO_{19}$, *Sci. Rep.* 11 (2021) 18342. DOI: 10.1038/s41598-021-97684-8

[3] Turchenko V., Kostishin V.G., Trukhanov S., Damay F., Balasoiu M., Bozzo B., Fina I., Burkhovetsky V.V., Polosan S., Zdorovets M.V., Kozlovskiy A.L., Astapovich K.A., Trukhanov A., Structural features, magnetic and ferroelectric properties of $SrFe_{10.8}In_{1.2}O_{19}$ compound, *Mater. Research Bulletin* 138 (2021) 111236. DOI: 10.1016/j.materresbull.2021.111236

[4] Trukhanov A.V., Turchenko V.A., Kostishin V.G., Damay F., Porcher F., Lupu N., Bozzo B., Fina I., Polosan S., Silibin M.V., Salem M.M., Tishkevich D.I., Trukhanov S.V., The origin of the dual ferroic properties in quasi-centrosymmetrical $SrFe_{12-x}In_xO_{19}$ hexaferrites, *J. Alloys Comp.* 886 (2021) 161249. DOI: 10.1016/j.jallcom.2021.161249

2. Applied Research

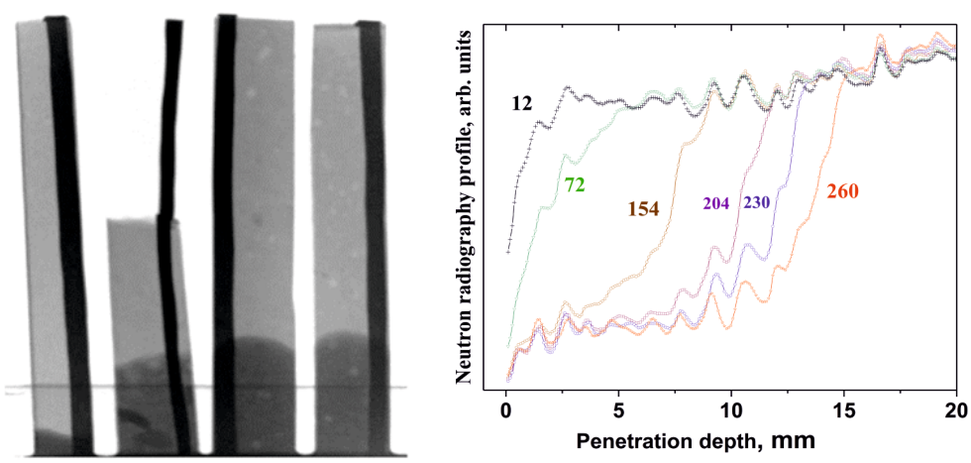
- Engineering
- Mechanical stresses
- Constructional materials
- Geophysics

Neutron microstructural analysis of promising cement materials for the construction of radioactive waste storage

Cooperation in the framework of the IBR-2 user program:
Reactor Physics Department, Nuclear Research Center, Atomic Energy Authority, Cairo, Egypt

Scientists from Egypt considered water penetration into special cement materials for preventing their deterioration

Cement mortars play a key role in the construction of buildings, being used in various formulas. The time it takes for cement-based mortars and concretes to set depends heavily on the presence of water in these materials. Chemical and biological agents carried by water are major factors in the deterioration of building materials. Transport of water through porous media like cement mortar is crucial for their durability and stability. Neutron radiography is a powerful non-destructive analytical tool with many applications in studying water absorption and infiltration in porous building materials such as mortar [1, 2], concrete, stones, and bricks [3]. Experiments on neutron radiography were performed at the neutron radiography and tomography facility NRT at the IBR-2 reactor of FLNP JINR. The capillary penetration coefficient, sorptivity, and capillary porosity were calculated from the neutron radiography data [1-3]. It was shown that the capillary absorption processes depend on the sealing material used to cover the surface of the investigated samples.



Neutron radiography images (NRT, IBR-2) of the cement mortar with penetrating water. The water front profile of the sample as a function of time in seconds.

[1] Nazarov K.M., Kichanov S.E., El Abd A., Taman M., Kozlenko D.P., Study of water infiltration into cement-based mortars using real-time thermal neutron radiography, *Eurasian Phys. Tech. J.* 17 (2020) 1. DOI: 10.31489/2020No1/39-45

[2] El Abd A., Taman M., Kichanov S.E., Hamad E., Nazarov K.M., Implementation of capillary penetration coefficient on water sorptivity for porous building materials: An experimental study, *Construction and Building Materials* 298 (2021) 123758. DOI: 10.1016/j.conbuildmat.2021.123758

[3] El Abd A., Kichanov S.E., Taman M., Nazarov K.M., Penetration of water into cracked geopolymer mortars by means of neutron radiography, *Construction and Building Materials* 256 (2020) 119471. DOI: 10.1016/j.conbuildmat.2020.119471

Neutron tomography analysis of novel cement materials for radioactive waste conditioning

Cooperation in the framework of the IBR-2 user program:
Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest, Romania

Scientists from Romania initiated complex microstructure analysis of special cement materials with improved mechanical properties

The problem of disposal and storage of solid radioactive wastes from nuclear industries is acute for governments, environmental and scientific communities of the countries that use and develop nuclear energy and technologies. Currently, new methods of synthesis and new chemical formulations of cement materials are actively being developed in order to improve their anti-corrosive and mechanical properties [1-3]. The method of neutron radiography and tomography at the NRT facility of the IBR-2 pulsed reactor of FLNP JINR is successfully employed to identify and analyze structural features of cement materials [1] that have a critical impact on the mechanical or chemical stability of final products [2]. The structural futures of the graphite inclusions [3] obtained from 3D neutron tomography data were used to calculate the mechanical properties of composite cement materials in the framework of several models that take into account both the shape and size of the graphite aggregates.

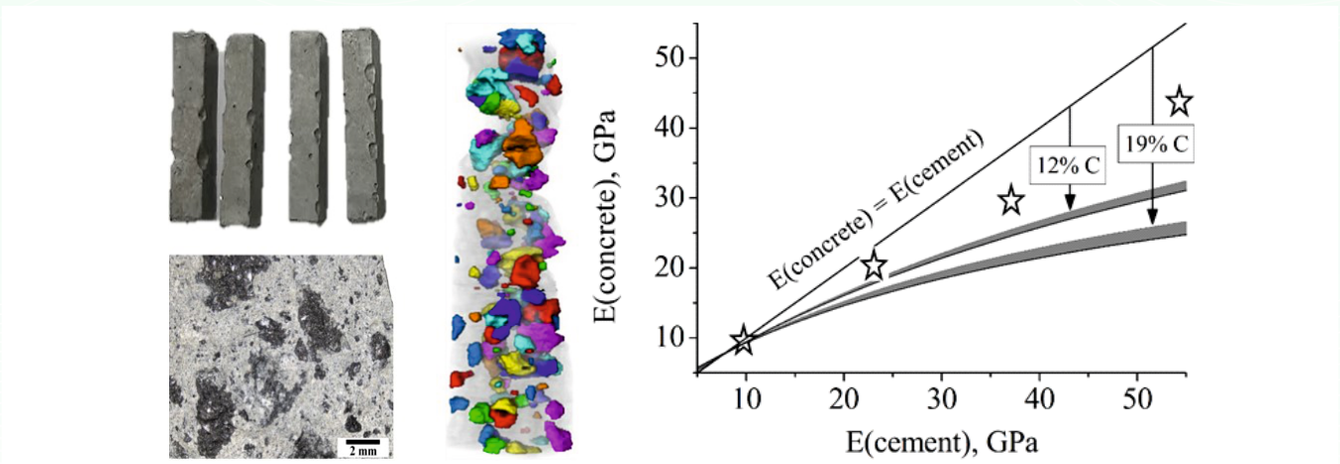


Photo and microscope images of mechanical cutting slices of cement samples with graphite inclusions together with 3D model from neutron radiography (NRT, IBR-2). Elastic properties of the studied composite cement materials are compared with those of a typical concrete material.

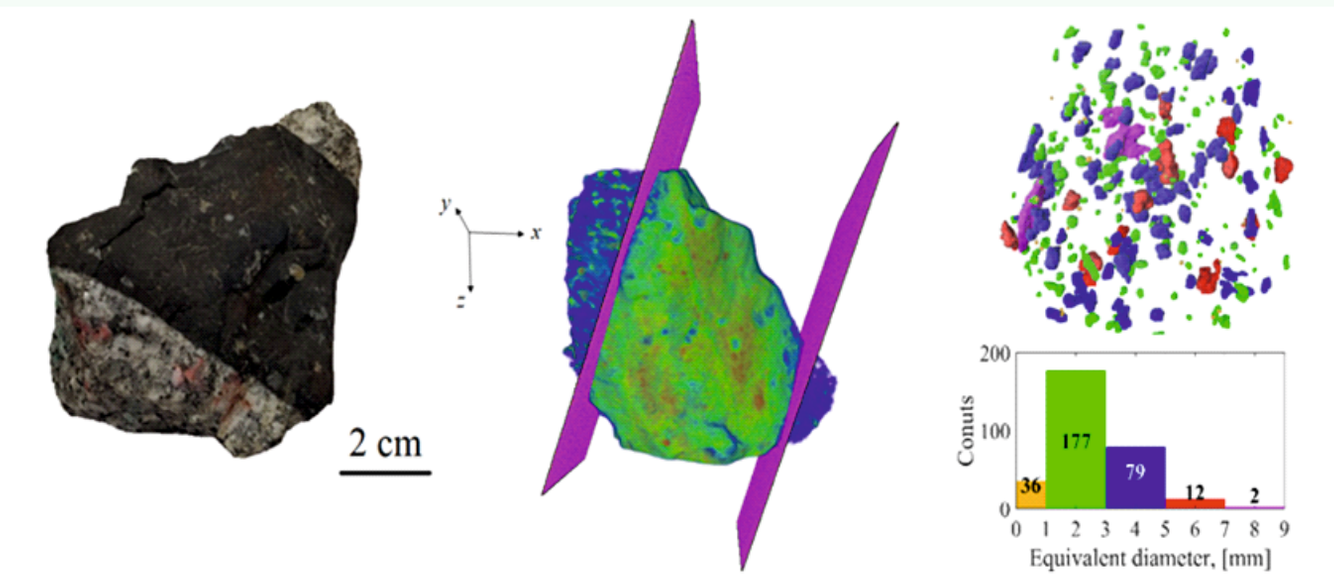
[1] Kichanov S.E., Nazarov K.M., Kozlenko D.P., Balasoiu M., Nicu M., Ionascu L., Dragolici A.C., Dragolici F., Savenko B.N., Neutron tomography studies of cement-based materials used for radiactive waster conditioning, *Romanian J. Phys.* 64 (2019) 803. https://rjp.nipne.ro/2019_64_1-2/RomJPhys.64.803.pdf
[2] Zel I. Yu., Kenessarin M., Kichanov S.E., Balasoiu M., Kozlenko D.P., Nazarov K., Nicu M., Ionascu L., Dragolici A.C., Dragolici F., Spatial distribution of graphite in cement materials used for radioactive waste conditioning: An approach to analysis of neutron tomography data, *Cement and Concrete Composites* 119 (2021) 103993. DOI: 10.1016/j.cemconcomp.2021.103993
[3] Zel I.Yu., Kenessarin M.R., Kichanov S.E., Nazarov K., Bălășoiu M., Kozlenko D.P., Pore segmentation techniques for the low-resolution data: application to the neutron tomography data of cement materials, *J. Imaging* 8 (2022) 242. DOI: 10.3390/jimaging8090242

Neutron tomography studies of lamprophyre dike samples: new approaches to the analysis of 3D imaging data

Cooperation in the framework of the IBR-2 user program:
Institute of Nuclear Physics, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan;
The Abdullayev Institute of Geology and Geophysics, Tashkent, Uzbekistan

Scientists from Uzbekistan initiated the detailed microstructure analysis of lamprophyre dike samples from the Koy-Tash granitoid intrusion

The neutron tomography is an effective method for studying the internal structure of various igneous, metamorphic rocks, cement materials, archaeological materials, etc. The high penetrating power of neutrons allows one to measure rather large volumes of rock materials, while high neutron imaging contrast between different minerals provides necessary conditions for successful phase segmentation and 3D analysis. Lamprophyre dikes, the representatives of igneous rocks, were studied using neutron tomography at the NRT facility of the IBR-2 pulsed reactor of FLNP JINR. Three-dimensional distributions of internal inclusions were obtained, and the analysis of their size distributions, shape, and orientation was used to reveal possible relationships between structural properties of the dike under study and the direction of the magma flow [1]. One of the studied dike samples was a combination of granodiorite walls and dike material with ocelli inclusions. It demonstrated the possibility for determining the orientation of the shape of the inclusions relative to the rock wall and revealing the relative orientation and direction of the magma flow.



Photography and reconstructed 3D model from neutron tomography data (NRT, IBR-2) of the lamprophyre dike sample together with segmented virtual planes of granite walls inside dike volume and spatial distribution of inner inclusions with their size distribution.

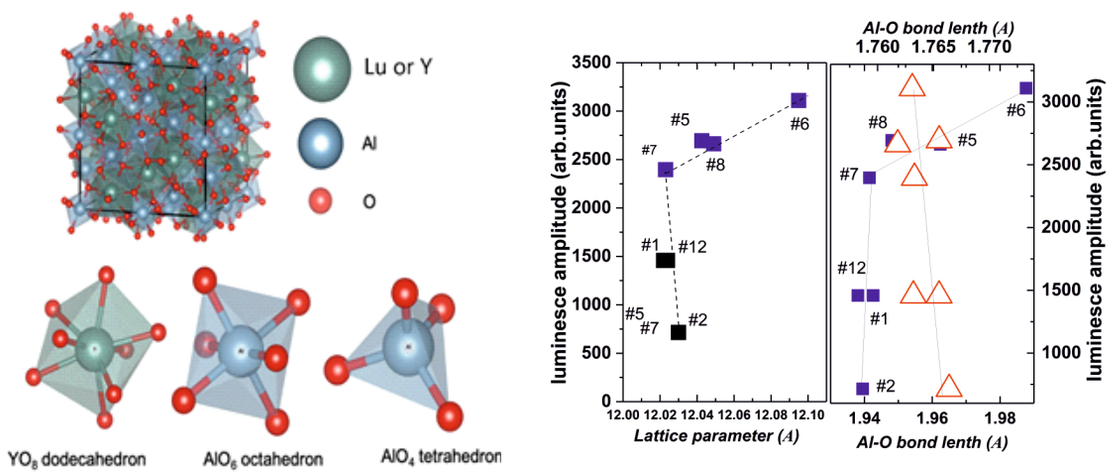
[1] Zel I., Abdurakhimov B., Kichanov S., Lis O., Myrzabekova E., Kozlenko D., Tashmetov M., Ishbaev K., Kosbergenov K., Neutron Tomography Studies of Two Lamprophyre Dike Samples: 3D Data Analysis for the Characterization of Rock Fabric, *J. Imaging* 8 (2022) 80. DOI: 10.3390/jimaging8030080

Structural aspects of the formation of optical properties in new luminescent materials: neutron diffraction studies

Cooperation in the framework of the IBR-2 user program:
Research Institute for Physical Chemical Problems of the BSU, Minsk, Belarus

Scientists from Belarus initiated the structure analysis of promising optical materials

Crystal phosphors based on lutetium aluminum garnets $Lu_3Al_5O_{12}:Ce^{3+}$ and yttrium aluminum garnets $Y_3Al_5O_{12}:Ce^{3+}$ in the form of single crystals, as well as alternative optical transparent ceramics obtained by solution-melt chemicals methods are of the current interest. They are characterized by high temperature stability of luminescence and low effects of temperature quenching in comparison with other phosphors. In this connection, it is important to study the evolution of their spectral luminescent and structural properties. Neutron powder diffraction measurements were performed on the DN-12 diffractometer at the IBR-2 reactor of FLNP JINR. In the studied garnet phosphors, the Al-O bond lengths for the octahedral oxygen coordination are expanded with the increase in the Ce concentration, while there are no evident changes in Al-O bonds in the tetrahedral oxygen coordination. The anisotropic modification of oxygen dodecahedra around Lu^{3+}/Y^{3+} and accordingly around optically active ion Ce^{3+} leads to a distortion of its crystallographic environment. It induces the redistribution of intensity bands of the doublet observed in luminescence spectra, relevant to two electron relaxation channels.



Schematic of the crystal structure of phosphors based on yttrium and lutetium aluminum garnets representing main structural units. Dependence of the luminescence intensity on the unit cell parameter and the Al–O bond lengths in the tetrahedral and octahedral oxygen environments obtained from neutron diffraction data.

[1] Kichanov S.E., Frolova E.V., Shevchenko G.P., Kozlenko D.P., Belushkin A.V., Lukin E.V., Malashkevich G.E., Rakhmanov S.K., Glazkov V.P., Savenko B.N., Investigation of structural features of the $Y_3Al_5O_{12}$: Ce3+/Lu2O3 crystal phosphors formed by the colloidal chemical method, *Phys. Solid State* 55 (2013) 813. DOI:10.1134/S1063783413040136

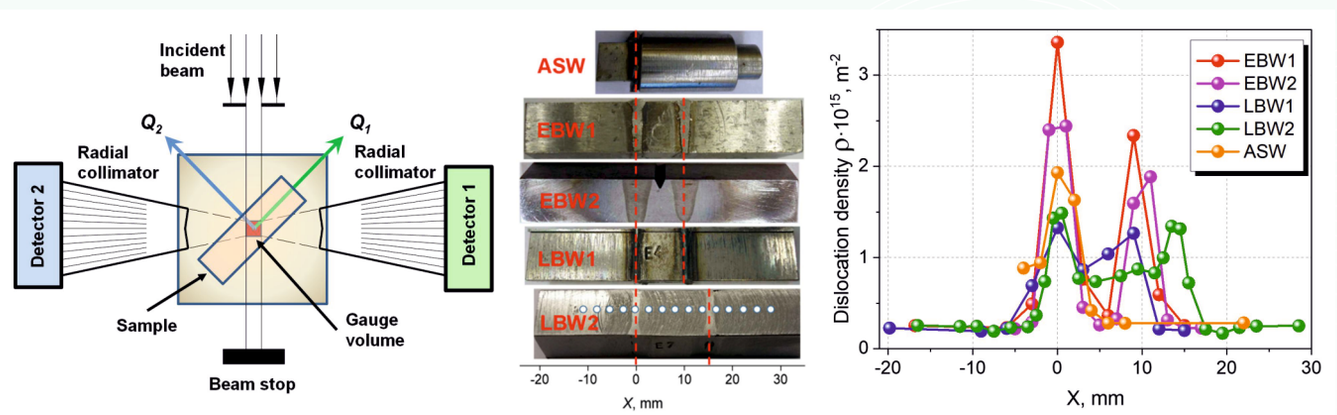
[2] Kichanov S.E., Shevchenko G.P., Tretyak E.V., Kozlenko D.P., Malashkevich G.E., Belushkin A.V., Savenko B.N., The structural and luminescent properties of $Lu_3Al_5O_{12}$: Ce^{3+}/Lu_2O_3 crystal phosphors prepared by colloid chemical synthesis, *J. Alloys Comp.* 613 (2014) 238. DOI:10.1016/j.jallcom.2014.06.034

Residual stresses and microstructural changes in nuclear reactor surveillance specimens reconstituted by various welding techniques

Cooperation in the framework of the IBR-2 user program:
Institute of Electronics of Bulgarian Academy of Sciences, Sofia, Bulgaria

Scientists from Bulgaria initiated the studies of residual stress distributions and microstructural changes in nuclear reactor surveillance specimens after reconstitution by various welding techniques

The monitoring of the metal condition of the reactor pressure vessel (RPV) during its lifetime for ensuring the integrity of the reactor vessel is a vital issue in nowadays nuclear power engineering. During reactor operation, RPVs are subjected to intense neutron irradiation, leading to the deterioration of reactor vessel steel and significant changes in its physical and mechanical properties, mainly manifested as increased brittleness. To monitor the RPV's metal condition, reference surveillance specimens are used. At certain intervals, these samples are removed from the reactor core and subjected to the Charpy impact tests, which assess the actual state (brittle or ductile) of the RPV material. Due to the limited number of surveillance samples, they are usually recovered by welding after the impact tests and returned to the reactor for further irradiation. This allows to increase the number of irradiated RPV steel samples to obtain representative and reliable data that are used to assess the radiation embrittlement of the RPV material to confirm or extend reactor lifetime. The reconstitution procedure must not significantly alter the structure and mechanical properties of the specimen's material. Therefore, it is essential to monitor the level of residual stresses in the reconstructed surveillance specimens after welding. In this work, a series of non-irradiated surveillance samples restored by various welding methods was investigated. Using high-resolution neutron diffraction [1], estimates of residual stresses, microstrains, dislocation densities, and crystallite sizes were obtained in the area around welds, which differ greatly from those in the original material [2].



Investigation of residual stresses and microstructural changes by high-resolution neutron diffraction (Fourier stress diffractometer FSD, IBR-2 of FLNP JINR) in a series of welded surveillance specimens.

[1] Bokuchava G.D., Petrov P., Papushkin I.V., Application of neutron stress diffractometry for studies of residual stresses and microstrains in reactor pressure vessel surveillance specimens reconstituted by beam welding methods, *J. Surface Investigation* 10(6) (2016) 1143. DOI: 10.1134/S1027451016050463

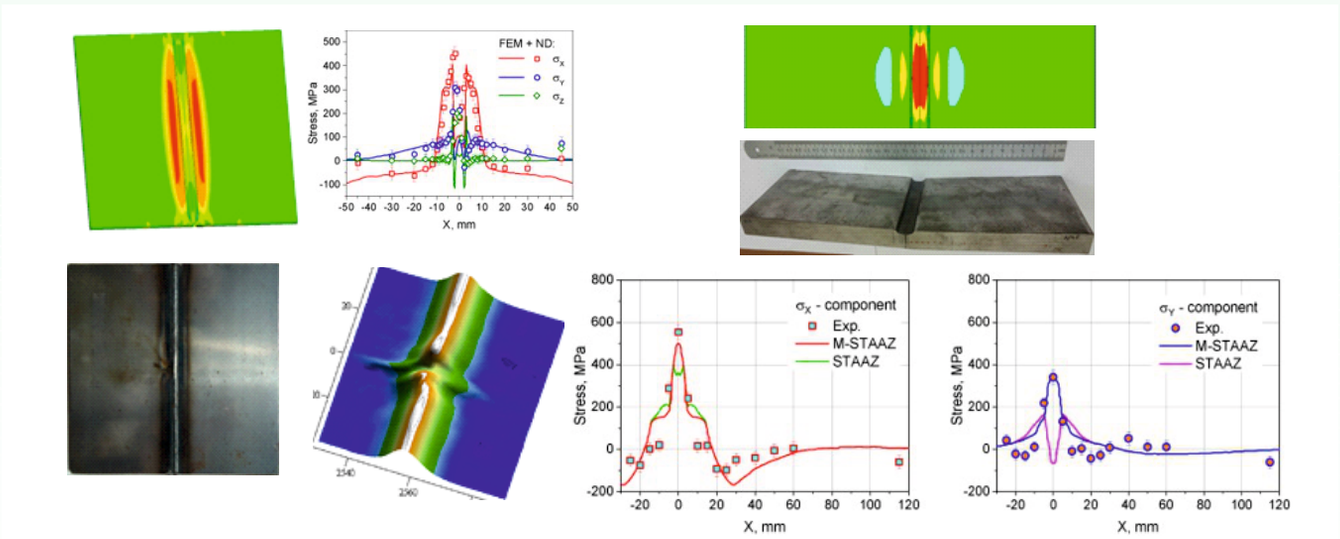
[2] Bokuchava G., Petrov P., Study of residual stresses and microstructural changes in Charpy test specimens reconstituted by various welding techniques, *Metals* 10(5) (2020) 632. DOI: 10.3390/met10050632

Residual stress analysis in welded joints by neutron diffraction and computer modeling

Cooperation in the framework of the IBR-2 user program:
Institute of Electronics of Bulgarian Academy of Sciences, Sofia, Bulgaria;
Brandenburg University of Technology, Cottbus, Germany

Scientists from Bulgaria and Germany initiated the combined experimental and computational studies of residual stress distributions and microstructural changes in nuclear reactor surveillance specimens after reconstitution by various welding techniques

Welding technologies are widely used in industry. Local areas of the heat-affected zone as a result of strong thermal effects during welding are subject to complex thermomechanical effects. The quantitative prediction of residual stress distribution is of great importance to ensure the quality and reliability of welds. To verify numerical models, reliable experimental data are required. Neutron diffraction helps much in it being a non-destructive method which does not change mechanical characteristics of the material and makes it possible to study it at a depth of several centimeters. The residual stress distributions after single-pass laser and multi-pass arc welding were experimentally measured on the FSD diffractometer at the IBR-2 reactor of FLNP JINR. Neutron data were used to verify numerical models of STAAZ and M-STAAZ welding processes. The developed numerical models are in good agreement with the diffraction results, which makes it possible to study the influence of various conditions and parameters of the welding process on the development of residual welding stresses. This information serves further as a basis for developing technological recommendations to obtain the desired level and profile of residual stresses in a specific product.



Comparison of residual stress distributions calculated by FEM and measured by neutron diffraction for single-pass laser and multi-pass arc welded specimens (Fourier stress diffractometer FSD, IBR-2).

[1] Genchev G., Doynov N., Ossenbrink R., Michailov V., Bokuchava G., Petrov P., Residual stresses formation in multi-pass weldment: A numerical and experimental study, *J. Constructional Steel Research* 138 (2017) 633. DOI: 10.1016/j.jcsr.2017.08.017

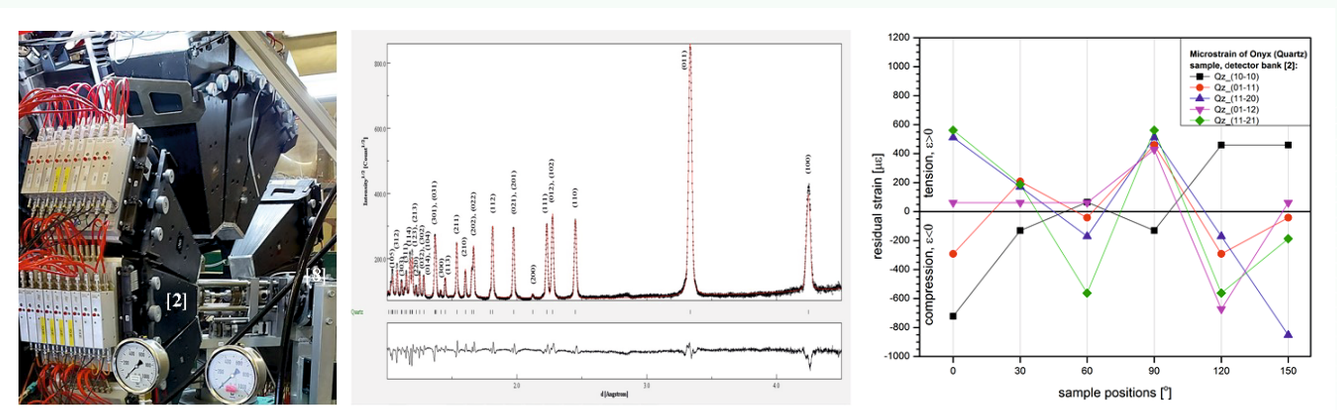
[2] Bokuchava G., Petrov P., Genchev G., Doynov N., Ossenbrink R., Michailov V., Residual stress analysis in welded joints by numerical simulation and high resolution neutron diffraction, *Romanian J. Phys.* 63 (2018) 904. https://rjp.nipne.ro/2018_63_7-8/RomJPhys.63.904.pdf

Investigation of applied and residual strains in geological materials

Cooperation in the framework of the IBR-2 user program:
National University of Mongolia, Ulaanbaatar, Mongolia;
Karlsruhe Institute of Technology, Karlsruhe, Germany

Scientists from Mongolia and Germany studied mechanical properties of polycrystalline quartzite under uniaxial load conditions to clarify effects of seismicity

The knowledge of the mechanical properties of rocks is of fundamental interest for better understanding of the geodynamic processes and for geotechnical applications such as mining and tunneling. Quartz constitutes a large volume of the earth's upper crust, which is about 60%. Therefore, studies of quartz and quartz-containing rocks are important for explaining some of the effects of seismicity. The distribution of earthquake impacts depends on the tectonic stress field of the earth and on the crystal and the mechanical properties of the rocks and rock layers. The response of the quartzite lattice to an applied uniaxial load was studied during in situ deformation experiments on the EPSILON diffractometer at the IBR-2 reactor of FLNP JINR. The strain in the quartz phase in the sandstone sample was measured at different loadings and the Young's moduli of the lattice planes of quartz for the Bragg reflections $(01\bar{1}1)/(10\bar{1}1)$, $(11\bar{2}0)$ and $(01\bar{1}2)/(10\bar{1}2)$ were determined. It was found that the determined Young's moduli of the listed Bragg reflections show lower values than those theoretically determined for single crystals. The difference is about 35.7 % for the $(01\bar{1}1)/(10\bar{1}1)$, 7.0 % for the $(11\bar{2}0)$ and 43.3 % for the $(01\bar{1}2)/(10\bar{1}2)$ lattice planes.



Investigation of residual strains in a polycrystalline quartzite rock sample on the EPSILON diffractometer, IBR-2.

[1] Badmaarag A., Sangaa D., Sikolenko V.V., Enkhtur L., Residual strain investigation of a polycrystalline quartzite rock sample using time-of-flight neutron diffraction, *Mongolian Geoscientist* 28 (2023) 27. DOI: 10.5564/mgs.v28i56.2451

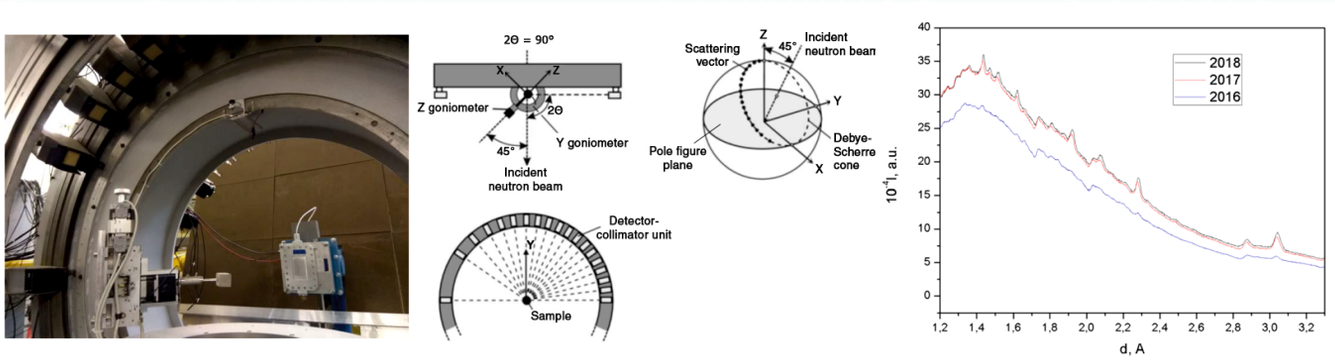
[2] Scheffzük Ch., Müller B., Breuer S., Badmaarag A., Schilling F.R., Applied strain investigation on a sandstone sample using neutron time-of-flight diffraction at the strain diffractometer EPSILON, IBR-2M Dubna, *Mongolian J. Phys.* 2 (2016) 433.

Study of aging of cement materials used for conditioning of aluminum radioactive wastes

Cooperation in the framework of the IBR-2 user program:
Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest, Romania

Scientists from Romania initiated structural studies of promising cement-based materials for conditioning of low and intermediate level radioactive wastes

Radioactive waste management is a crucial issue nowadays, as it involves conditioning wastes in concrete matrices that provide stable environment. Such kind of matrices is the main barrier to the migration of radionuclides in the environment from a radiation protection perspective. The cementitious materials used to encapsulate radioactive wastes need to meet certain acceptance criteria, including having stable chemical, physical, and mechanical properties over a period of 300 years or more. Therefore, the monitoring of the structure of these materials in time is an essential aspect for ensuring their safety and effectiveness. To improve the anticorrosive and mechanical properties of conditioning matrices, new methods and formulations have been developed for various types of radioactive wastes that are either being stored for a long period of time or disposed. In order to develop a suitable cement matrix for conditioning metallic radioactive aluminum, the addition of inorganic or organic compounds to cement pastes was investigated in order to reduce corrosion rates in alkaline solutions and obtain low permeability rates. The results of experiments carried out on the SKAT texture diffractometer of the IBR-2 reactor of FLNP JINR showed that for the samples containing aluminum powder, there is an increase in diffraction peaks in the neutron patterns, with the exception of the sample containing $Al_2(SO_4)_3$, $C_6H_8O_7$, and Pantarchol. In addition, in the sample containing CEM III + H2O + aluminum powder, a greater number of phases are observed as compared to the sample with $Al_2(SO_4)_3$ + $C_6H_8O_7$ + $LiNO_3$ + Pantarchol, but the latter reveals a more intense peak growth. Although the peak growth slows down after the first measurement, it does not stop completely. This increase in the peaks means that the structural changes in the sample continue, which could lead to anisotropic physical properties over time. From a structural stability perspective, therefore, a sample without $LiNO_3$ would be preferable.



Investigation of crystallographic texture of the cement sample (composed of CEM III + H_2O + Al(powder) + $Al_2(SO_4)_3$ + $C_6H_8O_7$ + Pantarhol + $LiNO_3$) at SKAT texture diffractometer, IBR-2.

[1] Lychagina T.A., Nikolayev D.I., Balasoiu M., Nicu M., Ionascu L., Dragolici A.C., Dragolici F., Aging studies of low pH cement-based materials used for aluminum radioactive waste conditioning, *Romanian J. Phys.* 64 (2019) 802. https://rjp.nipne.ro/2019_64_1-2/RomJPhys.64.802.pdf

3. Functional nanomaterials

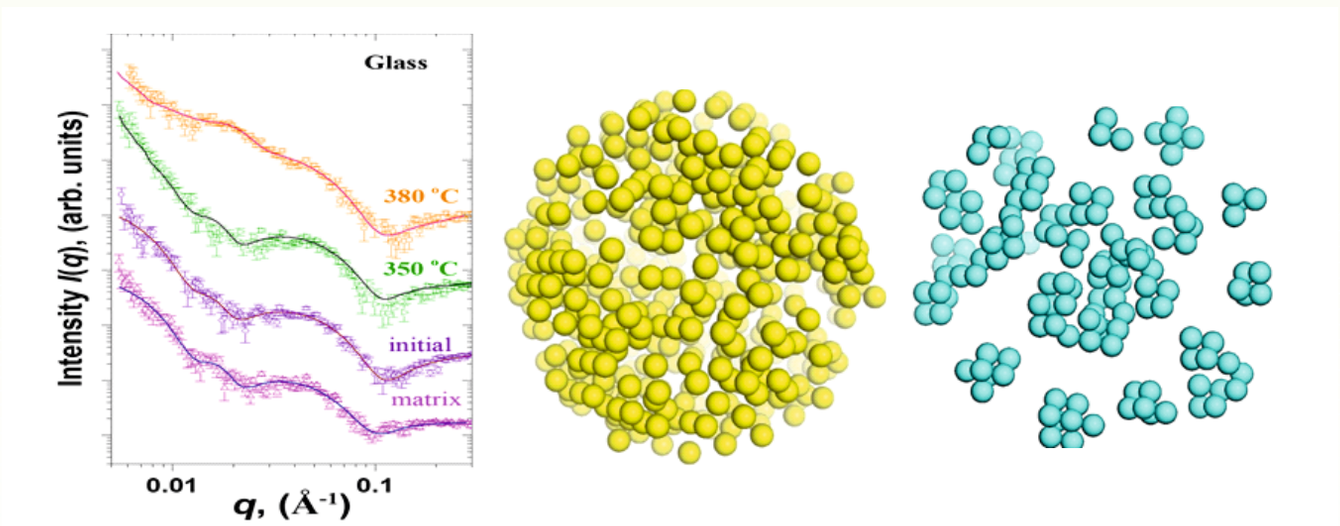
- Nanocomposites
- Polymers
- Surfactants
- Energy storage

Luminescent nanoparticles in glass materials: small-angle neutron scattering

Cooperation in the framework of the IBR-2 user program:
Belarusian State Technological University, Minsk, Belarus

Scientists from Belarus initiated studies of the nanoscaled structure of composite glass materials with promising optical properties

The composite glassy materials based on the nanoparticles embedded in a glass matrix have attracted the attention of the scientific community because of the unique physical phenomena related to the electron quantum confinement or unusual non-linear optical respond. The glasses with high optical transparency are excellent host materials for trapping luminescent nanoparticles. These nanostructured glassy materials provide higher quantum efficiencies of the up-conversion luminescence. In this work, detailed studies of the composite glasses were done by small-angle neutron scattering (SANS) on the YuMO spectrometer at the IBR-2 reactor of FLNP JINR. The results indicate a two-stage process of the formation of the luminescence nanoparticles in the studied composite glasses. At the first stage, relatively large amorphous nanoparticles of lead fluoride are formed in a glass matrix [1]. It is assumed that only the rare-earth ions are introduced into amorphous nanoparticles. The obtained structural data indicate the fragmentation of the initial amorphous nanoparticles into complex clusters consisting of smaller crystalline particles [2]. These small crystalline nanoparticles were assumed to be a center of the up-conversion luminescence in the studied composite glasses.



Evolution of SANS curves of the glasses with embedded optical nanoparticles following different temperature treatment. Reconstructed from SANS data structural model of a spatial arrangement of amorphous or crystalline luminescent nanoparticles inside initial glass matrix and in thermally treated glasses.

[1] Kichanov S.E., Kozlenko D.P., Gorshkova Yu.E., Rachkovskaya G.E., Zakharevich G.B., Savenko B.N., Structural studies of nanoparticles doped with rare-earth ions in oxyfluoride lead-silicate glasses, *J. Nanoparticle Research* 20 (2018) 54. DOI:10.1007/s11051-018-4156-z

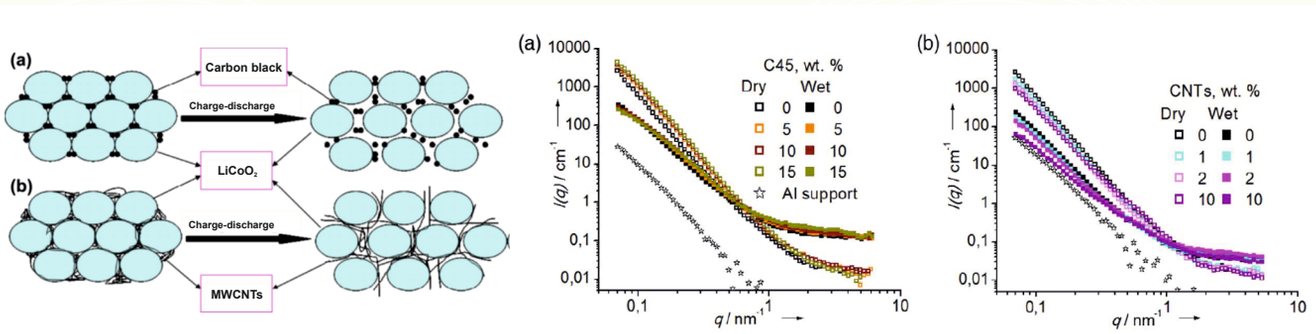
[2] Kichanov S.E., Gorshkova Yu.E., Rachkovskaya G.E., Kozlenko D.P., Zakharevich G.B., Savenko B.N., Structural evolution of luminescence nanoparticles with rare-earth ions in the oxyfluoride glass ceramics, *Mater. Chem. Phys.* 237 (2019) 121830. DOI:10.1016/j.matchemphys.2019.121830

Carbon-based additives for improving electrode materials in lithium-ion batteries

Cooperation in the framework of the IBR-2 user program:
Institute of Nuclear Physics, Ministry of Energy of the Republic of Kazakhstan, Almaty;
Gumilyov Eurasian National University, Astana, Kazakhstan;
Dubna State University, Dubna, Moscow Region, Russia

Scientists from Kazakhstan and Russia studied microstructure of electrode materials for lithium-ion batteries to improve their specific energy capacity

Small-angle neutron scattering (SANS) was applied to study the effect of conductive carbon additives (soot, graphene, graphene oxide and carbon nanotubes (CNTs)) on the porous structure of electrodes for lithium-ion batteries including $LiFePO_4$, $Li_4Ti_5O_{12}$, $LiNiMnCoO_2$ and others [1]. The experiments were performed on the YUMO instrument at the IBR-2 reactor of FLNP JINR. To separate the scattering by closed and open pores, the electrodes were wetted with a deuterated electrolyte, which made it possible to match the scattering by open pores. It was found that the used additives change the porosity of the electrodes to different degrees and affect the wettability of the material both due to the different efficiency of the embedding into the pores, and due to the changes in the matrix. Thus, the CNT network embedded in the electrode layer provides its greater wettability by an electrolyte compared to widely used carbon black. This results in better electrode performance. The structural analysis made it possible to improve and optimize the manufacturing technology of large-area LFP-based electrodes. It was demonstrated that the use of CNTs as conductive additives opens up prospects for the production of electrodes with an area capacity of more than 5 mAh/cm^2. The practical applicability of the considered electrode technology was proven on a pouch cell prototype with specific energy density of 150 Wh×kg^{-1}/295 Wh×l^{-1}.



Structure research of cathode materials (based on LFP) with carbon additives by SANS (YuMO, IBR-2) for improving capacity of lithium-ion batteries.

[1] Napolskiy F., Avdeev M., Yerdauletov M., Ivankov O., Bocharova S., Ryzhenkova S., Kaparova B., Mironovich K., Burlyaev D., Krivchenko V., On the use of carbon nanotubes in prototyping the high energy density Li-ion batteries, *Energy Technology* 8 (2020) 2000146. DOI:10.1002/ente.202000146

[2] Yerdauletov M., Avdeev M.V., Tomchuk A.A., Napolskiy F.S., Janseitov D.M., Krivchenko V.A., Nanoscale structure of positive electrodes for lithium-Ion batteries with graphene-based additives according to small-angle neutron scattering, *J. Surface Investigation*, 17 (2023) 460. DOI:10.1134/S1027451023020246

Composite nanoparticles based on periodic porous silica

Cooperation in the framework of the IBR-2 user program:
Pavol Jozef Šafárik University in Košice, Košice, Slovakia;
Comenius University Bratislava, Bratislava, Slovakia;

Scientists from Slovakia initiated the investigations of nanocomposite systems designed primarily for biomedical applications

The extraordinary properties inherent in the periodic nanoporous material on the basis of amorphous silica (large active surface area, regular and perfectly ordered pores along with chemical stability, heat resistance and biocompatibility) interest the scientific community with their enormous application potential in catalysis, cryomagnetic refrigeration, engineering, and environmental industry to name but a few. By virtue of the unique properties of neutrons, insight into the inner structure and matter organization of this kind of systems was facilitated for the first time on the YuMO instrument at the IBR-2 reactor of FLNP JINR. Structural characteristics of nanocomposite series consisting of iron oxide or gadolinium oxide nanoparticles (NPs) embedded in the regular pores of amorphous silica matrix were investigated. Rigorous experimental support documented regular nanopores organized in the cubic or hexagonal superlattice and confirmed the presence of NPs in the body of examined matrices, providing additional information on their shape, concentration and size distribution. Scattering superposition principle employed in the model conception allowed for tailoring its fundamental characteristics, and rendered it a potent and versatile tool for a wide range of applications. All of the examined systems have exhibited extraordinarily high values of magnetic entropy change (up to 70 J kg^{-1} K^{-1}) at low temperatures with the absence of thermal hysteresis, indicating their perspective utilization in cryogenic refrigeration.

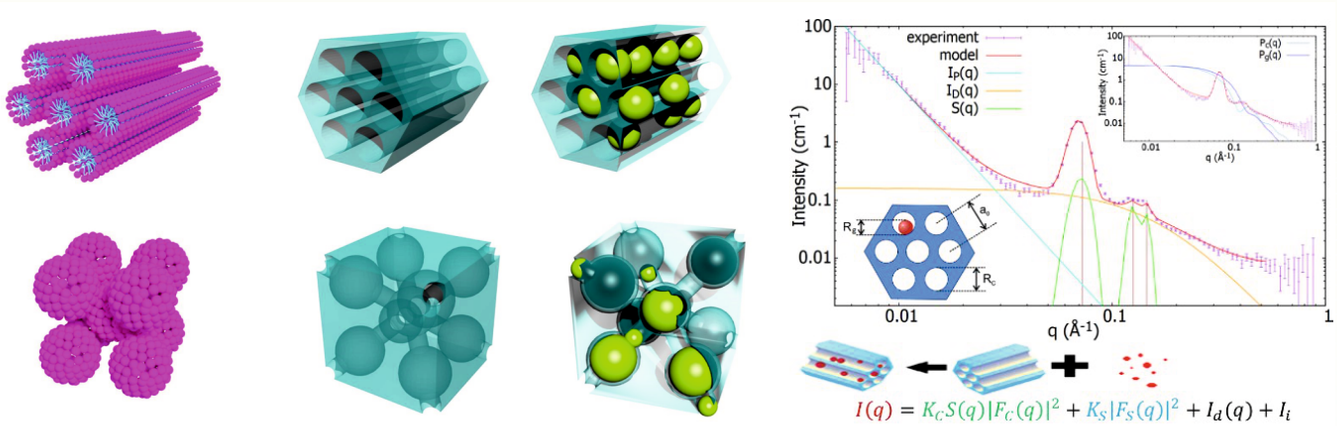


Illustration of the SBA-15 (upper raw of the left-hand panel) and SBA-16 (lower raw of the left-hand panel) nanocomposite preparation and structure organization functionalized by the introduction of Fe_2O_3 or Gd_2O_3 nanoparticles. The right-hand panel illustrates the model analysis of the SANS data.

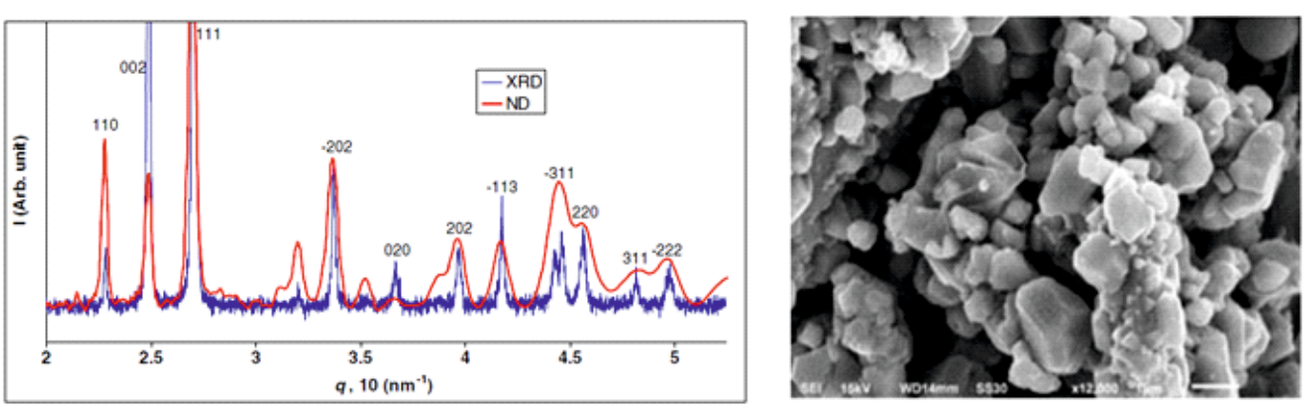
[1] Zeleňáková A., Hrubovčák P., Kapusta O., Kučerka N., Kuklin A., Ivankov O., Zeleňák V., Size and distribution of the iron oxide nanoparticles in SBA-15 nanoporous silica via SANS study, *Scientific Reports* 9 (2019) 15852. DOI:10.1038/s41598-019-52417-w
[2] Zeleňáková A., Hrubovčák P., Berkutova A., Šofranko O., Kučerka N., Ivankov O., Kuklin A., Girman V., Zeleňák V., Gadolinium-oxide nanoparticles for cryogenic magnetocaloric applications, *Scientific Reports* 12 (2022) 2282. DOI:10.1038/s41598-022-06132-8

Structure investigation of graphene nanocomposite CuO–rGO

Cooperation in the framework of the IBR-2 user program:
Physics Department Faculty of Science Cairo University, Giza, Egypt;
Institute of Solid State Physics RAS, Chernogolovka, Moscow, Russia

Scientists from Egypt and Russia initiated microstructure studies of a new low-cost nanocomposite for anodes in lithium-ion batteries to improve their performance characteristics

The increasing demand on lithium-ion batteries (LIBs) arises from their high-performance energy conversion and storage. Anodes of the commercial batteries are usually made from graphite. Many researches consider graphene oxide (GO) as a promising component of anodes in LIBs. Defects generated on the GO surface during the oxidation stage act as anchoring sites for deposition of nanoparticles. Nanosized transition-metal oxides are promising for anode materials in LIBs and supercapacitors. The use of CuO decorates reduced graphene oxides (rGOs); enhanced lithium storage characteristics and cycle stabilities has been reported. In this work, the research team uses a one-step synthesis of CuO–rGO using Cu nitrate, GO solution, and reducing agent hydrazine hydrate. The investigation of the structure and related properties of these promising materials is critically needed. The properties of CuO–rGO nanocomposites are difficult to be explained without knowing their nanostructure. This work focused on the structural investigation by X-ray diffraction, neutron diffraction complementing the FTIR data on the electronic composition of CuO–rGO nanocomposites. Characterization by different techniques confirms the reduction of graphene oxide and formation of CuO–rGO. The CuO nanocrystals are uniformly distributed on graphene sheets. Neutron and X-ray diffraction prove the formation of single phase of CuO monoclinic crystal system with space group C2/c. So, CuO–rGO nanocomposite was successfully prepared by simple precipitation method. The preparation process was tested and characterized by different techniques. The crystallite size was about 40 nm and the lattice strain was about $8*10^{-4}$. The prepared nanocomposite can find application for energy storage devices.



Neutron (RTD, IBR-2) and X-ray diffraction patterns and SEM image of nanocomposite under study.

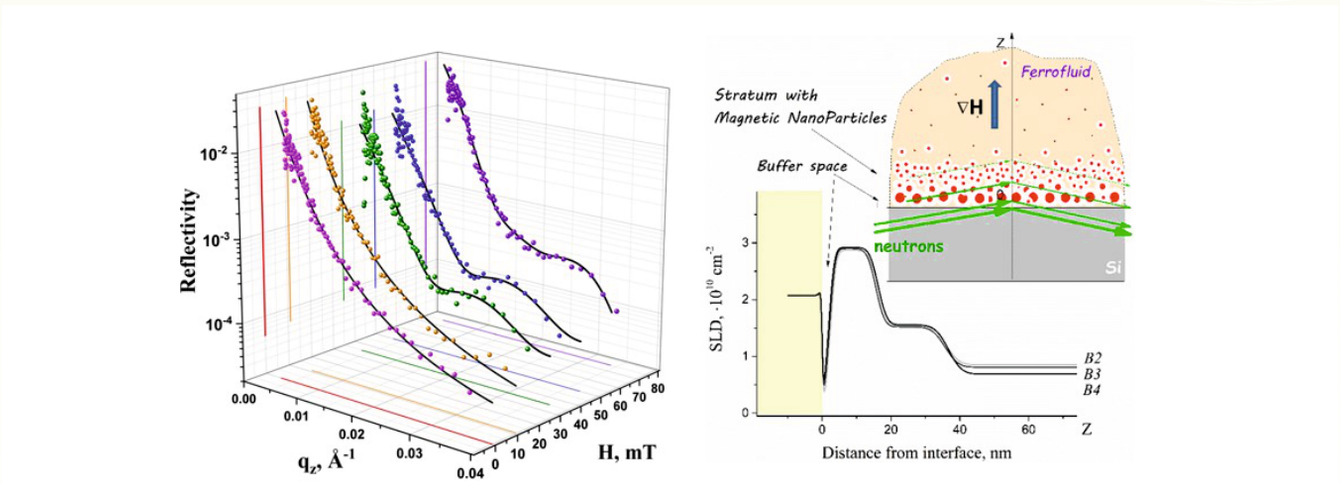
[1] Abdel-Aal S.K., Beskrovnyi A.I., Ionov A.M., Mozhchil A.M., Abdel-Rahman A.S., Structure investigation by neutron diffraction and X-ray diffraction of graphene nanocomposite CuO–rGO prepared by low-cost method, *Physica Status Solidi A* 218 (2021) 2100138. DOI: 10.1002/pssa.202100138

Ferrofluids at interfaces in external fields

Cooperation in the framework of the IBR-2 user program:
Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia;
University of Pretoria, Pretoria, South Africa

Scientists from Slovakia and South Africa studied adsorption of magnetic nanoparticles from ferrofluids on planar interfaces induced by magnetic and electric fields

Assembling of magnetic nanoparticles (MNPs) at planar interfaces are of current interest for various potential applications in catalysis, optics, and magnetic data storage. In this regard, an important step is the study of ferrofluids - suspensions of colloidal magnetic nanoparticles coated with various stabilizing agents (surfactants, polymers), whose properties can be controlled by external magnetic and in some cases (dielectric ferrofluids) electric fields. The study is related to the direct present-day use of ferrofluids as additives in electrolytes of high-voltage transformers for regulating thermal properties, where nanoparticles of magnetic materials interact with electrodes in the presence of a strong electric field, which, in turn, affects the dielectric breakdown voltage. Adsorption of MNPs under magnetic and electric fields was followed by neutron reflectometry on the GRAINS instrument at the IBR-2 reactor of FLNP JINR. At a sufficiently high field gradient, the formation of several adsorption layers with different filling densities of nanoparticles is observed. The discovered sensitivity of ferrofluids to external fields expands the possibilities of controlling the behavior of such systems under the combined action of magnetic and electric fields.



Formation of an adsorption layer of magnetic nanoparticles at the ferrofluid–crystal interface in an external magnetic field according to neutron reflectometry data (GRAINS, IBR-2).

[1] Nagornyi A.V., Petrenko V.I., Rajnak M., Gapon I.V., Avdeev M.V., Dolnik B., Bulavin L.A., Kopcansky P., Timko M., Particle assembling induced by non-homogeneous magnetic field at transformer oil-based ferrofluid/silicon crystal interface by neutron reflectometry, *Appl. Surf. Sci.* 473 (2019) 912. DOI:10.1016/j.apsusc.2018.12.197

[2] Selyshchev P.A., Petrenko V.I., Rajnak M., Dolnik B., Kurimskye J., Kopcansky P., Timko M., Bulavin L.A., Non-uniform distribution of ferrofluids spherical particles under external electric field: Theoretical description, *J. Mol. Liq.* 278 (2019) 491. DOI: 10.1016/j.molliq.2019.01.001 0167-7322

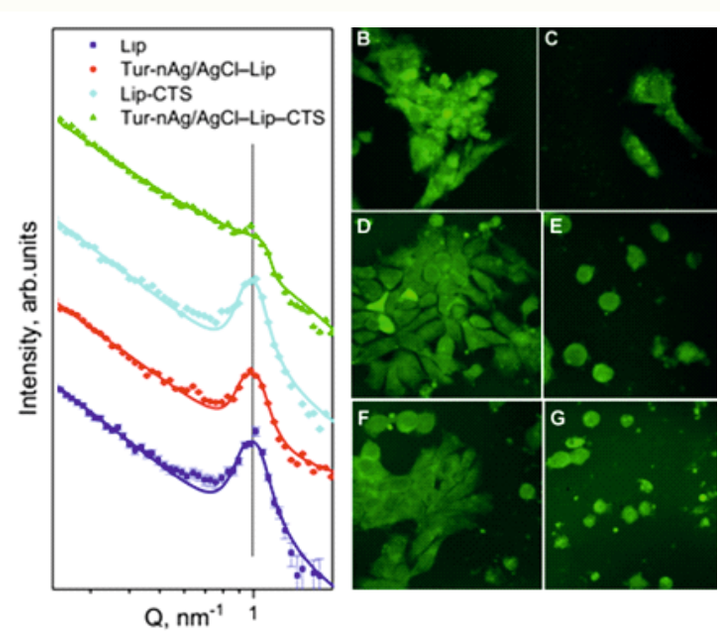
[3] Karpets M., Rajnak M., Petrenko V.I., Gapon I.V., Avdeev M.V., Bulavin L.A., Timko M., Kopcanský P., Electric field-induced assembly of magnetic nanoparticles from dielectric ferrofluids on planar interface, *J. Mol. Liq.* 362 (2022) 119773. DOI:10.1016/j.molliq.2022.119773

Characterization of biohybrids based on turmeric and silver/silver chloride nanoparticles

Cooperation in the framework of the IBR-2 user program:
University of Bucharest, Bucharest-Măgurele, Romania;
University "Politehnica" of Bucharest, Bucharest, Romania;
National Institute for Lasers, Plasma and Radiation Physics, Ilfov, Romania;
"Horia Hulubei" National Institute of Physics and Nuclear Engineering, Romania;
University of Nis, Leskovac, Serbia

Scientists from Romania and Serbia studied new materials based on biomimicking lipid bilayers loaded with special nanoparticles

The phyto-development of nanomaterials is one of the main challenges for scientists today, as it offers unusual properties and multifunctionality. This research concerned new materials based on biomimicking lipid bilayers loaded with chlorophyll, chitosan, and turmeric-generated nano-silver/silver chloride particles. These "green" hybrid systems are an important alternative in cancer treatment, as well as in health problems associated with drug-resistant infections. The structure organization of liposomes was investigated by small-angle neutron scattering (SANS) on the YuMO spectrometer at the IBR-2 reactor of FLNP JINR. Suspensions of multilamellar lipid vesicles (MLVs) were prepared in biological PBS buffer. The repeat distances d of the multilamellar liposomes were determined by fitting the diffraction peaks by the Gaussian function. All SANS curves have a diffraction peak in a region of Q-value of about 1 nm^{-1}. It means that the prepared liposomes have a multilamellar structure with the repetition distance of $d \approx 6.4$ nm. The bio-impact of the obtained biohybrids was studied in terms of antimicrobial hemolytic, and antiproliferative activities. It was shown that only the bio-based materials containing biomimicking lipid bilayers proved to be the most effective against the investigated cancer cells.



Left: SANS curves (YuMO, IBR-2) for samples of soybean lecithin liposomes with and without chitosan, liposomes associated with turmeric extract with silver/silver chloride nanoparticles with and without chitosan. Symbols are experimental data and lines are fits.

Right: morphological evaluation of BJ cells (B,C), HepG2 cells (D, E) and HT-29 cells (F,G) treated with the studied antitumoral biohybrids.

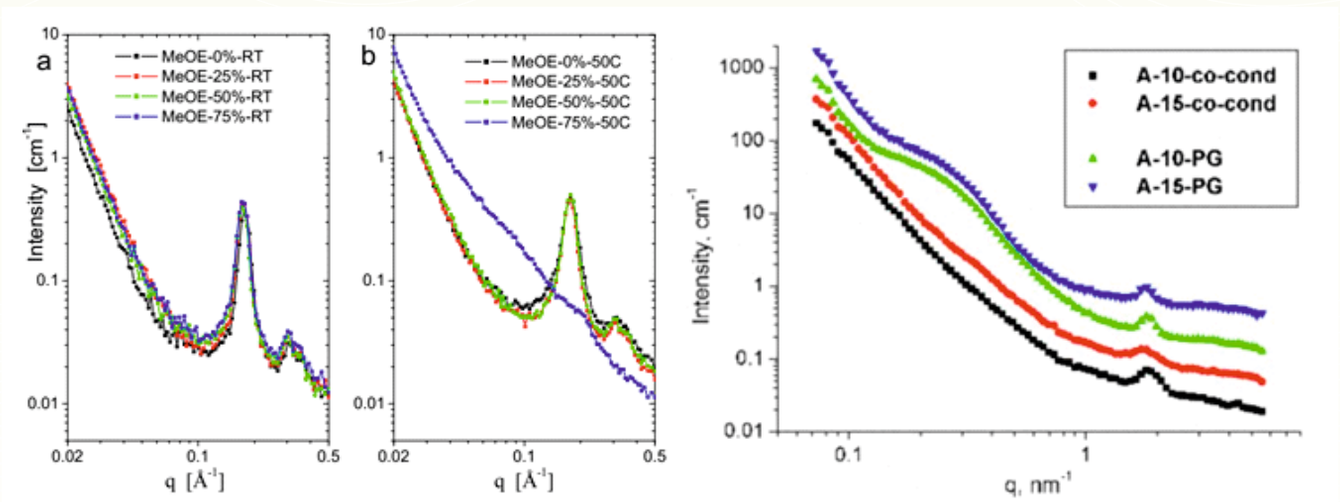
[1] Barbinta-Patrascu , Gorshkova Y., Ungureanu C., Badea N., Bokuchava G., Lazea-Stoyanova A., Bacalum M., Zhigunov A., Petrovic S., Characterization and antitumoral activity of biohybrids based on Turmeric and silver/silver chloride nanoparticles, *Materials* 14 (2021) 4726. DOI: 10.3390/ma14164726

Structural and adsorptive properties of iron oxide-silica nanocomposites

Cooperation in the framework of the IBR-2 user program:
"Coriolan Drăgulescu" Institute of Chemistry, Timişoara, Romania;
National Institute for R&D in Electrochemistry and Condensed Matter, Timişoara, Romania;
West University of Timișoara, Romania;
Politechnica University of Timişoara, Romania

Scientists from Romania initiated detailed studies of a functionalized nanocomposite

Decontamination of toxic pollutants by porous nanomaterials with high removal efficiency became a topic of intense studies. The functionalization of mesoporous materials based on silica nanoparticles is used to regulate the adsorption properties. Here, the structure of a number of iron oxide-silica nanocomposite materials were studied [1-3] by small-angle neutron scattering (SANS) on the YuMO instrument at the IBR-2 reactor of FLNP JINR. All samples show the typical organized structure of MCM-41 type, exhibiting the (100), (110), (200) reflections of the hexagonal pore structure [1]. Also, SANS curves fitted with Monte Carlo least square minimization algorithms provided structural information about iron oxide-silica nanocomposites prepared using different catalysts. It turned out that the studied nanocomposites have the properties of porous materials, such as xerogels, with the magnetite nanoparticles embedded in the fractal-like networks [3].



SANS (YuMO, IBR-2) for nanocomposites prepared at RT (a) and 50 ºC (b) together with the parent and the functionalized mesoporous silica samples (right). A-0 refers to the calcined sample prepared only with tetraethoxysilane (TEOS), and A-0-60C is the same material prior to calcination.

[1] Putz A.-M., Ivankov O.I., Kuklin A.I., Ryukhtin V., Ianăşi C., Ciopec M., Negrea A., Trif L., Horváth Z.E., Almásy L., Ordered mesoporous silica prepared in different solvent conditions: Application for Cu (II) and Pb (II) adsorption, *Gels* 8 (2022) 443. DOI: 10.3390/gels8070443

[2] Putz A.-M., Ciopec M., Negrea A., Grad O., Ianăşi C., Ivankov O.I., Milanović M., Stijepović I., Almásy L., Comparison of structure and adsorption properties of mesoporous silica functionalized with aminopropyl groups by the co-condensation and the post grafting methods, *Materials* 14 (2021) 628. DOI: 10.3390/ma14030628

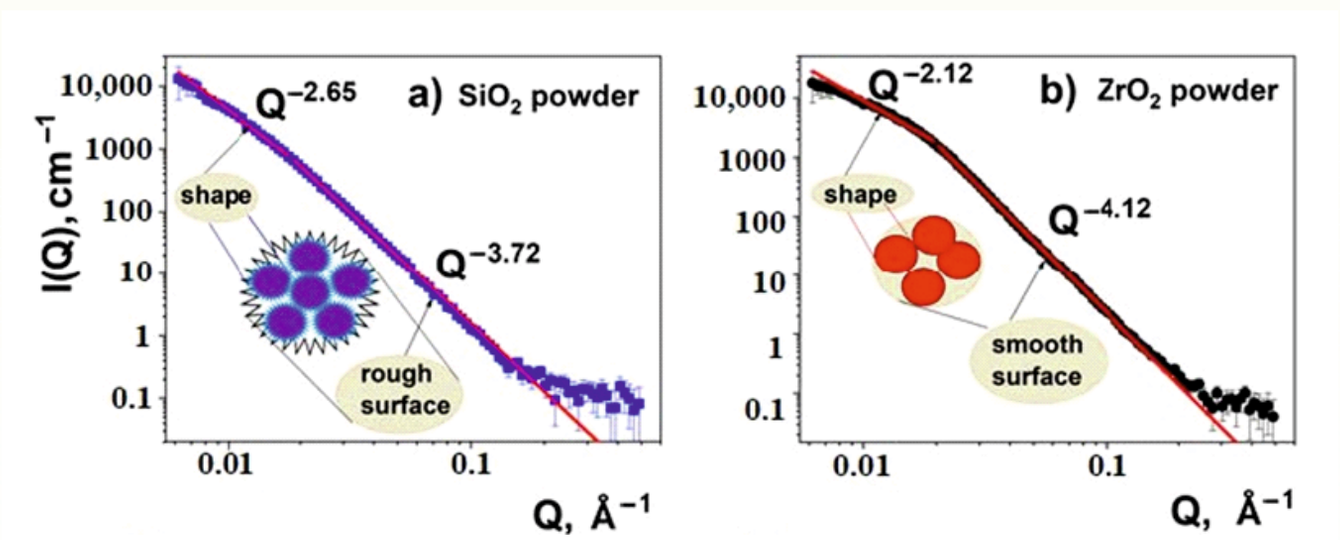
[3] Cătălin I., Ianăşi P., Negrea A., Ciopec A., Ivankov O.I., Kuklin A.I., Almásy L., Putz A.-M., Effects of catalysts on structural and adsorptive properties of iron oxide-silica nanocomposites, *Korean J. Chem. Eng.* 38 (2021) 292. DOI: 10.1007/s11814-020-0675-2

Nanoparticle filled high-density polyethylene composites

Cooperation in the framework of the IBR-2 user program:
ANAS Institute of Radiation Problems, Baku, Azerbaijan;
Azerbaijan University of Architecture and Construction, Baku, Azerbaijan

Research team from Azerbaijan initiated intensive study of new thin-film nanocomposites based on high-density polyethylene with nanoparticles of SiO_2 and ZrO_2 as fillers

The structure and properties of polymer nanocomposites is of current interest in materials science. This is because nano-sized fillers allow for reaching a high total volume in the filler/matrix interfacial region while preserving its relatively small thickness. As compared to bulk composites, it is possible to alter the properties of the material by changing the concentration of nano-fillers. The influence of amorphous SiO_2 and crystalline ZrO_2 on the structural properties of their nanocomposites with high-density polyethylene (HDPE) was studied. In the case of the nano- ZrO_2 filler small-angle neutron scattering (SANS) together with SEM showed poor interfacial adhesion and the presence of voids in the interfacial region. SANS investigations also showed that these voids are filled with a temperature increase due to the flipping motions of polymer chains. The effect was accompanied by a partial aggregation of the filler. For the nano-SiO_2 filler, the lamellar thickness and the degree of crystallinity increased with increasing the filler loading, but the ordering of the lamellae is disrupted even at a filler content of only a few percent. The revealed different impact of the two fillers on the composite structure was analyzed in terms of nanoparticle surface properties and their affinity to the HDPE matrix.



Small-angle neutron scattering data (YuMO, IBR-2) for SiO_2 and ZrO_2 fillers in HDPE with schematic representation of structural differences for two types of fillers distributed in polymer films.

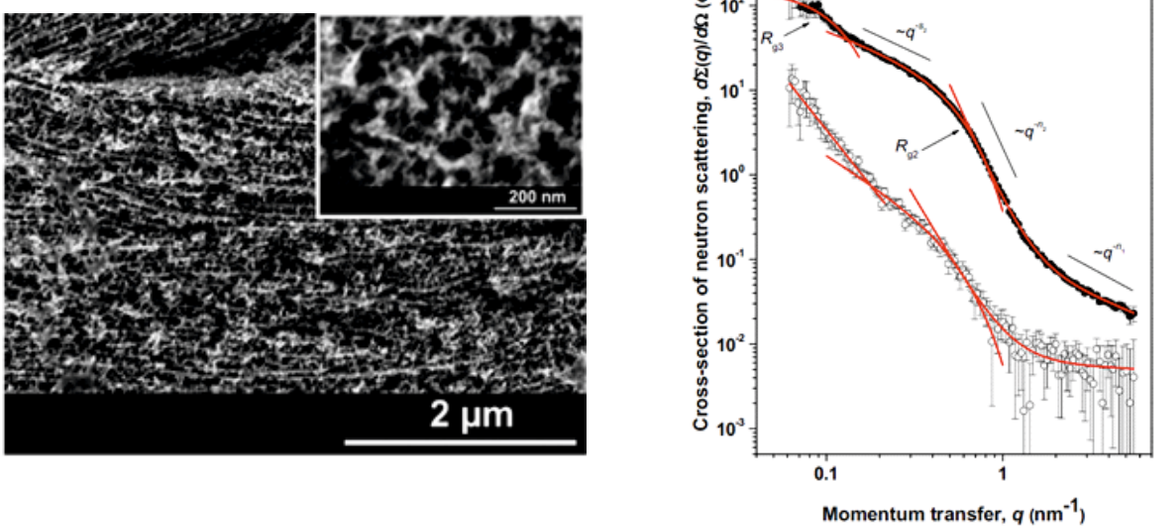
[1] Nabiyev, A.A. , Olejniczak, A. , Islamov, A.Kh. , Pawlukojc A., Ivankov O.I., Balasoiu M., Zhigunov A., Nuriyev M.A., Guliyev F.M., Soloviov D.V., Azhibekov A.K., Doroshkevich A.S., Ivanshina O.Yu., Kuklin, A.I., Composite films of HDPE with SiO_2 and ZrO_2 nanoparticles: The structure and interfacial effects, *Nanomaterials* 11 (2021) 2673. DOI: 10.3390/nano11102673

Carbon cryogels with high porosity

Cooperation in the framework of the IBR-2 user program:
Vinca Institute of Nuclear Sciences, University of Belgrade, Serbia;
Kazan Federal University, Kazan, Russia;
Kurnakov Institute of General and Inorganic Chemistry of RAS, Moscow, Russia;
Petersburg Nuclear Physics Institute NRC KI, Gatchina, Russia;
Grebenshchikov Institute of Silicate Chemistry of RAS, St. Petersburg, Russia

Scientists from Serbia and Russia initiated the studies of the microstructure of carbon cryogels - a promising class of high-porosity nanomaterials

The carbon cryogels (CCs) show significant potential in a wide variety of applications, from absorbents and catalysts to supercapacitors and fuel cells. This is due to their high specific surface area, multimodal pore-size distribution, electrical conductivity, and thermo-mechanical stability. In the present study, the CC material was prepared by a sol-gel process from resorcinol with formaldehyde and heat treatment in the inert atmosphere. The Brunauer Emmett Teller (BET) measurements, X-ray diffraction (XRD), Raman spectroscopy, Fourier-transform infrared spectroscopy (FT-IR), differential thermal analysis with thermogravimetric measurements (DTA-TG), scanning electron microscopy (SEM), and small-angle X-ray scattering (SAXS) analysis, as complementary techniques, were used to characterize the obtained CC. It was found that the obtained CC is a porous amorphous material with high open porosity (≈82.5%) and complex porous structure organization. Using the small-angle neutron scattering (SANS) with the contrast variation technique and the adsorption of deuterated water by carbon cryogel it was possible to separately study the structure of open and closed pores, as well as to estimate both the volume fraction of closed pores ($\varphi_{closepore} \approx 1\%$) and the total porosity ($\varphi_{total} \approx 83.5\%$) of the obtained CC.



Structure characterization of carbon cryogels with high porosity by EM and SANS (YuMO, IBR-2).

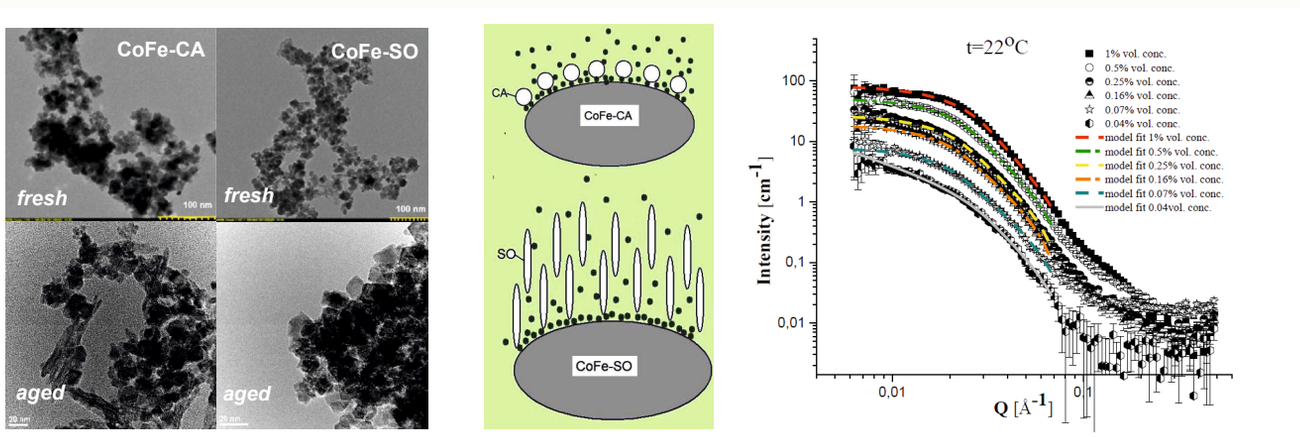
[1] Matovic B., Gorshkova Yu.E., Kottsov S.Yu., Kopitsa G.P., Butulija S., Minovic Arsic T., Cvijovic-Alagic I., Carbon cryogel preparation and characterization, *Diamond & Related Materials* 121 (2022) 108727. DOI: 10.1016/j.diamond.2021.108727

Ageing of cobalt ferrite nanoparticles and their fate in the environment

Cooperation in the framework of the IBR-2 user program:
"Politehnica" University of Bucharest, Romania;
West University of Timisoara, Timisoara, Romania;
"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania;
"Alexandru Ioan Cuza" University, Faculty of Physics, Iasi, Romania;
"Horia Hulubei" Institute of Physics and Nuclear Engineering, Bucharest, Romania

Scientists from Romania studied time evolution of microstructure of ferrofluids with special magnetic properties

In the last decades, magnetic nanoparticles (MNp) in ferrofluids attracted the interest of a large scientific community. Due to their special properties based mainly on the low dimensionality and superparamagnetism, new possibilities for nanotechnology engineering, nanomedicine, environmental protection arise. The stability in time is a critical feature of MNp, straightly related to the usability in various areas. This research dealt with CoFe-CA MNPs capped with citrate anion (CA) single layer and CoFe-SO MNPs capped with sodium oleate (SO) double layer. The aged suspensions were clearly affected by agglomeration and sedimentation [1]. Using small-angle neutron scattering (SANS), three populations of nanostructures of short chain aggregates were identified. Also, the concentration effect in $CoFe_2O_4$/LA/SDS-Na/H_2O ferrofluids at several temperatures was studied by SANS [2]. The found structural changes at high temperatures wasa explained as a consequence of a partial aggregation of the fractal type.



TEM images for freshly prepared and one year aged samples of CoFe-CA and CoFe-SO (left). Metal ion release at the surface of CoFe-CA and at the surface of CoFe-SO MNPs (center) [1]. Modelling of experimental SANS curves (YuMO, IBR-2) for $CoFe_2O_4$/LA/SDS-Na/H_2O ferrofluids with different concentration (right) [2].

[1] Popescu L., Buzatu D., Balasoiu M., Stan C., Vasile B. S., Sacarescu L., Creanga D., Ivankov O., Soloviov D., Balasoiu-Gaina A.-M., Study on ageing of cobalt ferrite nanoparticles and their fate in the environment, *Romanian Journal of Physics* 64 (2019) 818.
https://rjp.nipne.ro/2019_64_9-10/RomJPhys.64.818.pdf
[2] Balasoiu M., Buzatu D., Ivankov O., Balasoiu-Gaina A.-M., Lysenko S., Astaf'eva S., Stan C., Dimensionality of CoFe2O4/LA/SDS-Na/H2O ferrofluid sample with different dilution from SANS-curves modelling, *UPB Scientific Bulletin A* 82 (2020) 249.
https://www.scientificbulletin.upb.ro/rev_docs_arhiva/full650_476140.pdf

Transformations of worm-like surfactant micelles in solutions

Cooperation in the framework of the IBR-2 user program:
Faculty of Physics, Lomonsov Moscow State University, Moscow, Russia

Scientists from Russia applied neutron scattering to relate the structure of giant surfactant micelles with specific rheological properties of solutions

Solutions of so-called giant (worm-like) surfactant micelles are characterized by specific rheological properties due to extended micellar chains which can entangle and form spatial networks, imparting high viscoelasticity to aqueous solutions. These viscoelastic systems are used in a wide variety of applications ranging from life science lubricants to oil fracturing fluids. In this work, the effect of a water-soluble monomer (acrylamide) at different salt content on the structure and rheological properties of micellar solutions of an anionic surfactant (potassium oleate) was studied by small-angle neutron scattering (SANS) measured on the YuMO instrument at the IBR-2 reactor of FLNP JINR. It was found that at low salt levels, when the worm-like micelles are linear, acrylamide causes them to shorten and become spherical micelles as a result of its incorporation into the micellar crown. This leads to a drop in the viscosity of the solution. At a high salt content, which ensures the existence of branched worm-like micelles, the monomer first triggers their transition into long linear chains, which increases viscoelasticity, and then the transition into rods. Thus, the influence of the monomer on the rheological properties differs significantly for linear and branched micelles. Experimental approaches were supported by model calculations, including molecular dynamics (MD) simulations.

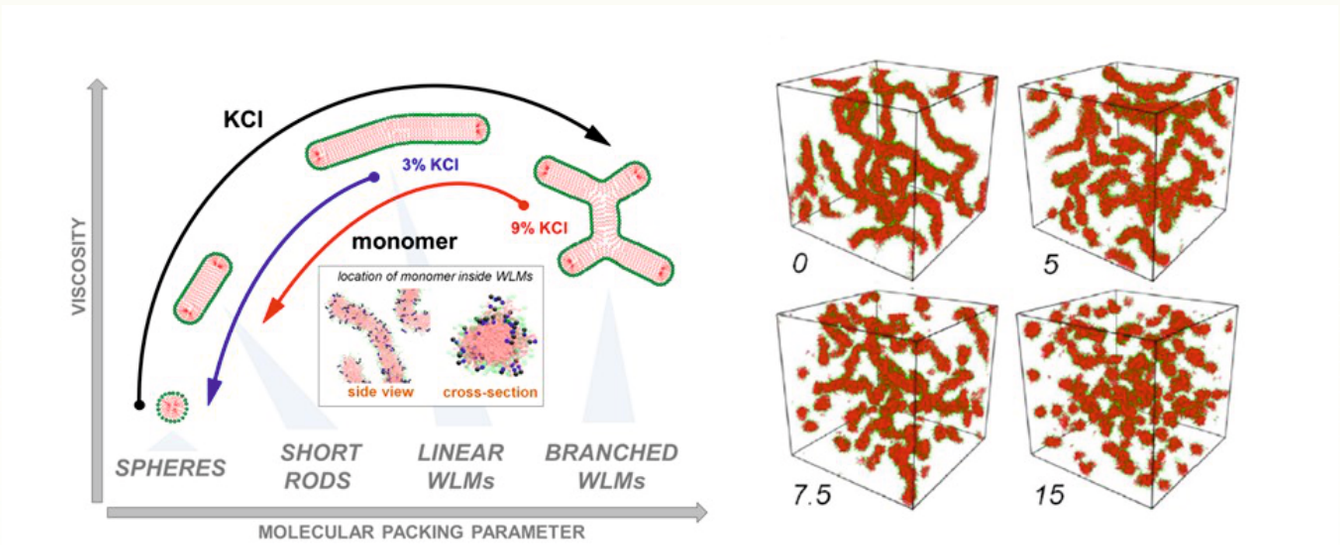


Diagram of the state of a surfactant solution with a transition to worm-like micelles, which is induced by the monomer and addition of salt (KCl) obtained by SANS and other methods, as well as results of MD modeling of self-assembly of surfactant molecules for different monomer/surfactant ratios.

[1] Ospennikov A.S., Gavrilov A.A., Artykulnyi O.P., Kuklin A.I., Novikov V.V., Shibaev A.V., Philippova O.E., Transformations of wormlike surfactant micelles induced by a water-soluble monomer, *J. Col. Interface Sci.* 602 (2021) 590. DOI: 10.1016/j.jcis.2021.05.062

[2] Shibaev A.V., Kuklin A.I., Torocheshnikov V.N., Orekhov A.S., Roland S., Miquelard-Garnier G., Matsarskaia O., Iliopoulos I., Philippova O.E., Double dynamic hydrogels formed by wormlike surfactant micelles and cross-linked polymer, *J. Col. Interface Sci.* 611 (2022) 46. DOI: 10.1016/j.jcis.2021.11.198

4. Life Sciences

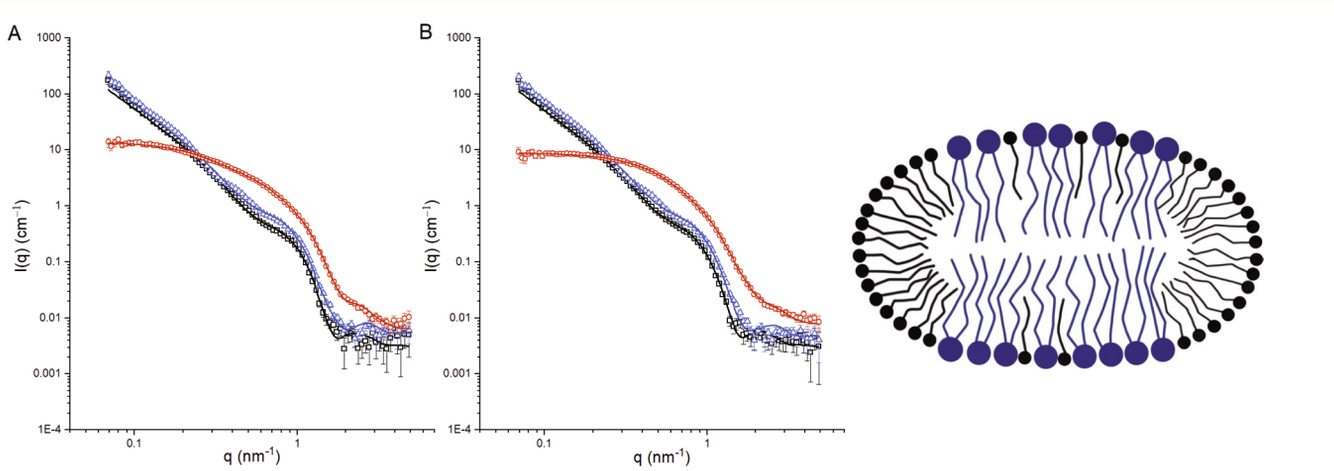
- Membranes
- Proteins
- Biorelevant colloids

Solubilisation of model mammalian membrane by DDAO surfactant

Cooperation in the framework of the IBR-2 user program:
Faculty of Pharmacy, Comenius University Bratislava, Bratislava, Slovakia

Scientists from Slovakia investigated whether a frequently used surfactant DDAO is toxic to the living environment

N,N-dimethyl-1-dodecanamine-N-oxide (DDAO) is an amphiphilic molecule commonly used in products of daily use, such as dishwashing liquids and surface cleaners, cosmetics and pharmaceutical formulations. Notwithstanding its relevant environmental concentrations being low, monitoring its toxic actions on wild animals and humans is needed. Solubilisation of model biomembranes of dioleoylphosphatidylcholine (DOPC) and DOPC+cholesterol induced by DDAO surfactant was studied. Pore formation in lipid bilayer was studied by fluorescence probe leakage method, while the changes in the size of lipid aggregates upon increasing DDAO concentration were followed turbidimetrically. The small-angle neutron scattering (SANS) was used to study the structural parameters of the bilayers in unilamellar liposomes and the geometry of the aggregates created after the addition of DDAO. With the increase of its molar ratio, a transition from liposomes into mixed micelles – best described by cylinders with elliptical cross section was observed. The cross-sectional dimensions of the cylinders suggested that the central part of the ellipse is formed by lipid+DDAO mixed bilayer that is stabilized by a DDAO-rich rim. Further increase in DDAO concentration caused a decrease in the major radius of the ellipse and shortening of the cylinders. Within the experimental error, the results were not considerably influenced when one third of DOPC molecules was substituted with CHOL (DOPC:CHOL = 2:1).



SANS curves (YuMO, IBR-2) for samples containing aggregates of DOPC (A) and DOPC+cholesterol (B) mixed with various amounts of DDAO. Right-hand schematic shows a representation of elliptical cross section of the mixed micelle after solubilization (components: DOPC - two chained, DDAO - single chained).

[1] Želinská K., Gallová J., Huláková S., Uhríková D., Ivankov O., Solubilisation of model membrane by DDAO surfactant – partitioning, permeabilisation and liposome-micelle transition, *General Physiology and Biophysics* 39 (2020) 107. DOI: 10.4149/gpb_2019056

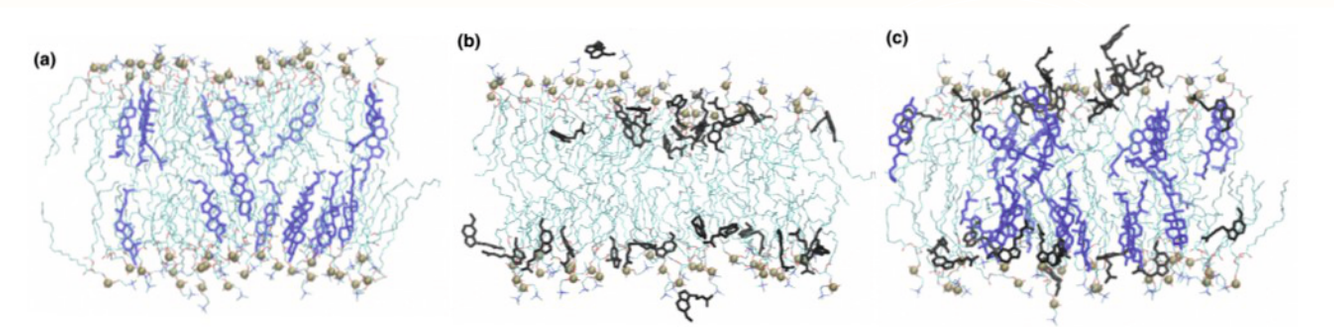
[2] Želinská K., Interaction of model membranes with surfactants and antimicrobial peptide, *Dissertation thesis*, Faculty of Pharmacy, Comenius University Bratislava (2022).

Competitive effects of cholesterol and melatonin in model lipid membranes

Cooperation in the framework of the IBR-2 user program:
Comenius University Bratislava, Bratislava, Slovakia;
P.J. Šafárik University in Košice, Košice, Slovakia;
Dubna State University, Dubna, Russia

Scientists from Slovakia and Dubna documented how to control the fluidity of biomembranes using ubiquitous biomolecules cholesterol and melatonin

The impact of cholesterol and melatonin on the static and dynamical properties of model biomembranes was researched utilizing neutron reflectometry on GRAINS reflectometer and small-angle neutron scattering on YuMO instrument at the IBR-2 reactor of FLNP JINR. These studies were complemented by Raman spectroscopy and molecular dynamics simulations. It was shown that the impact of cholesterol and melatonin is opposite and competitive in the case of three-component systems lipid/cholesterol/melatonin - cholesterol induced an increase in the bilayer thickness, while melatonin induces a decrease in the bilayer thickness. Commensurately, a projected area per lipid decrease was demonstrated with increasing the concentration of cholesterol, and the lipid area increases with increasing the concentration of melatonin. The observed condensing effect of cholesterol and fluidizing effect of melatonin appear in an additive manner upon their mutual presence. Cholesterol and melatonin preferentially accumulate in different membrane regions, presumably affecting the conformation of lipid hydrophobic moieties differently, and in turn having distinct impacts on the structure of the entire membrane. These findings may be relevant for understanding the effects of age-related changes in cholesterol and melatonin concentrations, including those in the brains of individuals with Alzheimer's disease.



Representations of the lipid membrane with 28 mol% of cholesterol (a), 26 mol% of melatonin (b), and with both compounds (21 mol% cholesterol and 26 mol% melatonin).

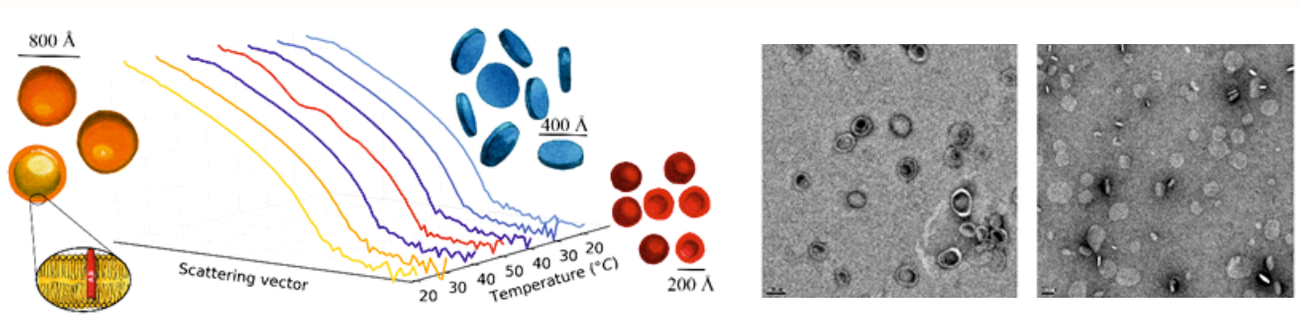
[1] Hrubovčák P., Dushanov E., Kondela T., Tomchuk O., Kholmurodov K., Kučerka N., Reflectometry and molecular dynamics study of the impact of cholesterol and melatonin on model lipid membranes, *European Biophys. J.* 50 (2021), 1025. DOI: 10.1007/s00249-021-01564-y
[2] Kondela T., Dushanov E., Vorobyeva M., Mamatkulov K., Drolle E., Soloviov D., Hrubovčák P., Kholmurodov K., Arzumanyan G., Leonenko Z., Kučerka N., Investigating the competitive effects of cholesterol and melatonin in model lipid membranes, *Biochim. Biophys Acta Biomembr.* 1863 (2021) 183651. DOI: 10.1016/j.bbamem.2021.183651

Amyloid-beta peptide triggered morphological changes of lipid membranes mimicking preclinical Alzheimer's disease

Cooperation in the framework of the IBR-2 user program:
Comenius University Bratislava, Bratislava, Slovakia;
P.J. Šafárik University in Košice, Košice, Slovakia;
Moscow Institute of Physics and Technology, Dolgoprudny, Russia;

Scientists from universities in Bratislava, Košice and Dolgoprudny recorded for the first time morphological changes of model membranes related to the onset of Alzheimer's disease

The amyloid-beta peptide (Aβ) is considered a key factor in Alzheimer's disease (AD) ever since the discovery of the disease. The understanding of its damaging influence has however shifted recently from large fibrils observed in the inter-cellular environment to the small oligomers interacting with a cell membrane. Small angle neutron scattering (SANS) measured on the YuMO instrument at the IBR-2 reactor of FLNP JINR showed for the first time spontaneous reformations between spherical unilamellar vesicles and discoidal bicelle-like structures. These changes in the membrane self-organization happened during the thermodynamic phase transitions of lipids and only in the presence of the peptide. Additional experiments revealed the presence of the morphological changes independent from the introduction of the charged lipids, cholesterol, and melatonin. The dramatic changes in the membrane's overall shape with parallel changes in its thickness were interpreted as the Aβ-triggered membrane damage and a consequent reorganization of its structure. The suggested process is consistent with an action of separate peptides or small size oligomers rather than large Aβ fibrils.



Suggested from SANS experiments schematic of the Aβ25–35 triggered membrane reorganizations during temperature changes. TEM images corroborate the presence of spherical unilamellar vesicles (left) and flat discoidal bicelle-like structures (right).

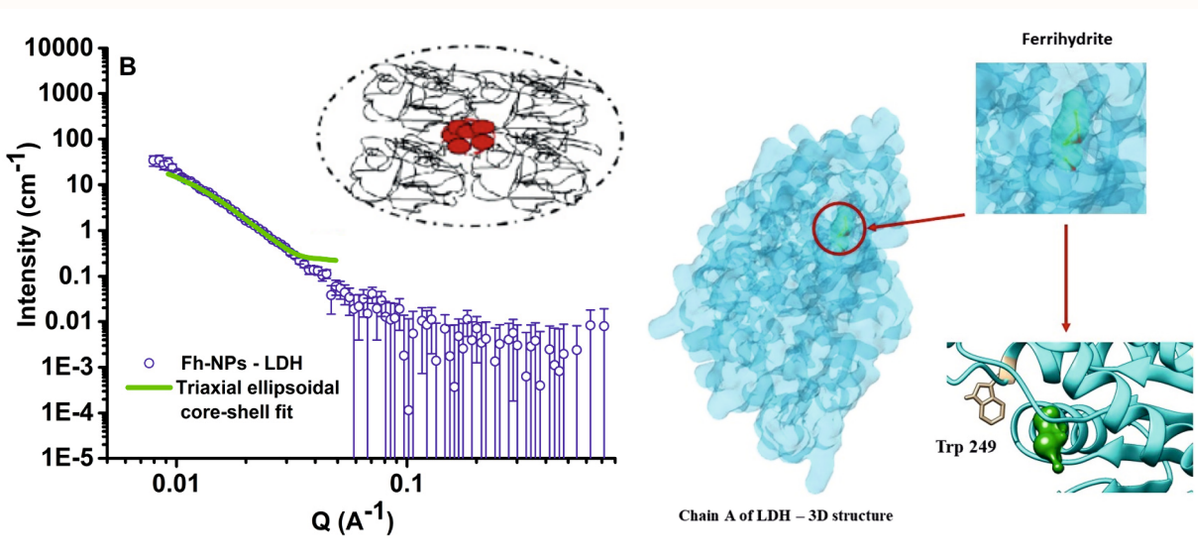
[1] Ivankov O., Murugova T.N., Ermakova E.V., Kondela T., Badreeva D.R., Hrubovčák P., Soloviov D., Tsarenko A., Rogachev A., Kuklin A.I., Kučerka N., Amyloid-beta peptide (25-35) triggers a reorganization of lipid membranes driven by temperature changes, *Sci. Reports* 11 (2021) 21990. DOI: 10.1038/s41598-021-01347-7
[2] Ivankov O., Badreeva D.R., Ermakova E.V., Kondela T., Murugova T.N., Kučerka N., Anionic lipids modulate little the reorganization effect of amyloid-beta peptide on membranes, *General Physiology and Biophysics* 42 (2023) 59. DOI: 10.4149/gpb_2022052
[3] Ivankov O., Kondela T., Dushanov E., Ermakova E., Murugova T., Soloviov D., Kuklin A., Kučerka N., Cholesterol and melatonin regulated membrane fluidity does not affect membrane's breakage triggered by amyloid-beta peptide, *Biophys. Chem.* 298 (2023) 107023. DOI: 10.1016/j.bpc.2023.107023

Ferrihydrite nanoparticles for biomedical applications

Cooperation in the framework of the IBR-2 user program:
Faculty of Physics, University of Bucharest, Măgurele, Romania;
"Horia Hulubei" National Institute of Physics and Nuclear Engineering, Măgurele, Romania;
Siberian Federal University & Kirensky Institute of Physics, SB RAS, Krasnoyarsk, Russia;
Moscow Institute of Physics and Technology, Dolgoprudny, Russia

Collaboration of scientists from Romania and Russia researched the properties of biogenic ferrihydrite nanoparticles interesting for various biomedical applications

Due to their characteristics (size, shape, chemical composition, solubility, charge, and surface roughness), nanomaterials can interfere at nanoscale with biomolecules and cells, which makes them promising devices with a variety of applications in biomedicine such as drug delivery systems, biopharmaceutics, biomarkers, tissue engineering, etc. An increased interest can be observed recently towards ferrihydrite nanoparticles (Fh-NPs). Small-angle neutron scattering (SANS) measured on the YuMO instrument of the IBR-2 reactor of FLNP JINR was used to obtain information on the morphology and dimensions of Fh-NPs (simple or doped with cooper or cobalt) and their effect on the fluidity of model lipid membranes. The results suggest that NPs interact slightly with the lipid head groups for short exposure times (1 h), but after a longer time, NPs can be found predominantly in the hydrophobic core of the membrane. The additional molecular docking studies show that ferrihydrite binds, with a low affinity, in close proximity to the metal binding site of human serum albium protein. The studies of biophysical effects of Fh-NPs – protein composites foresee their use in biological and medical applications and the development of new drugs for therapies and diagnostics of various diseases.



Left-hand panel shows SANS curve (YuMO, IBR-2) of Fh-NPs in a liquid suspension. Right-hand panel shows virtual screening and docking results for the best binding of ferrihydrite (green).

[1] Chilom C.G., Zorilă B., Bacalum M., Bălăşoiu M., Yaroslavtsev R., Stolyar S.V., Tyutyunnicov S., Ferrihydrite nanoparticles interaction with model lipid membranes, *Chem. Phys. Lipids* 226 (2020) 104851. DOI: 10.1016/j.chemphyslip.2019.104851

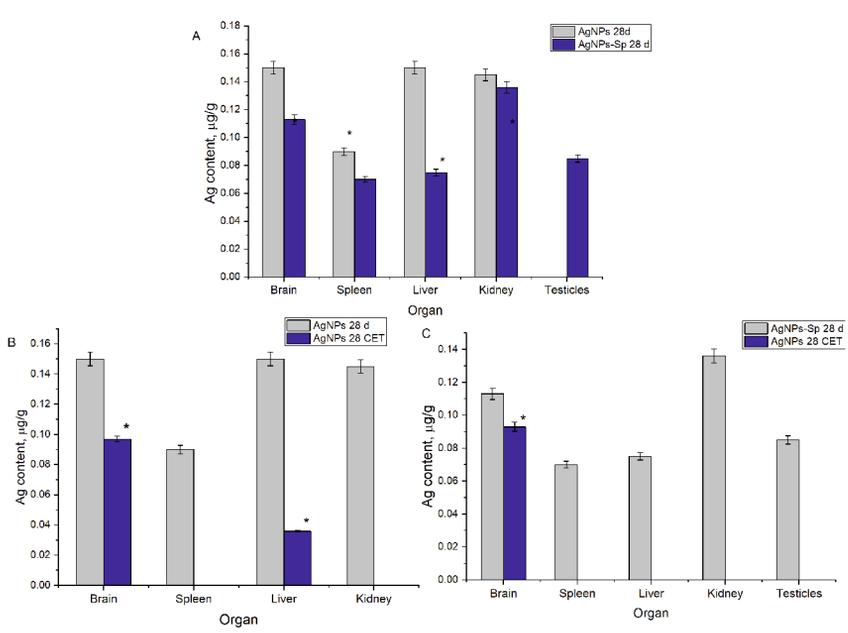
[2] Chilom C.G., Zorilă B., Bacalum M., Bălăşoiu M., Yaroslavtsev R., Stolyar S.V., Tyutyunnicov S., Ferrihydrite nanoparticles insights: Structural characterization, lactate dehydrogenase binding and virtual screening assay, *International J. Bio. Macromol.* 164 (2020) 3559. DOI: 10.1016/j.ijbiomac.2020.08.242

Accumulation and effect of silver nanoparticles functionalized with *Spirulina platensis* on rats

Cooperation in the framework of the IBR-2 user program:
Institute of Microbiology and Biotechnology, Technical University of Moldova, Chisinau, Moldova

Scientists from the Republic of Moldova investigated the effect of silver nanoparticles on animals in order to obtain more information about their toxicity

Silver nanoparticles (AgNPs) are among the most available nanomaterials produced on an industrial scale for various applications. Their extensive use can be associated with the risk of development of toxic effects on living organisms, including humans. The neutron activation analysis on the REGATA facility at the IBR-2 reactor of FLNP JINR was used to assess the accumulation of unmodified and functionalized *Spirulina platensis* biomass AgNPs in different organs of rats. Biofunctionalized nanoparticles showed a higher affinity for the brain and spleen, whereas the unmodified ones - for the liver and kidneys. There was no accumulation of nanoparticles in the ovaries, while in the testicles biofunctionalized nanoparticles were accumulated only. This selectivity can serve as a basis for the development of preparations based on targeted nanoparticles. During the clearance period, silver in the form of AgNPs-*Spirulina* was excreted from all organs, except the brain, whereas unmodified AgNPs were excreted completely from the spleen and kidneys, but the main part of the silver accumulated in liver and brain remained. Thus, both types of studied NPs easily crossed the blood–brain barrier in the direction of the brain, while the reverse flow was very low.



The content of silver in rats' organs: (A) animals administrated with AgNPs and AgNPs-*Spirulina* for 28 days, measured immediately after the end of the experiment; (B) animals administrated with AgNPs for 28 days with measurements after a clearance period; (C) animals administrated with AgNPs-*Spirulina* for 28 days after a clearance period.

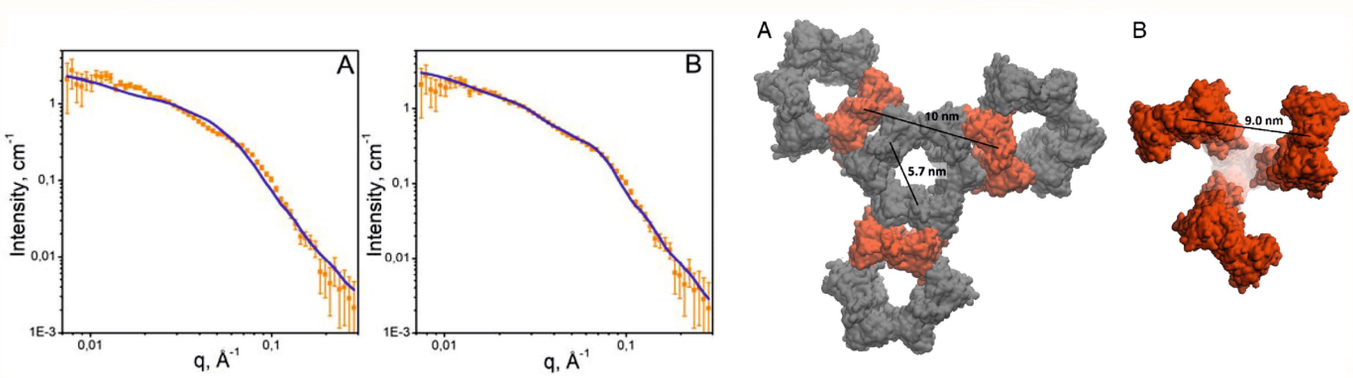
[1] Rudi L., Zinicovscaia I., Cepoi L., Chiriac T., Peshkova A., Cepoi A., Grozdov D., Accumulation and effect of silver nanoparticles functionalized with *Spirulina platensis* on rats. *Nanomaterials* 11 (2021) 2992. DOI:10.3390/nano11112992

The superstructure of two-component signaling systems in nature

Cooperation in the framework of the IBR-2 user program:
Moscow Institute of Physics and Technology, Dolgoprudny, Russia

Scientists from Russia led a research of the most abundant two-component signaling systems that are responsible for the communication of microorganisms

Two-component systems (TCS) are widespread signaling systems present in all domains of life. They are the most common signaling systems in prokaryotes but are absent in mammals, making them potential antimicrobial drug targets. TCS typically consist of a signal receptor/transducer and a response regulator. The receptors (histidine kinases, chemoreceptors and photoreceptors) are often embedded in the membrane and have a similar modular structure. Chemoreceptors were shown to function in highly ordered arrays, with trimers of dimers being the smallest functional unit. However, much less is known about photoreceptors. The small-angle neutron scattering (SANS) experiments performed on the YuMO instrument at the IBR-2 of FLNP JINR showed that detergent-solubilized sensory rhodopsin II in complex with its cognate transducer forms dimers at low salt concentration, which associate into trimers of dimers at higher buffer molarities. When fitted an atomistic model of the whole complex into the SANS data, the obtained results suggested that the trimer of dimers is "tripod"-shaped and that the contacts between the dimers occur only through their cytoplasmic regions, whereas the transmembrane regions remain unconnected. The reported work opens up prospects for further successful use of SANS technique in studies of the TCS sensors, for which the huge conformational changes of the tertiary structure of the transducer after activation of the photosensor are expected.



SANS curves for TCS fitted to the theoretical curves calculated for a mixture of dimers and trimers of dimers which inter-dimer contacts are induced both between the transmembrane regions of dimers and their cytoplasmic tips (panels A) and those of dimers and "tripod"-shaped trimers of dimers (panels B).

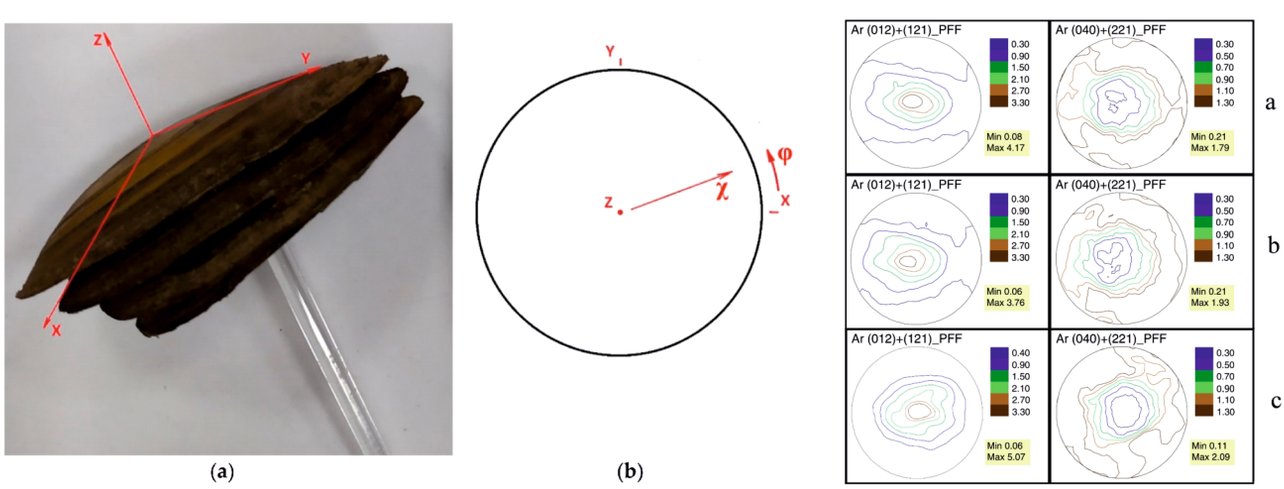
[1] Ryzhykau Yu.L., Orekhov P.S., Rulev M.I., Vlasov A.V., Melnikov I.A., Volkov D.A., Nikolaev M.Yu., Zabelskii D.V., Murugova T.N., Chupin V.V., Rogachev A.V., . Gruzinov A.Yu, Svergun D.I., Brennich M.E., Gushchin I.Yu., Soler-Lopez M., Bothe A., Büldt G., Leonard G., Engelhard M., Kuklin A.I., Gordeliy V.I., Molecular model of a sensor of two-component signaling system, *Scientific Reports* 11 (2021) 10774. DOI: 10.1038/s41598-021-89613-6

Investigation of crystallographic texture of freshwater bivalve mollusks

Cooperation in the framework of the IBR-2 user program:
Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest, Romania;
Danube Delta National Institute for Research and Development, Tulcea, Romania;
Borissiak Paleontological Institute, Russian Academy of Sciences, Moscow, Russia

Scientists from Romania and Russia initiated the investigation of crystallographic texture of the valves of bivalve mollusks

Bivalve mollusks of the family Unionidae are the dominant freshwater Eurasian bivalve mollusks. They inhabit water bodies with both flowing (rivers, streams) and stagnant water (lakes and ponds). Also, Unionidae are present in sea areas with low salinity, such as the Gulf of Finland in the Baltic Sea. These mollusks are an important component of human economic activity, and their fundamental ecosystem service is acting as a natural biofilter of freshwater bodies. The aim of this work was to reveal the features of the global crystallographic texture of the valves of some representative bivalve mollusks of the Unionidae family, to establish whether they change depending on the temperature and salinity of the water. Neutron diffraction, in contrast to X-ray diffraction, is a non-destructive method. Results of neutron experiments performed on the SKAT texture diffractometer at the IBR-2 reactor of FLNP JINR revealed that the pole figures of aragonite in the valves repeat their shape. The pole density maxima for U. pictorum from the Danube Delta and the Gulf of Finland in the Baltic Sea, living at different salinities and temperatures, differs by 0.41 mrd. The maximum value of the crystallographic texture for A. cygnea from the Danube Delta was also measured (5.07 mrd). In terms of texture sharpness, it surpasses the shell of marine bivalve mollusks, which are partially or completely composed of aragonite. Although U. pictorum and Mya arenaria Linnaeus, 1758 have different microstructures, their pole figures are very similar in isolines pattern, but differ in pole density maxima.



(a) (b)

Investigation of crystallographic texture of the bivalve mollusks using SKAT texture diffractometer, IBR-2.

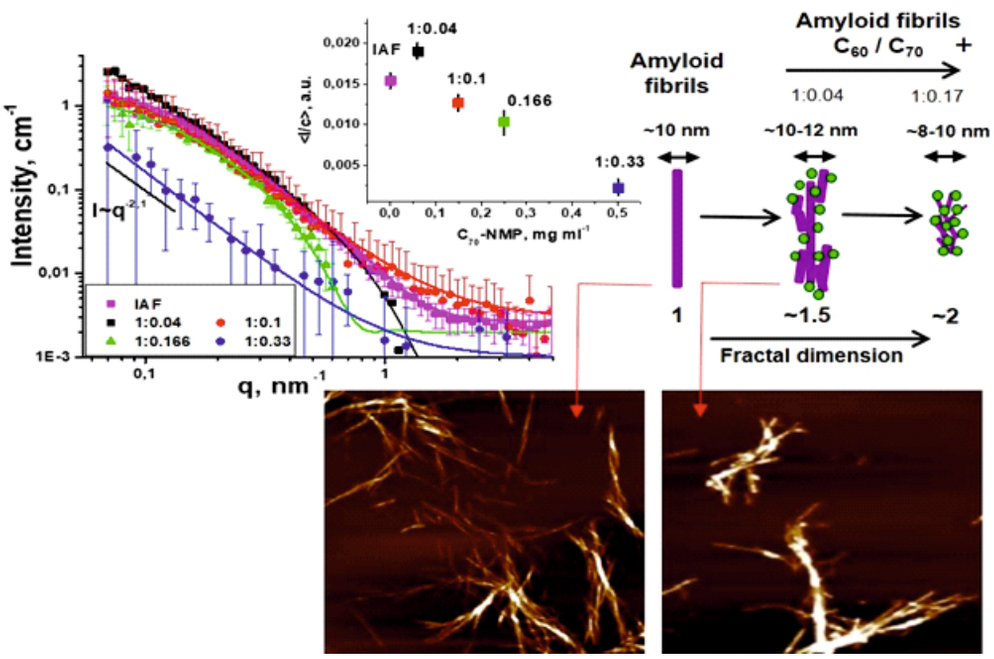
[1] Pakhnevich A., Nikolayev D., Lychagina T., Balasoiu M., Ibram O., Global Crystallographic Texture of Freshwater Bivalve Mollusks of the Unionidae Family from Eastern Europe Studied by Neutron Diffraction, *Life* 12 (2022) 730. DOI: 10.3390/life12050730

Fullerenes as effective disaggregating agents of amyloid fibrils

Cooperation in the framework of the IBR-2 user program:
Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

Scientists from Slovakia studied the interaction between fullerenes complexes with NMP molecules and model amyloids

Nowadays determining the disassembly mechanism of amyloids under nanomaterials action is a crucial issue for their successful future use in therapy of neurodegenerative and overall amyloid-related diseases. In this study the anti-amyloid disassembly activity of fullerenes C60 and C70 dispersed in 1-methyl-2-pyrrolidinone (NMP) towards amyloid fibrils preformed from lysozyme and insulin has been investigated using combination of different experimental techniques. Thioflavin T fluorescence assay and atomic force microscopy were applied for monitoring of disaggregation activity of fullerenes. It was demonstrated that both types of fullerene-based complexes are very effective in disassembling pre-formed fibrils and characterized by the low apparent half-maximal disaggregation concentration (DC50) in the range of ~22-30 μg ml^{-1}. Small-angle neutron scattering (SANS) was employed to monitor the different stages of the disassembly process with respect to the size and morphology of the aggregates. Based on the obtained results a possible disassembly mechanism for amyloid fibrils interacting with fullerene/NMP complexes was proposed. The study is a principal step in understanding of the fullerenes destruction mechanism of the protein amyloids, as well as provides valuable information on how macromolecules can be engineered to disassemble unwanted amyloid aggregates by different mechanisms.



A schematic view of the fibrils destruction stages upon interaction with fullerenes as follows from the analysis of SANS (YuMO, IBR-2) and AFM data.

[1] Siposova K., Petrenko V.I., Ivankov O.I., Musatov A., Bulavin L.A., Avdeev M.V., Kyzyma O.A., Fullerenes as an Effective Amyloid Fibrils Disaggregating Nanomaterial, *ACS Appl. Mater. Interfaces* 12 (2020) 32410. DOI: 10.1021/acsami.0c07964

5. Environmental sciences

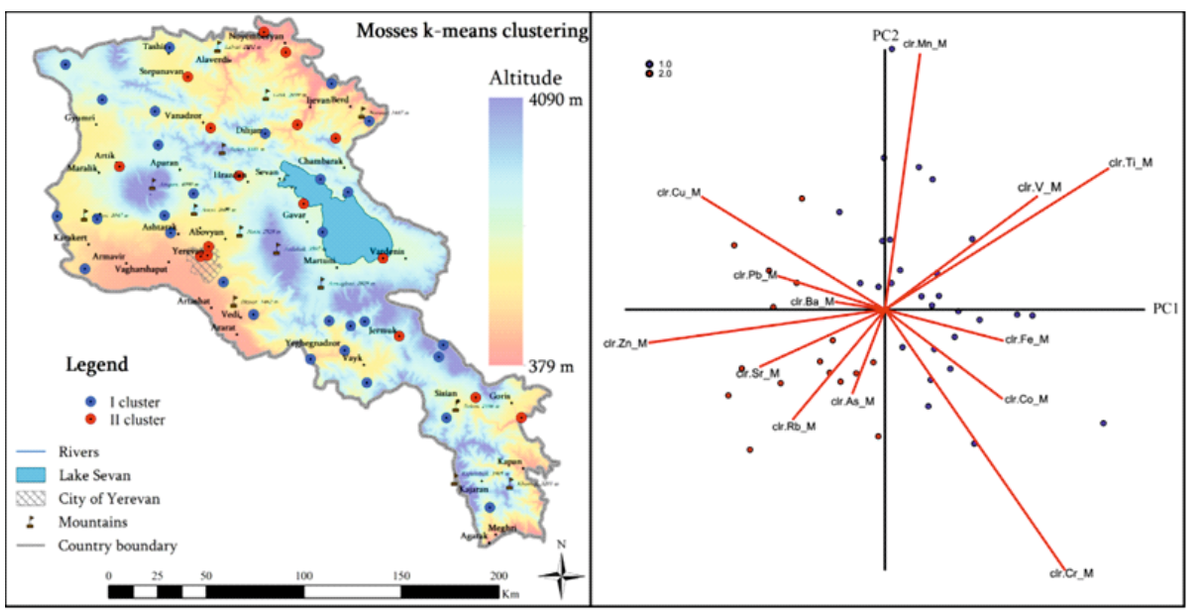
- Neutron activation analysis
- Monitoring of air, water and soil pollution
- Food safety and nanotoxicology

Factors conditioning the content of chemical elements in soil and mosses in Armenia

The Center for Ecological-Noosphere Studies NAS, Yerevan, Republic of Armenia

Scientists from Armenia investigated the level of air pollution in the country using moss biomonitoring technique

Over the past decades, the anthropogenic impact on the environment has increased significantly, which has led to the alteration of the quality of different environmental compartments, including air. The content of Cr, V, Ti, Sr, Rb, As, Zn, Co, Fe, Mn and Ba in moss samples collected in Armenia was determined using neutron activation analysis at the REGATA facility of the IBR-2 reactor in FLNP JINR. The obtained results showed that different natural and anthropogenic factors affect the content and spatial distribution of the studied elements in mosses. According to principal component analysis (PCA), studied elements do not form distinct groups. However, the 1st cluster was represented by Cr, Co, Fe, Ti, V, and Mn whereas the other studied elements (Cu, Pb, Zn, As, Sr, Ba, and Rb) were dominated in the 2nd cluster. At the same time, in both cases the samples displaying scattered distribution indicate the absence of any single feature determining the grouping of the studied moss samples. The results of this study can serve as a basis for identifying the most suitable sites in Armenia for the next moss survey study and creation of a scientifically based network of moss biomonitoring.



Spatial distribution of the mosses k-means clustering results and clr-biplot of the studied elements.

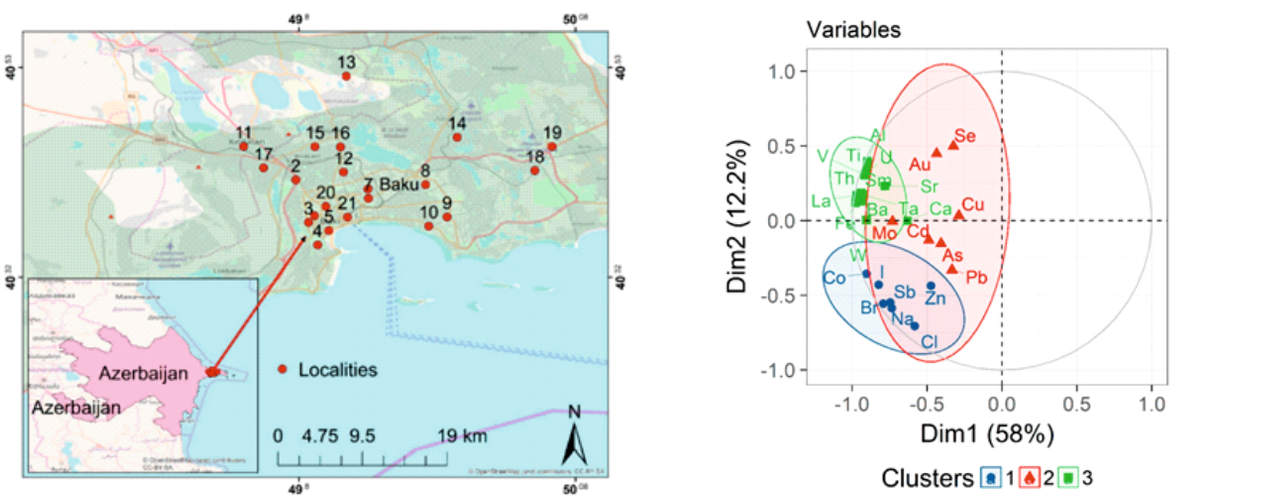
[1] Tepanosyan G., Sahakyan L., Gevorgyan A., Frontasyeva M., Factors conditioning the content of chemical elements in soil and mosses in Armenia. *Journal of Trace Elements and Minerals* 2 (2022) 100029. DOI: 10.1016/j.jtemin.2022.100029; *Archives of Environmental Contamination and Toxicology* 80 (2021) 350. DOI: 10.1007/s00244-020-00788-x

Assessment of atmospheric deposition of major and trace elements using neutron activation analysis and GIS technology: Baku – Azerbaijan

Baku State University, Baku, Azerbaijan;
National Nuclear Research Centre JSC, Baku, Azerbaijan

Scientists from research centers in Baku investigated the level of air pollution in the city

Air pollution is one of the global environmental problems causing severe damages to human health and ecosystems. A total of 34 elements were determined using neutron activation analysis at the REGATA facility of the IBR-2 reactor (FLNP JINR) in 21 moss bags (*Sphagnum girgensohnii*) exposed for three months at different locations in Baku. The significant values for the sea-salt elements, oil and gas industries and geogenic provenance of some elements were detected. Principal component analysis (PCA) allowed to identify the main sources of elements emissions including anthropogenic (Pb, As, Cd, Mo, Cu, Au, and Se), geogenic (Na, Cl, Br, I, Zn, Co and Sb), and mixed (V, Ti, Th, U, La, Sm, Ba, Ta, Fe, W, Ca, Sr, and Al) elements. In addition, it was discovered that the levels of anthropogenic elements were higher at the sites located in the vicinity of cement companies, paints manufacturing and oil and gas production. Significant concentrations of Th and U were notable near to the airport, which is, most probably, due to the building materials transported by weathering during the recent airport renovation. The obtained data can serve as a baseline in constituting local guidelines by regulatory bodies in the Republic of Azerbaijan.



Map of exposure sites in Baku (left) and biplot of the first two PCAs of 27 elements. Biplot illustrates 3 clusters (right).

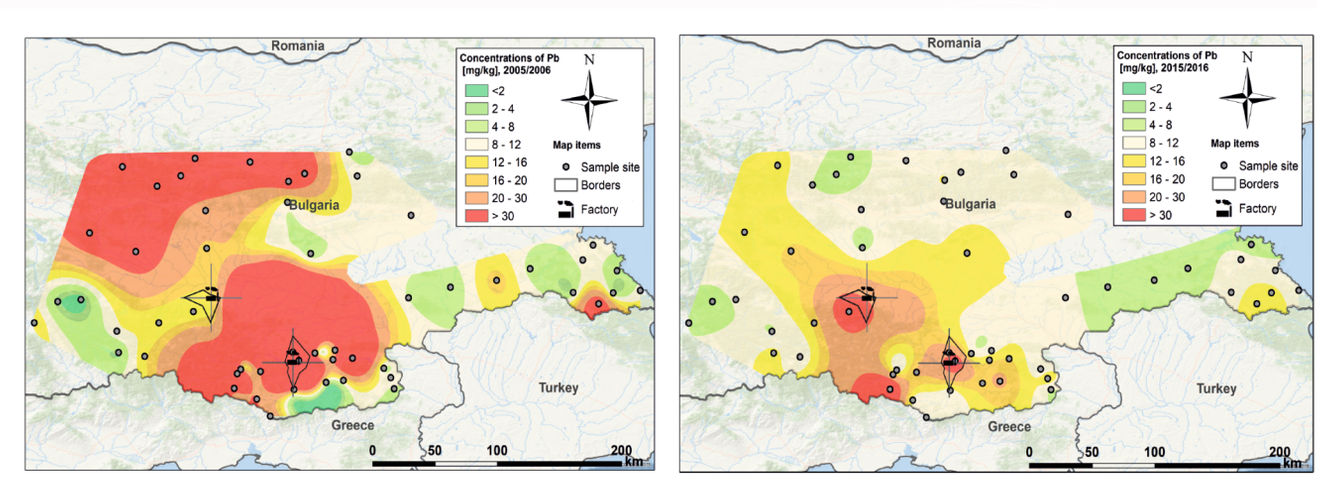
[1] Madadzada A.I., Badawy W.M., Hajiyeva S.R., Veliyeva Z.T., Hajiyev O.B., Shvetsova M.S., Frontasyeva M.V., Assessment of atmospheric deposition of major and trace elements using neutron activation analysis and GIS technology: Baku – Azerbaijan, *Archives of Environmental Contamination and Toxicology* 80 (2021) 350. DOI: 10.1007/s00244-020-00788-x

Multivariate assessment of atmospheric deposition studies in Bulgaria based on moss biomonitors: trends between the 2005/2006 and 2015/2016 surveys

Faculty of Physics and Engineering, Paisii Hilendarski University, Plovdiv, Bulgaria;
Agricultural University, Plovdiv, Bulgaria

Scientists from Plovdiv researched changes in the atmospheric deposition trends in Bulgaria using the moss biomonitoring technique

Moss biomonitoring technique was applied to investigate the changes in atmospheric deposition trends in Bulgaria between the 2005/2006 and 2015/2016 surveys. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor in FLNP JINR was used to determine the content of 34 major, minor and trace elements in mosses collected on the entire territory of the country. According to the obtained results, a strong decrease in the concentrations was revealed for most elements detected in mosses, except for Cu and K. Among toxic elements, a great reduction in the lead content was observed. The diagonal concentration pattern obtained for the 2005/2006 moss survey can be explained by the location of the open-pit copper mines and tailings in the regions of Chelopech, Zlatitsa, Elatsite, Pirdop, and Panagiyrishte, a non-ferrous plant near Plovdiv, as well as the Kardzhali Pb-Zn and adjacent mines and tailings in the south-east of the studied area. After the shutdown of the Kardzhali Pb-Zn plant in 2011, it is evident in the map for the 2015/2016 moss survey that the environmental situation in the region vastly improved, even though it is still affected by the tailings and quarries. In the decade between the two surveys, the effect of the shutdown of several major industrial facilities and the implementation of improved air pollution control systems was concluded.



Deposition maps for the elements Pb determined in the 2005/6 (left) and 2015/16 (right) ICP Vegetation moss surveys.

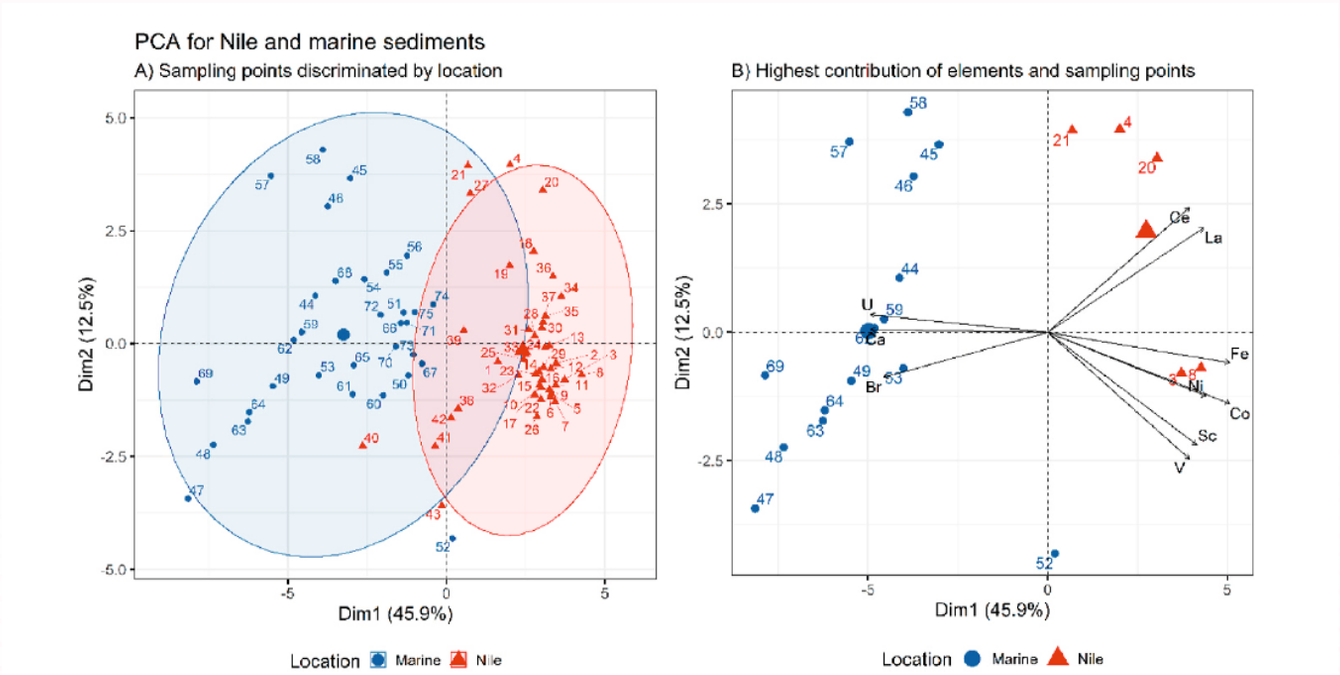
[1] Hristozova G., Marinova S., Motyka O., Svozilík V., Zinicovscaia I., Multivariate assessment of atmospheric deposition studies in Bulgaria based on moss biomonitors: trends between the 2005/6 and 2015/16 surveys, *Environmental Science and Pollution Research* 27 (2020) 39330.
DOI: 10.1007/s11356-020-10005-w

A review of major and trace elements in Nile River and Western Red Sea sediments: An approach of geochemistry, pollution, and associated hazards

Faculty of Science, Menoufia University, Shibin El-koom, Egypt;
Faculty of Science, Al-Azhar University, Assuit Branch, Assuit, Egypt

Scientists from Egypt researched the elemental composition of the surface sediments from the Nile River and Egyptian Red Sea

The Nile River flows through Egypt, forming one of the largest deltas, affected by ongoing anthropogenic activities due to densely inhabitants. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor in FLNP JINR was applied for the elemental analysis of sediments collected from two different origins along the Egyptian coastal areas of the Red Sea and along the Egyptian section of the basin of the Nile River and its delta. Significant amounts of V, Cr, and Zr were observed in Nile sediments, whereas, considerable concentrations of Br and Ca were found in marine sediments. Principal component analysis (PCA) showed that the sampling points with the highest contribution in the case of marine and Nile sediments are close to the phosphate mining and transportation, as well as to the natural geological occurrence of sediments. The discriminant analysis on both type of sediments suggested that their provenance is a mixed source from clay, silt, gravel, sand, and metabasic sources. The hazard index for almost all studied elements in the Nile and marine sediments for children and adults was slightly higher than the tolerable values.



Bi-plot of the first two PCAs illustrating the sampling points.

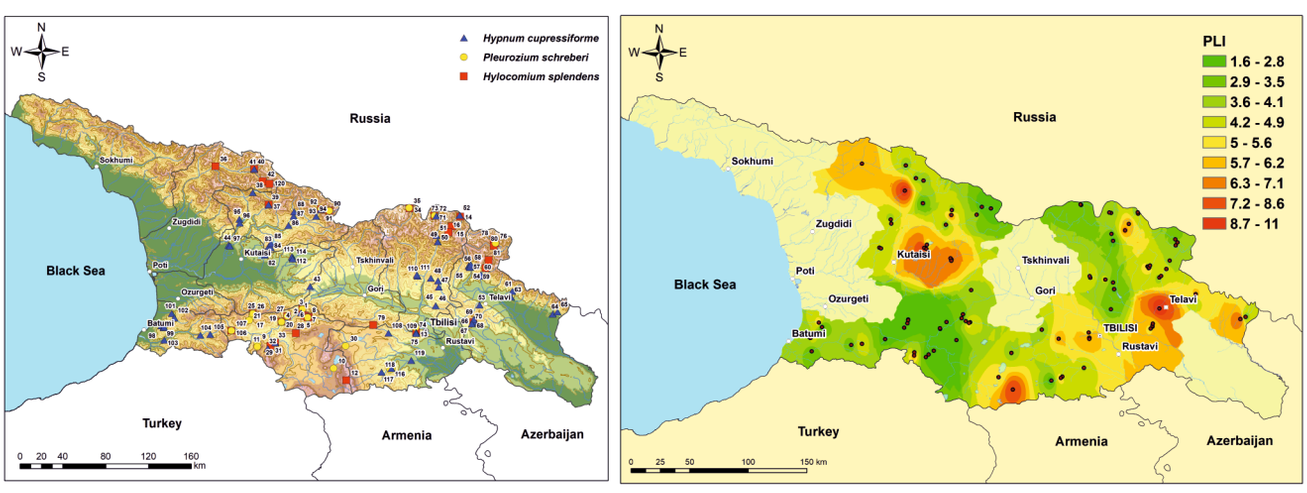
[1] Badawy W.M., Duliu O.G., El Samman H., El-Taher A., Frontasyeva M.V., A review of major and trace elements in Nile River and Western Red Sea sediments: An approach of geochemistry, pollution, and associated hazards, *Applied Radiation and Isotopes* 170 (2021) 109595.
DOI: 10.1016/j.apradiso.2021.109595

Characterization of trace elements in atmospheric deposition studied by moss biomonitoring in Georgia

I. Javakhishvili Tbilisi State University, Tbilisi, Georgia

Scientists from Tbilisi investigated the atmospheric deposition of trace elements in order to evaluate the air quality in Georgia

Air pollution is a serious worldwide problem caused by anthropogenic activities and is closely related to economics and human health. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor in FLNP JINR was used to determine the content of 38 elements in 120 moss samples collected in different regions of Georgia within the period of 2014-2017. The principal component analysis (PCA) was implemented to get information about the common geochemical features and to determine the provenance of the studied elements. The analysis showed a significant association of crustal elements, and the provenance of elements can be considered as a mixture of geogenic and anthropogenic sources (Zestafoni Ferroalloy Plant, Kutaisi Auto Mechanical Plant, Tsana and Uravi arsenic mines, Chiatura manganese mine, etc.). The high-risk index values were detected for 2015 and 2016 due to a significant contribution of As and Cd caused by arsenic wastes in Tsana and Koruldashi and emission from the Zestafoni Ferroalloy Plant, respectively. Considering the first dataset obtained, the characterization of inorganic air metal pollution in Georgia is an effective tool that might help the regulatory bodies to set the necessary laws and rules that control the emission of toxic elements in the atmosphere.



Map of sampling localities in Georgia (left) and spatial distribution of the pollution load index (PLI) of the determined element over all sampling sites (right)

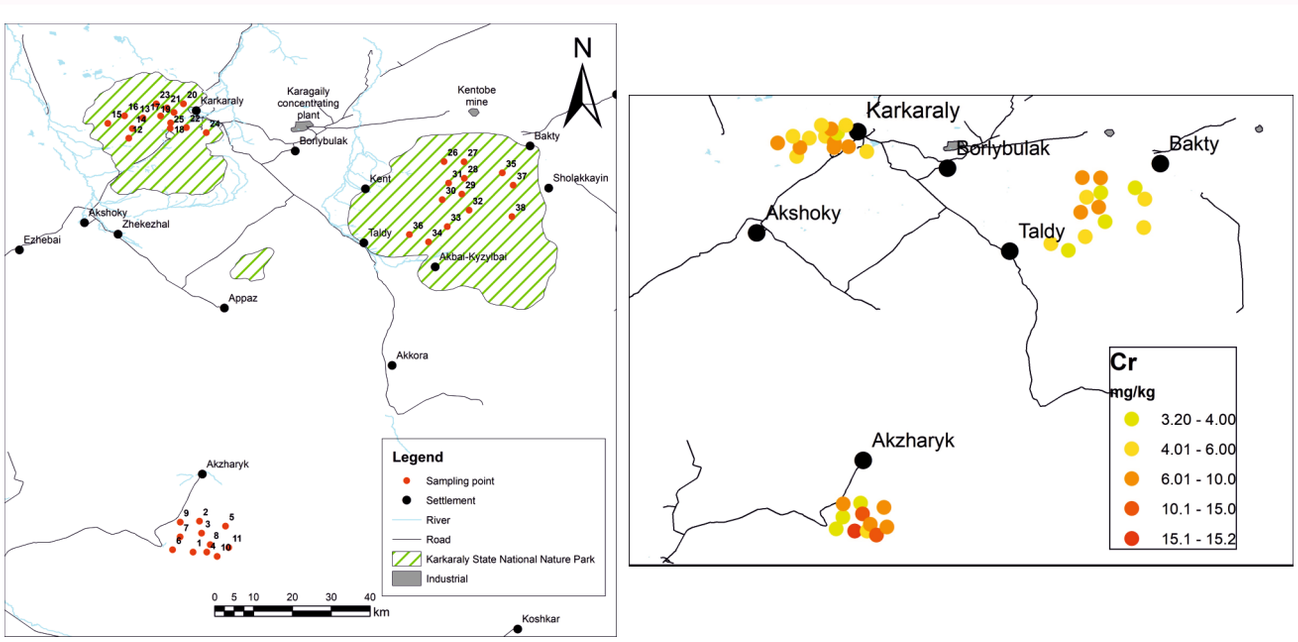
[1] Chaligava O., Shetekauri Sh., Badawy W.M., Frontasyeva M.V., Zinicovscaia I., Shetekauri T., Kvlividze A., Vergel K., Yushin N., Characterization of Trace Elements in Atmospheric Deposition Studied by Moss Biomonitoring in Georgia, *Archives of Environmental Contamination and Toxicology* 80 (2021) 350. DOI: 10.1007/s00244-020-00788-x

Mosses as bioindicators of air pollution with potentially toxic elements in area with different level of anthropogenic load in Karaganda region, Kazakhstan

L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

Scientists from Kazakhstan researched the elemental composition of mosses to assess the level of air pollution in the region

Currently, Karaganda region is one of the largest in Kazakhstan by industrial capacity, rich in minerals and primary commodities. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) was used to determine the content of 36 major, minor and trace elements in mosses collected at two territories with different level of anthropogenic load: the Karkaraly National Park and the Akzharyk settlement. The range of potentially toxic elements was extensive, with the highest concentrations found in the vicinity of the towns of Karkaralinsk and Akzharyk. According to the Mann–Whitney U Test ($p<0.05$) mosses collected in the Akzharyk village contained significantly higher concentrations of Na, Mg, Al, Cl, K, Ca, Se, V, Ni, Zn, Br, Rb, Sr, Zn, Cs, Ba, La, Ce, Th, Sm, Eu, Tb, Dy, Tm, Hf, Ta, Th. The main sources of air pollution in the studied areas are the soil erosion, mining, ore processing, industrial activities, transport and thermal power plants. This is due to nearby industrial zones such as the Karagaily mining and processing plant, as well as the Kentobe deposit. Ecological indices revealed unpolluted to moderately polluted environment conditions with low potential environmental risks for human health.



Sampling map of Karaganda region (left) and the content of Cr in mosses collected in Karaganda region (right)

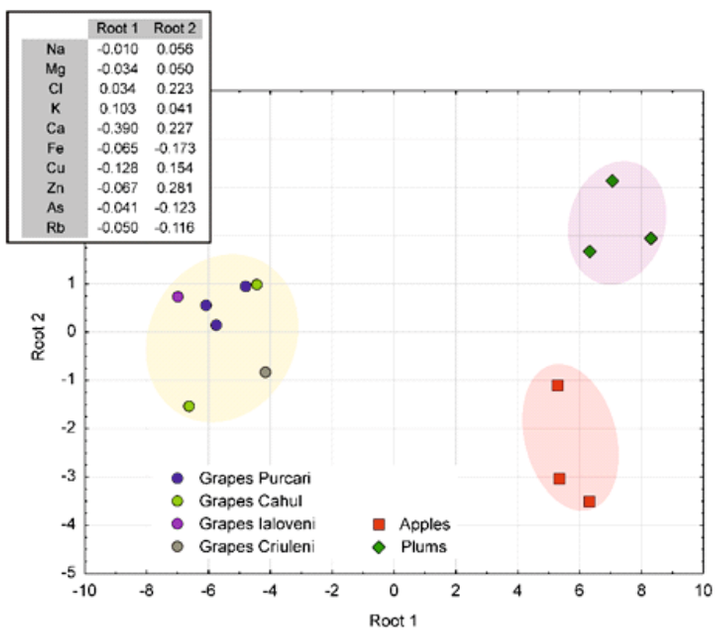
[1] Nurkassimova M., Omarova N., Zinicovscaia I., Chaligava O., Yushin N., Mosses as bioindicators of air pollution with potentially toxic elements in area with different level of anthropogenic load in Karaganda region, Kazakhstan, *J. Radioanalytical Nuclear Chem.* 333 (2024) 961. DOI: 10.1007/s10967-023-09334-0

Major and trace elements in Moldavian orchard soil and fruits: Assessment of anthropogenic contamination

Technical University of Moldova, Chisinau, Republic of Moldova;
University of Bucharest, Magurele (Ilfov), Romania

Collaboration of scientists from Republic of Moldova and Romania researched the elemental composition of soils and fruits to assess the level of their contamination

The relationship between food and health becomes critically important, as consumers now demand healthy, tasty and natural products, grown in uncontaminated environments. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) was used to determine the content of 40 elements in soils and 22 elements in fruits (apples, plums and grapes) collected in four different zones of the Republic of Moldova. According to the obtained results, the soil was moderately contaminated with As, Br, Cd and Sb. In all analyzed fruits the most abundant major element was K, while among microelements - Fe, Zn and Cu. Daily intake values calculated for Co, Fe, Mn, Ni, Zn, As, and Sb varied greatly depending on fruits sort and place of provenance. The potential health hazard index values for all elements, except Sb, were lower than 1.0, suggesting that analyzed fruits are safe for consumption. The discriminant analysis allowed to classify fruits under study by the type and place of provenance.



The result of Discriminant Analysis illustrating the existence of three clusters, each of them consisting of a single type of fruits.

[1] Zinicovscaia I., Sturza R., Duliu O.G., Grozdov D., Gundorina S., Ghendov-Mosanu A., Duca Gh., Determination of major and minor elements in Moldavan fruits by neutron activation analysis and assessment of their provenance, *International Journal of Environmental Research and Public Health* 17 (2020) 7112. DOI:10.3390/ijerph17197112

The impact assessment of CuO nanoparticles on the composition and ultrastructure of *Triticum aestivum L.*

National Institute for R&Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania; Babeș-Bolyai University, Faculty of Biology and Geology, Cluj-Napoca, Romania

Scientists from universities in Cluj-Napoca researched the effect of CuO nanoparticles on the elemental composition of wheat

Multiple applications of nanoparticles (NPs) in various areas of industry and science, such as medicine, pharmacology, electronics, biology, or agriculture, are directly related to their release into environmental multimedia. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) was applied to evaluate the elemental composition of *Triticum aestivum L.* plants subjected to chemically- and green-synthesized CuO NPs. In the wheat control sample, 34 elements were determined, but only 14 of them were identified in the exposed wheat samples. All wheat samples exposed to chemical or biogenic CuO NPs showed changes in elemental accumulation in plant tissues. Exposure to chemically obtained CuO NPs led to a more obvious alteration of the element profile compared to control and biogenic CuO NPs. Application of CuO NPs caused the accumulation of K, Br, Al, and Zn and the decrease of Cl, Na, Ba, and Sr in wheat samples, regardless of the type of NPs applied. The application of chemically obtained NPs induced the most significant changes by blocking the assimilation of Fe, Mo, As, Sb, and Sm and favoring much higher accumulation of Br than biogenic NPs. The decrease in chlorophylls and carotenoids in plants is correlated with increase in antioxidant capacity, and occurs with increase of Mo, Al, Mg, K, Zn, and Ca content.

Ranking of element content in each type of investigated plants

Parameter	Control Soil	Soil with CuO-NP	Soil with CuO-NP-cel	Soil with CuO-NP-bth
Elements determined in plants	Cl > Fe > K>Ca > Mg>Na > Ba > Zr > Al > Cr>Rb > Zn > Ni > Sr > Ce > Mn > La > Nd > Co > Sc > Th > As > Hf > Sm > Cs > U>Br > Sb > Ta > Eu>Tb > Yb > Tm > Mo	K > Cl > Ca > Mg > Br>Na > Al > Zn > Rb > Cu > Mn > Ba > Sr	K > Cl > Ca > Mg > Br>Na > Al > Zn > Rb > Cu > Mn > Ba > Sr	K > Cl > Ca > Mg > Na>Al > Fe > Zn > Rb > Mn > Ba > Br > Sr > Mo > As>Sb > Sm

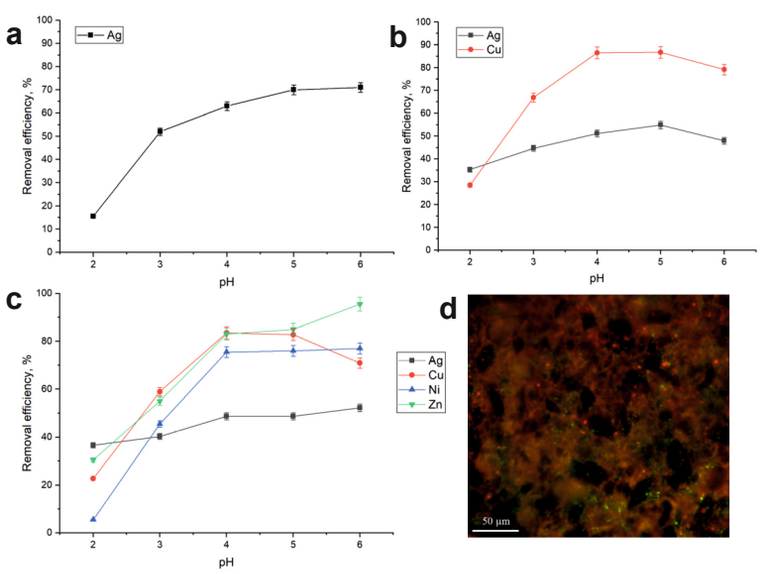
[1] Lung I., Opriș O., Sorana M.L., Culicov O., Ciorîță A., Stegărescu A., Zinicovscaia I., Yushin N., Vergel K., Kacso I., Borodi Gh., Pârvu M., The impact assessment of CuO nanoparticles on the composition and ultrastructure of Triticum aestivum L, *International Journal of Environmental Research and Public Health* 18 (2021) 6739. DOI: 10.3390/ijerph18136739

Application of *Shewanella Xiamenensis* placed on zeolite in treatment of silver-containing effluents

Frumkin Institute of Physical Chemistry, Russian Academy of Science, Moscow, Russia;

Scientists from Russia developed environmentally-friendly adsorbent for wastewater treatment

The recovery of silver from industrial wastewater is of practical importance due to silver resources limitations and its environmental impact. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) was applied to evaluate the adsorption capacity of *Shewanella xiamenensis* biofilms formed on zeolite (bio-zeolite) applied for the treatment of silver-containing effluents. The adsorption of metal ions on bio-zeolite was pH dependent; the optimal pH for the highest metal removal of 55-95% was in the range of 4.0–6.0. The maximum adsorption capacities of silver on bio-zeolite calculated from the Langmuir model were 14.8 mg/g (Ag system), 32.5 mg/g (Ag-Cu system) and 12.8 mg/g (Ag-Cu-Ni-Zn system). The adsorption was shown to be a spontaneous process endothermic or exothermic in nature depending on the metal ion, which is driven by entropy. Metal ions' removal from silver-containing effluents by bio-zeolite is a physico-chemical adsorption process rather than a pure physical or chemical adsorption process. *Shewanella xiamenensis* biofilms formed on zeolite can be considered as an excellent candidate for the treatment of silver-containing complex effluents.



Influence of pH on metal removal from studied synthetic solutions by bio-zeolite: (a) Ag (b) Ag-Cu, (c) Ag-Cu-Ni-Zn systems and (d) image of the Shewanella xiamenensis biofilm formed on zeolite

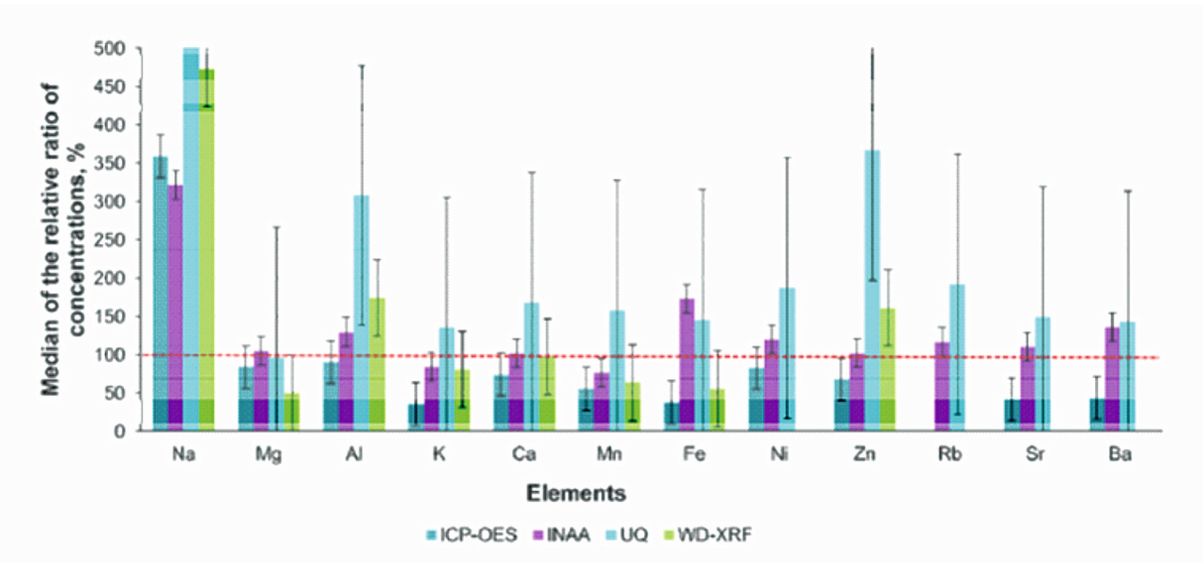
[1] Zinicovscaia, I.; Yushin, N.; Grozdov, D.; Safonov, A. Application of *Shewanella xiamenensis* placed on zeolite in treatment of silver-containing effluents, *Minerals* 13 (2023) 179. DOI: 10.3390/min13020179

Comparison of non-destructive techniques and conventionally used spectrometric techniques for determination of elements in plant samples (coniferous leaves)

Faculty of Chemistry, University of Belgrade, Belgrade, Serbia;
Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia;
Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

Collaboration of scientists from Serbia researched the analytical possibilities of several techniques of elemental analysis

Determination of samples elemental composition is a critical task in environmental studies. The neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) along with other analytical techniques, including inductively coupled plasma mass spectrometry (ICP-MS), was applied for the elemental analysis of 49 plant samples of four conifer tree species. Relative ratios of concentrations obtained using NAA were always in the range of 70–130 % compared to ICP-MS concentrations, except for Na (332 %), Fe (173 %) and Ba (136 %), which indicated that the technique produced results that were most similar to the ICP-MS results. The statistically significant correlation was found for all elements within the comparison of ICP-MS and NAA. Thus, NAA, being a non-destructive spectroscopic technique, can be successfully applied to the analysis of plant samples, which is valuable because sample preparation for this technique can be fast and satisfies well the principles of green chemistry.



Median values of the relative ratios of concentrations obtained using different techniques compared with ICP-MS concentration. Error bars represent standard deviations.

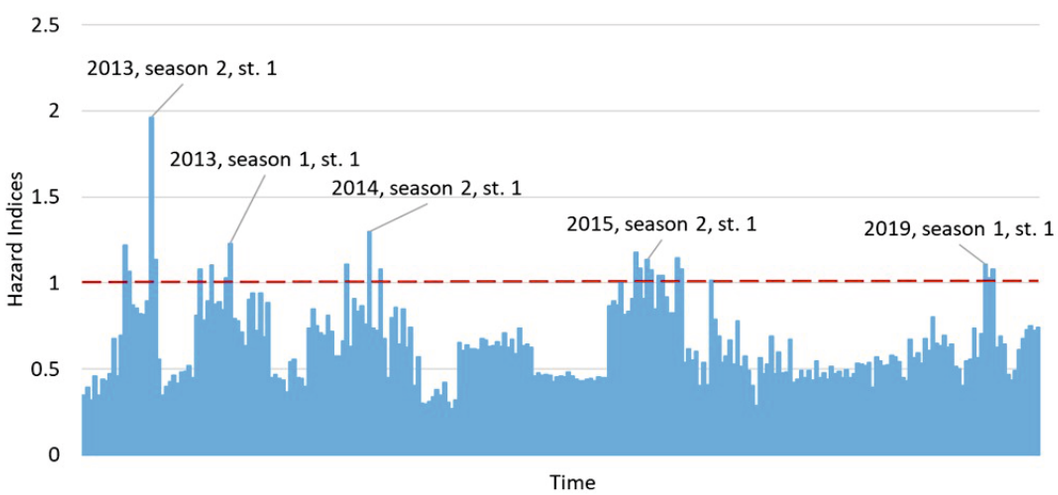
[1] Orlić J., Aničić Urošević M., Vergel K., Zinicovscaia I., Stojadinović S., Gržetić I., Ilijević K., Comparison of non-destructive techniques and conventionally used spectrometric techniques for determination of elements in plant samples (coniferous leaves), *Journal of the Serbian Chemical Society* 87 (2022) 69. DOI: 10.2298/JSC210921101O

Temporal trends of risks in consumption of wild and farmed mussels in 2013-2019 in the Saldanha Bay area (South Africa)

School for Science and Technology, Faculty of Military Science, Stellenbosch University, South Africa

Scientists from South Africa assessed the risks in consumption of wild and farmed mussels in the Saldanha Bay area of South Africa

The bivalve molluscs are an important group of food in many countries around the world, including South Africa. The levels of 24 macro- and microelements were determined by neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor (FLNP JINR) in mussel samples collected during the period of 2013-2019 from three sites with different natural features in the Saldanha Bay area. The combination of approaches in the risk assessment helped to detect the group of harmful elements for human health. In general, the wild and farmed mussels demonstrated low levels of risks for human health during the entire studied period, except for intakes of such elements as Fe and Zn in several cases. Based on the applied approaches, Cr, Fe, Ni, Zn, As and I in wild mussels can pose possible health risks to potential consumers in several cases during 2013-2019. It was concluded that the safe level of weekly consumption rate should be less than 100 g/week per person, according to the highest calculated values of concentrations.



Temporal trends in hazard indices (HI) calculated on sums of target hazard quotients (THQs) for Al, V, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Sr, Sb, I, Cs, U. The labels designated: year, season (1 – Winter, 2 – Autumn), station. Columns exceeding red dashed line indicate possible cumulative risks for human health.

[1] Nekhoroshkov P., Bezuidenhout J., le Roux R., Zinicovscaia I., Yushin N., Frontasyeva M., Temporal trends of risks in consumption of wild and farmed mussels in 2013-2019 in the Saldanha Bay area (South Africa), *Journal of Food Composition and Analysis* 131 (2024) 106193. DOI: 10.1016/j.jfca.2024.106193

Modeling of the arsenic uptake by *Brassica perviridis* (L. H. Bailey) (Spinach Mustard) growing on different soils collected in Northern Vietnam

Institute of Nuclear Science and Technology,Vietnam Atomic Energy Institute, Hanoi, Vietnam;
Institute of Physics of Vietnamese Academy of Science and Technology, Hanoi, Vietnam;
Hanoi Irradiation Center –Vietnam Atomic Energy Institute, Hanoi, Vietnam

Collaboration of scientists from Vietnam researched the food safety of Brassica perviridis cultivated on contaminated soils

Evaluation of the arsenic content in food has always been an important issue due to its high toxicity. This is especially relevant for Vietnam, a country with high arsenic contamination. The content of As and Fe in the vegetable *Brassica perviridis* depending on the conditions of plant growth and soil parameters was determined by neutron activation analysis (NAA) at the REGATA facility of the IBR-2 reactor in FLNP JINR. The obtained data showed that the As uptake in the *Brassica perviridis* plants grown in northern Vietnam could be presented as a function of soil parameters such as pH, organic carbon content, and Fe content, but, at the same time, does not depend on the As content in soil. Particularly high Fe content in Vietnamese soils contribute to the As immobilization and prevent its uptake by plants. Regression Data Analysis was used to extract a model function with good corresponding statistics: correlation factor R > 0.97, the probability p-value of independent variable coefficients in the range from 1.86E-07 to 0.007, and the significance F of the model < 1.49E-11. The obtained values demonstrate the reliability and the trueness of the applied model at the given soil characteristics and conditions of plants cultivation.

The main parameters of the model developed to describe As uptake by *Brassica perviridis*

Specie	Brassica Perrividis	Fe concentration in soil, g/kg	8.07– 164
Soil types	23 natural soils	Plantation	Plant distance 4-5 cm, as by the way of planting BP vegetables for food
As concentration in soil, mg/kg	1.34– 28.80	Irritation	plants irrigated by the same water
pH	3.87 - 7.81	Soil fertilization	N fertilizer
Organic carbon (% OC)	0.14 - 3.16	Predicted model	$C_{As-P/P.N}$ = 0.0014*pH + 0.0095*OC – 6.52E-05*C_{Fe-S} R=0.97, R^2=0.94 Significance F = 1.48E -11

[1] Nguyen T.B.M., Trinh T.T.M., Zinicovscaia I., Khiem L.H., Vergel K., Tuan P.L., Anh H.L., Nguyen T.T. H., Modeling of the arsenic uptake by Brassica perviridis (L. H. Bailey) (Spinach Mustard) growing on different soils collected in Northern Vietnam, *Water, Air, & Soil Pollution* 235 (2024) 180.
DOI: 10.1007/s11270-024-06989-7

6. Cultural Heritage

- Neutron tomography
- Neutron diffraction
- Archeological markers

Non-destructive structural studies of Byzantine pottery fragments from the Dobrudja region of Romania

Cooperation in the framework of the IBR-2 user program:
Museum of National History and Archaeology, Constanţa, Romania;
Faculty of Applied Sciences and Engineering, Ovidius University, Constanţa, Romania

Scientists from Romania initiated studies of phase composition and spatial distribution of phases in pottery fragments from excavations in the Dobrudja region

The actively developed broad direction in the archaeometry is relieved by comprehensive studies of cultural heritage objects using methods of non-destructive testing, such as X-ray and neutron tomography, neutron activation analysis and others. The studies of the samples of Byzantine ceramics from excavations in the Dobrudja region (Romania) were performed [1, 2]. The phase composition and the spatial distribution of various phases of the pottery fragments was studied using neutron diffraction and tomography methods on the DN-6 and NRT instruments of the IBR-2 reactor of FLNP JINR. The obtained structural data revealed the presence of calcite grains and pores, as well as the uniformity of phase spatial distribution, which made it possible to systematize the studied fragments. Structural data obtained using neutron diffraction and tomography can serve as a basis for systematization and group analysis of Byzantine ceramic samples [2]. This allows one to make assumptions both about the sources of raw materials and about the location of the pottery workshops [1, 2].

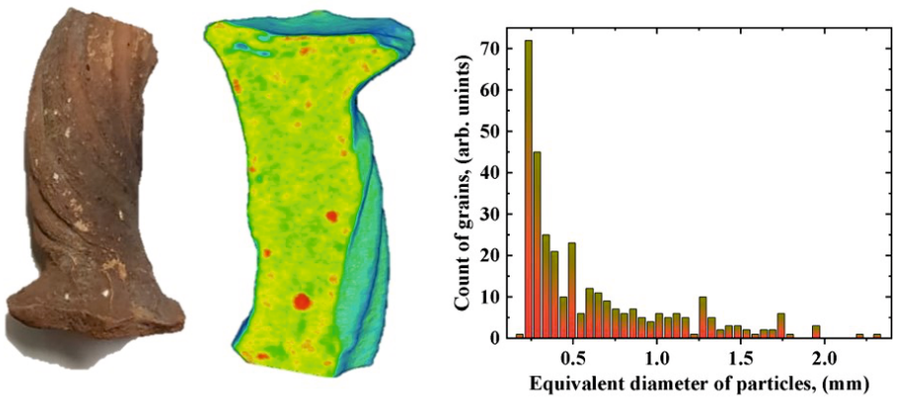


Photo and the longitudinal virtual slice of the 3D model after tomographic reconstruction of one of the studied pottery fragments. The distribution of the equivalent diameters of the observed silicate grains inside the ancient pottery sample is also presented.

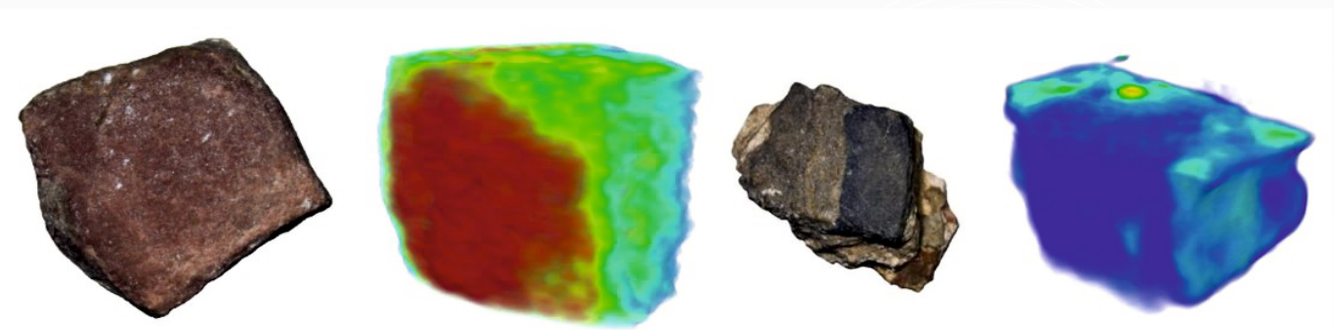
[1] Abdurakhimov B.A., Kichanov S.E., Talmaţchi C., Kozlenko D.P., Talmaţchi G., Belozerova N. M., Bălășoiu M., Belc M.C., Studies of ancient pottery fragments from Dobrudja region of Romania using neutron diffraction, tomography and Raman spectroscopy, *Journal of Archaeological Science: Reports* 35 (2021) 102755. DOI: 10.1016/j.jasrep.2020.102755
[2] Zhomartova A. Z., Abdurakhimov B. A., Talmațchi C., Kichanov S. E., Kozlenko D. P., Bălășoiu M., Talmațchi G., Șova C., Belc M.C., The systematic structural studies of some Byzantine ceramic fragments from Dobrudja region of Romania: Raman spectroscopy, neutron diffraction, and imaging data, *Archaeometry* 66 (2024) 787. DOI: 10.1111/arcm.12947

Non-destructive neutron methods for characterizing ancient Roman mosaic fragments

Cooperation in the framework of the IBR-2 user program:
Valahia University of Targoviste, Targoviste, Romania

Scientists from Romania made non-destructive neutron diagnostics of ancient Roman mosaics from the Roman Mosaic Museum in Constanta

One of the well-preserved examples of the cultural heritage from the Roman and Byzantine eras are mosaic fragments. Archaeologists and cultural researchers pay special attention to physical methods such as neutron diffraction and tomography, which provide a non-destructive way to examine the internal structure of objects also being sensitive to light elements. These methods allow for a high contrast between different materials and possess high penetrating power. In this study, the chemical and structural composition of decorative elements from ancient Roman mosaics at the Museum of Mosaics in Constanta, Romania, was reported. The non-destructive diagnostics of the mosaic samples was performed on the DN-6 neutron diffractometer and neutron radiography and tomography instrument operated at the IBR-2 reactor of FLNP JINR. The results of neutron diffraction were used to study the phase and mineral composition of mosaic fragments, and to obtain the unit cell parameters of the main phase components. Neutron tomography was applied to reconstruct the 3D spatial distribution of major phases, as well as to identify areas of corrosion and structural degradation, layers of paint on the mosaic fragments [1, 2]. The first results of neutron studies of cultural heritage items like mosaics demonstrate the possibilities of non-destructive control for rare cultural heritage objects, both in terms of historical restoring the manufacturing technology of ancient Roman and Byzantine mosaics [1], and the effects of structural and chemical degradation of valuable materials [2] in a polluted and sea air atmosphere of seaside Constanta, Romania.



A photo and the 3D model reconstructed from neutron tomography data of the fragments of ancient Roman mosaic.

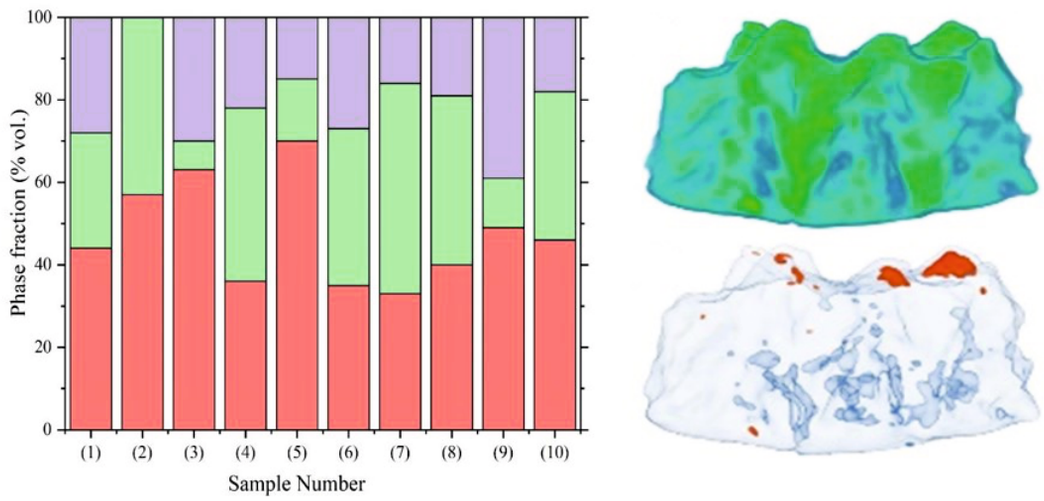
[1] Ion R.M., Bakirov B.A., Kichanov S.E., Kozlenko D.P., Belushkin A.V., Radulescu C., Dulama, I.D., Bucurica I.A., Gheboianu A.I., Stirbescu R.M., Teodorescu S., Iancu L., David M.E., Grigorescu R.M., Non-destructive and micro-invasive techniques for characterizing the ancient Roman mosaic fragments, *Appl. Sci.* 10 (2020) 3781. DOI: 10.3390/app10113781
[2] Ion R.M.; Bakirov B.A.; Kichanov S.E.; Gheboianu A.I., Ceramic artifacts investigations by nuclear techniques, *Scientific Bulletin of Valahia University-Materials and Mechanics* 19 (2023) 21 15. DOI: 10.2478/bsmm-2023-0013

Non-destructive neutron structural studies of objects of the cultural heritage of Kazakhstan

Cooperation in the framework of the IBR-2 user program:
Institute of Nuclear Physics, Almaty, Kazakhstan;
Gumilyov Eurasian National University, Astana, Kazakhstan;
Al-Farabi Kazakh National University, Almaty, Kazakhstan

Scientists from Kazakhstan initiated neutron tomography studies of ceramic fragments from historical community of the ancient Saka tribe

A significant number of ceramic artifacts found during various archaeological excavations can provide valuable information about daily life, the development of manufacturing techniques, trade relations, or the conquests of certain civilizations. In the frame of a non-destructive structural analysis, several ceramic fragments from an almost unstudied historical community of the ancient Saka tribe living in eastern Kazakhstan were selected. The internal structural features of the ceramic fragments were comprehensively tested using the neutron diffraction method on the DN-6 neutron diffractometer and neutron tomography method on the NRT beamline at the IBR-2 reactor of FLNP JINR. The composition of the phases and the internal pores revealed in the experiments were discussed in the context of the structural features of local clay deposits and the characteristics of ancient pottery manufacturing techniques. Based on the obtained structural information, the specific characteristics of ceramic production, including the temperature annealing processes for pottery fragments, were determined.



The relative proportions of quartz, feldspar, and mica in the ceramic fragments, based on neutron diffraction data (DN-6, IBR-2). The reconstructed from neutron tomography data (NRT, IBR-2) 3D model of a selected fragment with highlighted pores.

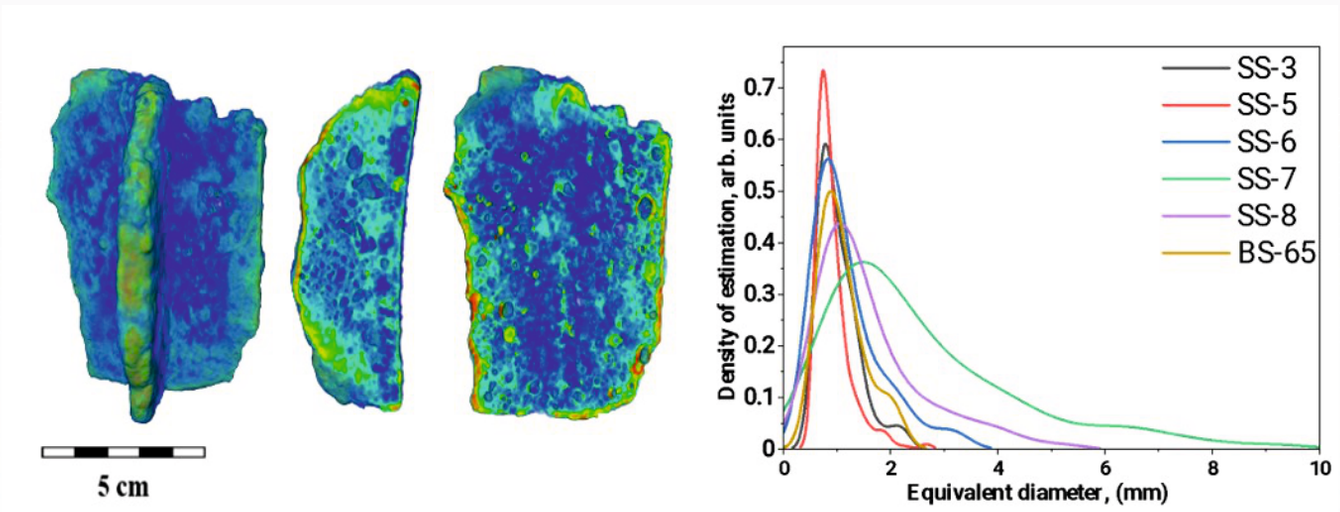
[1] Bakirov B.A., Zhomartova A.Z., Kichanov S.E., Zhumatayev R.S., Toleubayev A.T., Nazarov K.M., Kozlenko D.P., Nazarova A.M, Non-destructive neutron structural studies of ancient ceramic fragments of the cultural heritage of the Republic Kazakhstan, *Eurasian Journal of Physics and Functional Materials* 6 (2022) 56. DOI: 10.32523/ejpfm.2022060106
[2] Zhomartova A., Bakirov B., Kichanov S., Zhumatayev R., Toleubayev A., Shakenov S., Kozlenko D., Non-destructive structural studies of ceramic fragments of ancient tribes of Kazakhstan, *Eurasian Journal of Physics and Functional Materials* 7 (2023) 79. DOI: 10.32523/ejpfm.2023070201

Structural features of the fragments from cast iron cauldrons of the Medieval Golden Horde: neutron tomography data

IInstitute of Physics, Kazan Federal University, Kazan, Russia;
Khalikov Institute of Archeology, Tatarstan Academy of Sciences, Kazan, Russia

Archeologists and physicists from Kazan initiated neutron tomography studies of hidden porosity in ancient cast-iron cauldrons dating to the medieval Golden Horde period

The structural features of fragments from cast iron cauldrons of the medieval Golden Horde, which are representative of products from ancient iron casting processes, were analyzed. Two sets of iron-cast fragments from Selitrennaya settlement in the Lower Volga Region and Bolgar settlement in central Volga Region were selected. Neutron tomography studies of these fragments were conducted at a specialized experimental neutron radiography and tomography station NRT at the IBR-2 pulsed high-flux reactor. Based on the obtained 3D neutron tomography data, it was possible to identify and separate the internal pores inside these cast iron products. A preliminary conclusion is that the presence or absence of small internal pores can be associated with the location and casting technological processes of the foundries. The analysis of neutron tomography 3D data to obtain the size and form distributions, some morphological characteristics, and orientation of the internal pores in the cast iron fragments provided not only qualitative but also quantitative structural markers for cast iron objects. Thus, the versatility of porosity processes in the cast iron procedures in ancient workshops can be considered as structural markers to identify the locations of cast iron manufacturers, the presence of additional forging of cast iron products, as well as the features and primary composition of casting molds [2].



Reconstructed 3D model with examples of longitudinal and transverse slices from neutron tomography data (NRT, IBR-2). Distribution functions for the equivalent diameter of pores in cast iron fragments studied.

[1] Bakirov B., Smirnova V., Kichanov S., Shaykhutdinova E., Murashev M., Kozlenko D., Sitdikov A, Structural features of the fragments from cast iron cauldrons of the medieval Golden Horde: neutron tomography data, *J. Imaging* 9 (2023) 97. DOI: 10.3390/jimaging9050097

The study of ancient Greek kyathos using neutron tomography and radiography methods

IInstitute of Archeology of the Russian Academy of Sciences, Moscow, Russia

Archeologists from Moscow initiated studies of the structure of artefacts from the excavations of the Volna-1 soil burial ground

A series of kyathes found in the graves of the Volna-1 cemetery (Taman Peninsula, Russia) were studied by neutron tomography and X-ray diffraction to obtain information about hidden structural features and phase variety in the volume of metal objects. It was possible due to good neutron radiography contrast between components with different chemical compositions. Also, the kyathes are covered by a thick layer of corrosion, thus limiting the studies using other methods. Neutron tomographic experiments for a series of kyathes [1] were performed on the neutron radiography and tomography station NRT at the IBR-2 reactor of FLNP JINR. Based on the results of these experiments, it was found that the relative volume of corrosion varies significantly from sample to sample, ranging from 20% to 90% of the total volume. Additionally, the reconstructed 3D models allow for the identification of structural features of these objects. Some of the samples are cast monoliths, while others are composed of two prefabricated elements: a separate handle blank that was attached to a separate bowl using pins. In some cases, traces of repair work can be identified, such as the attachment of a handle to a bowl using a metal strip made of tin-lead bronze secured with large riveted pins.

Photo of several samples under study and reconstructed 3D models with highlighted elements of the construction of ancient bronze kyathes based on neutron tomography (NRT, IBR-2).

[1] Sudarev N.I., Saprykina I.A., Smirnova V.S., Mimokhod R.A., Kichanov S.E., Preliminary results of styding the kyathoi dating to the 5th-4th centuries BS from the graves of the Volna-1 cementry, *Kratkiye Soobshcheniya Instituta Arkheologii* 272 (2023) 326.

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NEUTRON RESEARCH AT IBR-2 FOR MEMBER STATES

Scientific Highlights

Frank Laboratory of Neutron Physics, 2024

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