



## Selected Applications of Magnetic Resonance

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The intensive development of magnetic resonance methods began after 1944, when E. K. Zavoiskii, Professor of Kazan State University (Russian Federation), discovered the phenomenon of electron paramagnetic resonance—EPR (Thesis for Doctor of Science, 1944). In 1946, two scientific teams of American scientists, headed by F. Bloch and E. M. Purcell, published articles on the observation of nuclear magnetic resonance (NMR) **in condensed matter** (Phys. Rev., 1946, v. 69, p. 127 and *ibid.*, p. 37, consequently). In 1950, H. G. Dehmelt and G. Krueger obtained spectra of nuclear quadrupole resonance—NQR (Naturwissenschaften, 1950, Bd. 37, S. 111). The goal of this special issue is to set off some perspective directions in the area of the magnetic resonance and its applications. Although the articles collected in a single issue cannot cover the variety of modern trends, they may give a flavor on the current state of the art of interesting researches, and we hope that this special issue to some extent demonstrates the multitude of applications of magnetic resonance.

In the science of the twenty-first century, great importance is attached to the problems of biology and medicine. One of the important achievements is magnetic resonance imaging (MRI)—an interdisciplinary field of science at the intersection of physics, chemistry, computer science, engineering and medicine. Two articles in this special issue are devoted to magnetic resonance imaging and related questions.

The article of Yu. A. Pirogov «Multi-nuclear MRI research» contains systemized results of long standing research in the Center for Magnetic Tomography and Spectroscopy (CMTS) of Moscow State University in the area of magnetic resonance imaging with nuclei other than protons. The scientific team of CMTS has modified the clinical low-field 0.5-T MRI scanner Bruker Tomikon S50, and it becomes possible to obtain MRI using 10 different types of nuclei in a weak magnetic field. The work clearly demonstrates that the multinuclear MRI has a great potential in both scientific research and development of practical (in particular, clinical) applications.

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The article «Advanced MRI-methods for evaluation of Parkinson`s disease» by U. Eichhoff is an original review concerning the applications of magnetic resonance imaging for early diagnostics and therapy of Parkinson`s disease. Parkinson`s disease is a progressive degenerative disease of the central nervous system. Its symptoms are expressed in the form of violations of the body`s motility and cognitive processes. In 2015, Parkinson`s disease affected 6.2 million people and resulted in about 117,400 deaths globally. In his article, U. Eichhoff describes in detail the causes of Parkinson`s disease and methods of its non-invasive identification. The susceptibility changes induced by iron in substantia nigra of the human brain make Susceptibility Weighted Imaging (SWI) and Quantitative Susceptibility Mapping (QSM) the preferred techniques for evaluation of Parkinson`s disease. Diffusion Tensor Imaging (DTI) and resting-state functional MRI (rs-fMRI) highlight the changes in structural and functional connectivities in the brain, which may explain the symptoms of the disease.

The following four articles reflect different aspects of solid matter studies.

The gallium–indium eutectic alloy is in a focus of modern research because of its great potential for microelectronics, wearable electronics, electronic skin, medical diagnosis, and soft robotics. Novel applications of the Ga–In alloy require better understanding of the effect of size reduction on its properties. This problem is considered in the article “Stabilization of  $\beta$ -Ga structure in nanostructured Ga-In alloy” by D. Yu. Nefedov and E. V. Charnaya with co-authors. They performed the NMR studies of the nanostructured Ga–In alloy within pores of the opal matrix.  $^{71}\text{Ga}$  and  $^{69}\text{Ga}$  NMR studies of the nanostructured eutectic Ga–In alloy embedded into opal porous matrix showed the emergence of the gallium-rich crystalline phase with a structure of  $\beta$ -Ga. This phase was stable under opal nanoconfinement while it is metastable in bulk.

Highly efficient thermoelectric materials have been attracting much attention because of their potential applications, especially for energy harvesting by waste heat. Recently, it was proposed to use magnetic semiconductors as effective thermoelectrics. One of the representatives of this class of compounds is the well-known semiconductor mineral chalcopyrite  $\text{CuFeS}_2$ . Chalcopyrite is an antiferromagnetic semiconductor that crystallizes in a zinc blende-type structure with four-coordinate cations and anions forming distinct corner-sharing tetrahedral whose unusual magnetic and electrical properties are still not yet completely understood. V.L. Matukhin and A. N. Gavrilenko with co-authors present the work “ $^{63,65}\text{Cu}$  NMR and EPR Study of Doped Chalcopyrite  $\text{Cu}_{1-x}\text{Pd}_x\text{FeS}_2$  Compounds” in which they show that the structure of chalcopyrite in the stoichiometric composition of  $\text{CuFeS}_2$  contains a significant number of defects that strongly distort the shape of resonance lines in NMR spectra of  $^{63,65}\text{Cu}$  nuclei. The addition of copper to the composition  $\text{Cu}_{1.02}\text{Fe}_{0.98}\text{S}_2$  significantly reduces the defectiveness of such a structure. Doping with palladium to the composition  $\text{Cu}_{0.99}\text{Pd}_{0.01}\text{FeS}_2$  also significantly reduces the defectiveness of the  $\text{CuFeS}_2$  structure, but noticeably less than in the  $\text{Cu}_{1.02}\text{Fe}_{0.98}\text{S}_2$  structure.

A.R. Gafarova and co-authors present the article “Quantum-chemical calculations in studying the conformation of  $\gamma$ -irradiated calcium gluconate”. Gluconic acid is widely used in food, metallurgy, cement and pharmaceutical industries. The

authors apply the gamma radiation to produce stable radicals from calcium compounds and to detect informative EPR spectra. The use of quantum-chemical calculations for the interpretation of EPR spectra is an important support for describing the objects under investigation. Three types of radicals are considered to explain the experimental EPR spectra of polycrystalline calcium gluconate irradiated with gamma-quanta. This made it possible to correctly describe the X- and Q-band EPR spectra of  $\text{CaGluc}2\cdot\text{H}_2\text{O}$  with one set of anisotropic parameters HFI and g-factors. The results demonstrate the possibility of using this method for the conformational analysis of the compounds studied.

Quantum magnonics is an emerging research field, with great potential for applications in quantum technologies, including quantum computing, processing and encoding information, forming hybrid quantum systems etc. In the article “Magnon quantization in the magnetic field gradient” by Yu. M. Bunkov, K. Yu. Dunichev, T. R. Safin, and M. S. Tagirov, the effect of magnon quantization in magnetized films of Yttrium Iron Garnet is investigated in the inhomogeneous magnetic field under the resonance RF pumping. It is shown that the obtained experimental data fit well with the magnon quantization in the triangular potential well and this system is an anharmonic. Thus, frequencies of excited levels are not equidistant and this is one of the conditions for using the system as a magnon qubit.

The low signal-to-noise ratio is a characteristic feature of NMR experiments in the Earth magnetic field. The main problem of the NMR spectroscopy of high resolution in this area is the ineffectiveness of signal accumulation due to fluctuations of the Earth magnetic field because of magnetic interferences from laboratory equipment and other magnetic field sources. The original solution to the problem was earlier proposed by J. Stepišnik with co-workers, who suggested using a second sensor to monitor changes of the resonance frequency caused by fluctuations in the Earth field. In the article of P. A. Kupriyanov and co-authors “To a question on possibilities of high-resolution NMR spectroscopy in the Earth magnetic field”, a relatively simple method has been developed to neutralize the Larmor frequency fluctuations without the second reference sensor. The home-built NMR-equipment allows the registration of the splitting in proton spectra, for example, due to the  $J$ -interaction with such nuclei as  $^{29}\text{Si}$  or  $^{13}\text{C}$  at their natural abundance (4.7 and 1.1%, respectively).

A number of NMR methods and different data processing procedures are applied in the article of A. Nagmutdinova, L. Brizi, P. Fantazzini, and V. Bortolotti “Investigation of the first sorption cycle of white Portland cement by  $^1\text{H}$  NMR” for the analysis of influence of drying/re-saturation cycles on the structure and components of White Portland Cement samples. In particular, the NMR signal from the component with lower mobility are analyzed by the Pake-Doublet theory in time-domain and two components are clearly detected, assigned to  $^1\text{H}$  nuclei of crystalline water in Ettringite and OH groups in Portlandite. The reversible changes of the solid components of cement samples have been observed. This is a new method to deeply investigate the changes of solid components during sorption cycles.

The last article of this special issue is devoted to the applications of nuclear quadrupole resonance (NQR): R.R. Khusnutdinov, G. V. Mozzhukhin, A.B. Konov, Y. Ozturk, and B. Z. Rameev. “Two-frequency planar gradiometer for distant NQR

detection of explosives". The methods of the remote NQR detection of solid explosives, narcotics and other important substances have been a subject of research for many decades. Almost all developments are based on the use of the resonance of  $^{14}\text{N}$  nuclei, since nitrogen atoms are usually present in specified substances. The attractiveness of the method is reduced by the relatively low sensitivity inherent in all radiospectroscopic methods. Therefore, researchers are striving to develop devices with improved sensitivity and noise immunity. The article of R.R. Khusnutdinov with co-authors is namely devoted to these aspects.

We hope that the publications presented in this issue will attract the attention of scientific community to the prospects of new MR developments and will stimulate further progress in the magnetic resonance and its applications. We would like to bring our gratitude to all the authors who have contributed to this special issue. We hope that humanity will overcome the pandemic and we wish everyone health and success in scientific activities!

This special issue will be published in a year when the Editor-in-Chief and our deeply respected Academician and Professor Kev M. Salikhov is celebrating his 85th birthday. We cordially wish Professor Kev Salikhov good health and further outstanding achievements in the Physics of Magnetic Resonance and its Applications!

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