Brief information about the project

Name of the project	AP14971722 «Defect structure of functional crystalline materials: X-ray and neutron diffraction studies»
Relevance	The real structure of a crystal - violation of the ideal long-range order due to the presence of various types of defects - affects almost all the main physical properties of crystalline materials, and often determines them. Among the methods for studying the defect structure of crystalline materials, the diffraction of short-wave radiation (X-rays and neutrons) is one of the most informative. A new method of neutron diffraction (Fourier diffractometry) has been developed at JINR (Dubna) at the IBR-2 pulsed reactor, combining the possibilities of high resolution and high aperture modes. Their parallel use on a HRFD (High Resolution Fourier Diffractometer) diffractometer makes it possible to obtain data on the structure and microstructure of crystals directly in the course of external action on the crystal or when external conditions change in situ and in real time. In addition, unlike transmission electron microscopy and X-ray diffraction, neutron diffraction provides volumetric data, which makes it possible to avoid the influence of local compositional inhomogeneities and surface effects. In the project, new information about the real crystal structure of several types of functional materials (iron-based alloys with a high coefficient of internal friction and giant magnetostriction) will be obtained by neutron diffraction. In addition, its changes in the course of structural phase transitions depending on external conditions will be determined. These results are necessary to solve some physical problems of functional intermetallic alloys. Equally, these results will be in demand by materials scientists who use iron-based functional alloys for practical applications.
Purpose	The purpose of this project is to develop a methodology for neutron diffraction studies of real crystalline materials with a defective structure and, with its help, to obtain new data on the effect of a real structure on the physical and physicochemical properties of materials.
Objectives	The main experimental method for determining the characteristics of the microstructural state of crystalline materials is the Bragg diffraction of X-rays or synchrotron radiation. In particular, in the diffraction experiment, in parallel with the structural data, information can be obtained about microstresses in crystallites and the characteristic sizes of coherent scattering regions. However, bulk functional materials, as a rule, consist of rather large crystallites and can be highly textured. These circumstances make structural analysis in the case of X-ray or synchrotron radiation with their narrow beams, when the irradiated volume contains not a very large number of crystallites, practically impossible. These difficulties are largely leveled if neutron diffraction is used. The

	penetrating power of neutrons is orders of magnitude greater than that of X-rays and electrons, and the cross-section of the neutron beam is at least 1 cm2. As a result, it is the "bulk" information that is recorded in the neutron experiment, which is practically not distorted by local fluctuations in composition and surface effects. Neutron diffraction is still relatively rarely used to determine the characteristics of the microstructural state of crystalline materials, since for this it is necessary to have a very high level of resolution of the diffractometer. In addition, to study phase transitions in real time, it is also required to have a very high level of light intensity of the diffractometer. Both of these conditions are fulfilled on a High-Resolution Fourier Diffractometer operating at the IBR-2 pulsed reactor at JINR (Dubna). The record-high resolution of the interplane distance ($\Delta d/d \approx 0.001$) on the PDVR is provided by the use of a fast Fourier interrupter and the correlation method of the diffraction data set. Disabling the correlation analysis puts the PDVR into a high-aperture mode, for which a high neutron flux (~107 n/cm2/s) and a sufficiently large solid angle of the detector system (Wd~ 0.2 cp) make it possible to use data accumulation times ts = 1 minute or less. Within the framework of the project, studies of changes in the atomic structure and microstructure of iron-based alloys (Fe-Ga, Fe-Al, etc.), which differ in unusual physical properties, will be carried out. In particular, the composition of Fe-27Ga is known for its record magnetostriction compared to other iron-based double alloys (about 400 ppm) [1], respectively, the analysis of the phase diagram and properties of Fe-Ga alloys is actively conducted by a variety of methods (review [2] and references therein). X-ray diffraction will be used for preliminary characterization of samples. Neutron diffraction experiments will be carried out at JINR on the FDVR diffractometer in a wide temperature range (20-900 ° C). The samples will be heated in a specialized high-temperature furnace (standard ILL) with a linear temperature increase or with isothermal annealing at certain fixed temperatures. The combination of real-time neutron diffraction in in-situ mode with continuous temperature scanning and measurements of high-resolution diffraction spectra at certain fixed temperatures will provide unique data necessary to understand the relationship of the structure and microstructure of alloys with their most important technological properties (plasticity, magnetostriction, internal friction, etc.).
Expected and achieved results	The project is aimed at obtaining information about functional alloys, which is of fundamental importance both for the theory of ordering alloys and for

	constructing models of the interaction of microstructure and physical characteristics of materials. At the same time, these data will be important for materials scientists, first of all, for constructing real phase diagrams of the state. The fundamental nature of the results will ensure the possibility of their publication in international scientific journals. It is assumed that, based on the results of the experiments, it will be possible to publish two articles in J-level journals. Alloys and Compounds. According to the results of the first year of the project, the publication of books or chapters in books, as well as patenting of the results is not expected. The scientific effect of the project will consist in obtaining completely new scientific information. The economic effect is possible, but it should take some time. Potential users of the project results will be physicists dealing with problems of intermetallic alloys, and material scientists using functional iron-based alloys for practical applications. During the implementation of the project, it is planned to publish at least 2 (two) articles in journals from the first three quartiles by impact factor in the Web of Science database or having a CiteScore percentile in the Scopus database of at least 50 (fifty), as well as at least 1 (one) article or review in a peer-reviewed foreign or domestic publication recommended by the CCSON. The publication of the results obtained will be carried out in accordance with subparagraph 1.1 of section 7 of the current tender documentation. The publication of the project results in highly rated journals with an impact factor will expand the publication activity of Al-Farabi Kazakh National University. At the same time, participation in the preparation and publication of the results of young scientists will allow them to gain invaluable experience in this area, as well as increase their scientometric indicators. Also, within the framework of the project, it is planned to prepare a PhD dissertation, this topic will be offered to doctoral students in 2022 when they enter the specialty "Nuclear Physics". The results of the project, in addition to publications, will be presented in the form of scientific reports at a number of international conferences and scientific schools. The participation of young scientists in these conferences will allow establishing new scientific connections for further research, with the aim of developing this direction in Kazakhstan.

	The social effect of the successful implementation of the project is to develop and strengthen the skills and experience in conducting scientific research of young promising scientists of Kazakhstan, as well as attracting them to science, to new directions that are most in demand in the world. So the participation of young scientists in the development of this topic will allow them to gain invaluable experience and become highly qualified specialists not only in their country, but also in the world. It is important to note that the results of the project will form a serious scientific and technical foundation for further advanced research in Kazakhstan in the field of development of construction technology, materials and construction. The implementation of the project will also contribute to building Kazakh-Russian cooperation with leading scientific groups working in the field of neutron physics, with the aim of developing the Kazakh scientific school. The training and consolidation of scientific personnel from among students in the field of science and education will be carried out, allowing to form effective research teams in the future. Thus, the implementation of the project will be closely linked with PhD doctoral and master's theses performed by Kazakhstani students as part of their studies. The target consumers of the results obtained will be international research centers and companies for obtaining, studying and optimizing the microstructure of composite cement materials for the needs of the nuclear industry.
Research team members with their identifiers (Scopus Author ID, Researcher ID, ORCID, if available) and links to relevant profiles	1. Mukhametuly Bagdaulet, KazNU named after Al-Farabi, "6D060500-Nuclear Physics", PhD, H-index = **4**, ORCID 0000-0001-7485-3231. 2. Balagurov Anatoly Mikhailovich, Prof., Doctor of Physical and Mathematical Sciences, H-index = 37, Scopus ID 7006758479
List of publications with links to them	**1. Mukhametuly, B.,** Bobrikov, I.A. Balagurov, A.M. «Neutron diffraction analysis of the microstructure of dispersion-hardening steels» Physics of Metals and Metallography Volume 117, Issue 10, 1 October 2016, Pages 1047-1053. (https://doi.org/10.1134/S0031918X16100045) (Q4, IF= 0.877, Процентиль – 55%) **2.** Balagurov, A.M., Bobrikov, I.A. **Mukhametuly, B.**, Sumnikov, S.V, Golovin, I.S. Coherent cluster atomic ordering in the Fe-27Al intermetallic compound. JETP Letters Volume 104, Issue 8, 1 October 2016, Pages 539-545.

	(https://doi.org/10.1134/S0021364016200078), (Q3, IF= 1.532, Процентиль – 55%) **3.** **Mukhametuly, B.,** Bokuchava G.D., Papushkin I.V., Sumin V.V., Aznabayev D. Microstrain in Dispersion-Hardened Steels. Physics of Particles and Nuclei Letters Volume 10, Issue 2, March 2013, Pages 157-161. (https://doi.org/10.1134/S1547477113020040) (Q4, IF= 0.527, Процентиль – 55%) **4.** **B. Muhametuly**, S. E. Kichanov, E. A. Kenzhin, D. P. Kozlenko, K. M. Nazarov, A. A. Shaimerdenov, E. Bazarbaev, E. V. Lukin. Concept of the Facility of Neutron Radiography and Tomography at the Research Reactor WWR-K in Almaty, Kazakhstan Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques. 13, 877–879 (2019). (https://doi.org/10.1134/S1027451019050082), (Q3, Процентиль – 21%) **5.** K.M.Nazarov, **B.Mukhametuly**, S.E.Kichanov, T.K.Zholdybayev, A.A.Shaimerdenov, K.B.Karakozov, D.S.Dyussambayev, M.T.Aitkulov, M.Yerdauletov, P.Napolskiy, M.Kenessarin, E.K.Kalymkhan, N.A.Imamverdiyev, S.H.Jabarov, Non-destructive analysis of materials by neutron imagin gat the TITAN facility, Eurasian Journal of Physics and Functional Materials, 2021, 5(1), стр. 6–14. DOI:10.32523/ejpfm.2021050101 (Q4, Процентиль – 14%) **6.** K.Nazarov, **B.Muhametuly,** E.A.Kenzhin, S.E.Kichanov, D.P.Kozlenko, E.V.Lukin, A.A.Shaimerdenov. New neutron radiography and tomography facilityat theWWR-K reactor, Nuclear Instruments and Methodsin Physics Research Section A. 2020, V.982,164572. (https://doi.org/10.1016/j.nima.2020.164572), (Q2, IF= 1.455, Процентиль – 59%) **7.** **B.Muhametuly**, D.P.Kozlenko, E.A.Kenzhin, S.E.Kichanov, E.V.Lukin, A.A.Shaimerdenov, K.Nazarov, B.N.Savenko. The First Scientific Results Obtained Using the Experimental Setup for Neutron Radiography and Tomography at the WWR-K Reactor, JINR News, 2020, No.1, p.20-23. DOI: 10.13140/RG.2.2.15838.38721 **8.** Bauyrzhan A.B., Koltochnik S.N., Aitkulov M.T., **Mukhametuly B**., Burtebaev N.T., Neutron-physical parameters at the outlet of the WWR-K reactor beam tube, Eurasian Journal of Physicsand Functional Materialsthis link is disabled, 2019,3(3), стр. 219–225. https://doi.org/10.29317/ejpfm.2019030303 (Q4, Процентиль – 14%) K. M. Nazarov, S. E. Kichanov, E. V. Lukin, I. Yu. Zel, D. P. Kozlenko, T. K. Zholdybayev, **B. Muhametuly**, M. Kenessarin, A. V. Rutkauskas, A. Yskakov, M. O. Belova.,

	A comparative study of promising filter materials for neutron imaging facilities, Eurasian Journal of Physicsand Functional Materialsthis link is disabled, 2021, Vol 5, No 4 стр. 169–180. DOI: 10.32523/ejpfm.2021050401, (Q4, Процентиль – 14%)
Patents	-