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ֆիզիկամաթեմատիկական գիտությունների թեկնածուի
գիտական աստիճանի հայցման ատենախոսություն

ՍԵՂՄԱԳԻՐ

ԵՐԵՎԱՆ 2026

INSTITUTE OF APPLIED PROBLEMS OF PHYSICS

SHAHVERDYAN ARUS

DYNAMIC DIFFRACTION OF X-RAYS AND THERMAL NEUTRONS IN THE PRESENCE OF TEMPERATURE GRADIENT AND ACOUSTIC WAVES IN SINGLE CRYSTALS

Thesis for the degree of Candidate of Physical and Mathematical Sciences
Specialty 01.04.07- “Condensed Matter Physics”

ABSTRACT

YEREVAN 2026

Ատենախոսության թեման հաստատվել է Ֆիզիկայի կիրառական պրոբլեմների ինստիտուտում

Գիտական ղեկավար՝ ֆիզ.-մաթ. գիտ. թեկնածու **Վ. Ռ. Քոչարյան**

Պաշտոնական ընդդիմախոսներ՝ ֆիզ. մաթ. գիտ. դոկտոր, պրոֆեսոր,
Արամ Ազատի Սահարյան
ֆիզ. մաթ. գիտ. թեկնածու,
Վահրամ Պատվականի Մկրտչյան

Առաջատար կազմակերպություն՝ «Ա. Ի. Ալիխանյանի անվան ազգային գիտական լաբորատորիա» (ԵՖԻ) հիմնադրամ

Ատենախոսության պաշտպանությունը կայանալու է 2026թ. օգոստոսի 27-ին ժամը 12:00-ին Ֆիզիկայի կիրառական պրոբլեմների ինստիտուտի 053 Մասնագիտական խորհրդի նիստում: Հասցեն՝ ք. Երևան 0014, Հր. Ներսիսյանի փ. 25:

Ատենախոսությանը կարելի է ծանոթանալ ՖԿՊԻ գրադարանում:
Սեղմագիրն առաքված է 2026թ. հուլիսի 23-ին:

Մասնագիտական խորհրդի գիտական քարտուղար ֆիզ.-մաթ.գիտ.թեկնածու **Հ.Ֆ. Խաչատրյան**

The thesis theme is approved at the Institute of Applied Problems of Physics

Scientific supervisor: Candidate of Phys. Math. Sciences **V.R. Kocharyan**

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Aram Azat Saharian
Candidate of Phys. Math. Sciences
Vahram Patvakan Mkrtchyan

Leading organization: "A. I. Alikhanyan National Science Laboratory (Yerevan Physics Institute)" foundation

The thesis defense will take place at 12:00 on August 27, 2026, during the session of Specialized Council 053 of the Institute of Applied Problems of Physics. Address: 25, Hr. Nersessian Str., Yerevan 0014, Republic of Armenia.

The thesis is available in the Institute of Applied Problems of Physics library.
The abstract was distributed on 23 July 2026

Scientific secretary of the Specialized Council Candidate of Phys. Math. Sciences **H. F. Khachatryan**

GENERAL DESCRIPTION OF THE THESIS

Relevance of the work: Investigation methods using electromagnetic waves and neutron beams with wavelengths on the order of angstroms are employed in a wide variety of fundamental, scientific-technical, and applied problems. They allow to study of the internal structure of various materials and systems, including biological, organic, and microelectronic components. The solution of these problems requires rapid control of beam parameters during experiments, such as selecting primary beam energy, adjusting the angular position of beam propagation, and performing focusing or defocusing. Typically, these tasks are performed using specialized goniometric systems or pre-fabricated mirrors with specific geometries. In other words, changing any beam parameter requires reconfiguring the experimental setup, where the speed of mechanical system adjustments severely limits the time efficiency.

External influences with controllable parameters, such as acoustic oscillations, temperature gradients, and static electric fields, applied to single crystals, can provide high-speed methods for reshaping or reconfiguring X-ray and neutron beams. Research devoted to revealing the peculiarities of the intensity redistribution of reflected X-ray beams in crystal lattices under the influence of external acoustic waves or specific thermal fields is of great importance. Several new phenomena have been discovered, in particular, the phenomenon of full pumping from the transmitted direction to the reflected direction, as well as the control of energy, spectral width, and focal length of reflected X-ray beams. This creates significant opportunities for the design and development of X-ray and neutron optical elements with controllable parameters. From this perspective, research aimed at the effective control of short-wave radiation characteristics such as energy, monochromaticity, focal length, and angular divergence is both important and relevant.

The aim of the thesis: The main objective of the work is to investigate the crystal lattice deformations arising from external acoustic waves or specific temperature distributions in single crystals and the formation of a dynamic scattering wave field of hard X-ray radiation and thermal neutrons in these lattices. Specifically:

- To investigate the parameters of diffracted X-ray beams in single crystals of the biphthalate family under the influence of acoustic waves.
- To investigate the peculiarities of X-ray beam intensity redistribution in quartz single crystals in the presence of orthogonal acoustic waves.

- To investigate the parameters of X-ray beams reflected under Laue diffraction geometry in single-crystal plates of different cuts under a temperature gradient applied perpendicular to the same atomic planes.
- To investigate the focusing phenomena of reflected thermal neutrons and X-rays in quartz single crystals with weak deformations.

To achieve this objective, the following practical tasks were solved:

— Generation of monochromatic X-ray beams with $\Delta\theta \approx 5''$ angular divergence and $\Delta\lambda/\lambda \approx 10^{-5}$ energy dispersion, as well as collimated polychromatic beams with $\Delta\theta \approx 10'' \div 30''$ angular divergence.

— Preparation of flat single-crystal plates in the form of rectangular parallelepipeds with high-quality processed surfaces, various orientations relative to crystallographic axes (cuts), and thicknesses, with conductive layers deposited on their surfaces.

— Development and fabrication of various crystal holders for the simultaneous excitation of orthogonal acoustic waves and the application of corresponding temperature gradients in piezoelectric crystals.

Scientific novelty: It has been experimentally shown that:

- Crystals of the biphthalate family excited by acoustic waves can be used as elements of controllable X-ray optics, particularly for obtaining intensity-modulated radiation.
- By simultaneously exciting longitudinal and transverse acoustic waves in a quartz single crystal, it is possible to control both the intensity and the propagation direction of a reflected X-ray beam. It is particularly important to note that independent transverse acoustic waves allow for intensity control, while longitudinal waves enable control of the reflected beam's direction.
- In crystal samples with different cuts, the parameters of the deformation field formed under the same temperature gradient values applied perpendicular to the $(10\bar{1}0)$ reflecting atomic planes differ significantly. Specifically, the bending radius of the atomic plane in an X-cut crystal is always significantly smaller than in a Z-cut crystal.
- Under the same temperature gradient values, an X-cut quartz single crystal allows pumping an X-ray beam from the primary direction to the reflected direction with greater energy and angular aperture (up to 2 times) compared to a Z-cut crystal.

Theoretical research has shown that:

- In a deformed lattice of a single crystal caused by a temperature gradient, Bragg diffraction of thermal neutrons under Laue geometry leads to a significant increase in the reflected beam intensity and beam compression (focusing).
- By changing the crystal lattice deformation parameter, it is possible to control the intensity and focal length of the reflected beam.

Practical importance: The obtained results can be used for exciting acoustic waves in piezoelectric crystals, studying their parameters, investigating deformations in single crystals, analyzing the processes of chemical reactions, and creating optical elements for X-ray radiation and neutrons. Furthermore, they are applicable in X-ray lithography, condensed matter physics, X-ray spectroscopy, microscopy, X-ray diagnostics, and other applied fields.

The basic results to be defended are as follows:

- First-time investigation of the behavior of diffracted X-ray beams as a function of the amplitude of an acoustic wave excited along the thickness of biphthalate family single crystals, demonstrating their potential as elements for controllable X-ray optics for intensity-modulated radiation.
- First-time investigation of X-ray diffraction from atomic planes in a quartz single crystal under simultaneous kHz and MHz acoustic waves under Laue geometry. It is shown that by varying the amplitude of transverse (MHz) acoustic waves, one can control reflected beam intensity and monochromaticity, while varying longitudinal (kHz) wave amplitude controls the beam direction.
- Experimentally investigated the peculiarities of deformation fields and X-ray reflection parameters in X-cut and Z-cut quartz plates under temperature gradients, it is shown that X-cut crystals are more efficient for controlling X-ray parameters than Z-cut crystals.
- A new type of X-ray spectrometer with controllable parameters (resolution, luminosity) was developed, which made it possible to increase the resolution up to 2 times compared to other spectrometers.
- The dependence of the diffraction focusing behavior of thermal neutrons in weakly deformed single crystals on the radius of curvature of the reflecting planes was theoretically studied. It was shown that, depending on the radius of curvature, the focus

inside the crystal shifts toward the exit surface, while outside the crystal, it shifts in the opposite direction.

Presentation of the Work: The results presented in the thesis have been reported and discussed at international conferences: «Electron, Positron, Neutron and X - Ray Scattering under External Influences», Yerevan-Meghri: 2015, 2017, 2019, 2021, 2023, 2025; «Электронно-лучевые технологии и рентгеновская оптика в микроэлектронике-КЭЛТ», Черноголовка- Россия 2021; «1st, II and III, IV International Scientific School–Conferences on Acoustophysics named after Academician A. R. Mkrtchyan», Yerevan – Sevan, Armenia, 2022, 2023, 2024, 2025; International Symposium «Radiation from Relativistic Electrons in Periodic Structures», RREPS, 2023; «Charged & Neutral Particles Channeling Phenomena», Channeling-2023, as well as in general and laboratory seminars at the Institute of Applied Problems of Physics of the NAS of the Republic of Armenia.

Publications: The main results of the thesis are published in 22 works: 8 scientific articles and 14 conference proceedings.

Structure and Volume: The thesis consists of an introduction, four chapters, and a conclusion, totaling 118 pages, including 20 figures and a list of 105 references.

CONTENT OF THE THESIS

In the Introduction, the relevance of the thesis topic is substantiated, and the objective of the research work, its scientific novelty, practical significance, and the main provisions presented for defense are formulated.

The first chapter presents a detailed analysis of the literature on X-ray diffraction phenomena from crystals subjected to external static (temperature gradient, uniaxial compression, etc.) and dynamic (bulk and surface acoustic waves) influences. A brief overview of theoretical and experimental research related to the topic and an analysis of existing scientific results are presented. Some theoretical foundations are also presented, based on which research related to the presented dissertation was conducted.

In the second chapter, several peculiarities of the spatio-temporal parameters of X-ray beams formed as a result of Laue geometry Bragg diffraction in various single crystals under the influence of external acoustic waves are investigated.

In the first paragraph of this chapter, to expand the possibilities for obtaining controllable X-ray beams and to search for new materials, the peculiarities of the intensity redistribution of diffracted radiation from potassium and rubidium biphthalate crystals under acoustic oscillations were investigated. X-ray diffraction studies of the crystal samples were conducted on a TRS laboratory diffractometer using a two-crystal scheme (see Fig. 1). Their amplitude-frequency characteristics were measured, and the resonant frequencies of the electromagnetic signals from the generator for exciting thickness-mode acoustic oscillations were determined: for rubidium biphthalate f_1 = 737.288 kHz and for potassium biphthalate f_2 = 794.648 kHz:

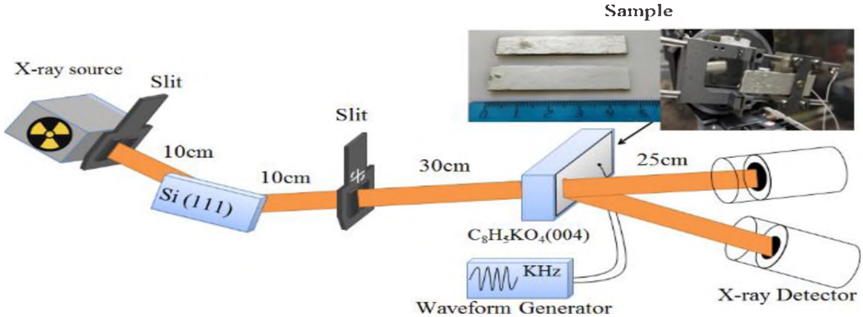

Fig. 1. Experimental setup and photographs of the samples, as well as the sample installed on the diffractometer with its holder.

During the investigation, the dependence of the intensity of X-ray beams reflected from the (004) atomic planes of potassium and rubidium biphthalate crystals on the crystal rocking angle around the precise Bragg angle was recorded in the presence of acoustic oscillations with different amplitudes in the crystals.

The dependencies shown in figure 2 indicate that the peak value of the rocking curve increases by one and a half to two times in the presence of acoustic oscillations, while no change in the shape of the rocking curve is observed. For the rubidium biphthalate crystal, the half-width of the rocking curve also remains unchanged. This indicates that there is a pumping from the transmitted direction to the reflected direction. In this regard, the single crystal of rubidium biphthalate stands out, for which intensity redistribution from the transmitted to the reflected direction is observed without broadening of the rocking curve, which can be used for obtaining intense, monochromatic, and modulated X-ray beams.

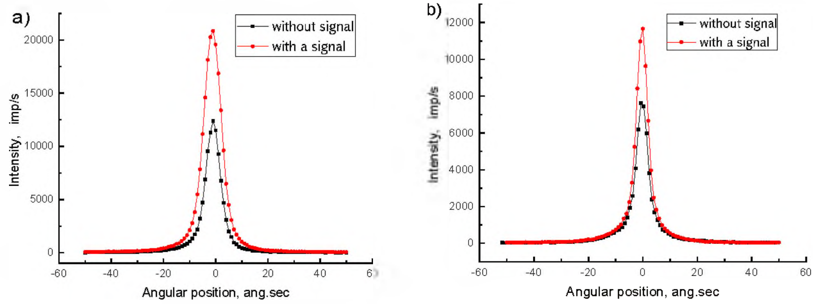

Fig. 2. Dependence of the intensity of X-ray radiation reflected from the (004) atomic planes of potassium (a) and rubidium (b) biphthalate crystals on the crystal rocking angle around the Bragg angle (1) in the absence and (2) in the presence of acoustic oscillations.

In the second paragraph, for the purpose of controlling the intensity and propagation direction of X-ray beams, the rocking curves of X-ray beams reflected from the $(11\bar{2}0)$ atomic planes of a quartz single crystal under Laue geometry were investigated from different regions of the crystal. Their behavior was studied in the absence of acoustic waves, in the presence of thickness-mode and length-mode acoustic waves, and simultaneously in the presence of acoustically excited oscillations along both length and thickness.

As seen in figure 3, the investigations show that the presence of length-mode acoustic oscillations in the single crystal leads to a change in the half-width of the rocking curve of the $(11\bar{2}0)$ reflecting atomic planes. The magnitude of this change depends on the region of beam incidence on the crystal, and the rocking curve is widest in the regions of oscillation where the interplanar distances change the most. In the case of thickness-mode acoustic oscillations, the opposite picture is observed: bending of the reflecting atomic planes occurs, which leads to a change in intensity (increase), while the reflection angle and the half-width of the rocking curve do not change. From curve 4, it is evident that in the presence of simultaneous length and thickness-mode orthogonal acoustic oscillations in the crystal sample, the behavior of the rocking curve half-width change along the crystal is the same as in the case of only length-mode acoustic oscillations (curve 2). This indicates that longitudinal acoustic waves are responsible for the change in the half-width of rocking curves, leading only to a change in interplanar distance, while transverse acoustic waves are responsible for the bending of the reflecting atomic planes, leading to a 2 to 3-fold increase in the intensity of the reflected beam.

Therefore, the obtained results indicate that a system with a resonator-crystal configuration allows for simultaneous excitation of acoustic waves along both thickness and length in a quartz single crystal, and simultaneously controls the intensity and direction of the reflected X-ray beam. Moreover, independent transverse acoustic waves allow for intensity control of the beam, while longitudinal acoustic waves control the direction of the reflected beam.

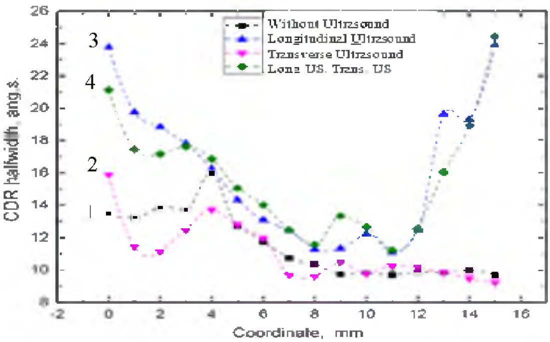

Fig. 3. Half-widths of rocking curves obtained from different regions of a quartz single crystal: (1) without acoustic waves; (2) with transverse acoustic waves; (3) with longitudinal acoustic waves; (4) with orthogonal acoustic waves.

In the third paragraph, for the purpose of developing and creating acousto-optic elements for simultaneous and effective control of X-ray radiation spatiotemporal parameters, the behavior of the intensity and rocking curves of X-ray beams reflected from $(10\bar{1}1)$ atomic planes under Laue geometry, depending on the parameters of orthogonal acoustic waves excited in a quartz single crystal, were investigated. A crystal-resonator with a special structure (Fig. 4a) was prepared on a 38x10x1 mm^3 quartz single crystal of X-cut to excite acoustic oscillations in mutually perpendicular directions. To ensure independent control of the parameters of acoustic waves excited in mutually perpendicular directions, the surfaces of the single crystal were coated with two pairs of conductive contacts: one pair was used for exciting length-mode acoustic oscillations, and the other pair for exciting thickness-mode acoustic oscillations. The results of the investigation showed that such a crystal-resonator allows for the simultaneous excitation of two independent mutually perpendicular acoustic waves and provides independent control of the parameters of these oscillations in the MHz and kHz ranges. In the investigation of the behavior of the intensity and rocking curves of X-ray beams reflected from $(10\bar{1}1)$ atomic planes under Laue geometry, depending on the parameters of orthogonal acoustic waves excited in a quartz single crystal, it was observed that X-ray-acoustic redistribution occurs, manifested by an increase in the diffracted radiation intensity due to the formation of thickness-mode standing acoustic waves, as well as an increase in the rocking curve half-width (obtaining a double-peak rocking curve) caused by the formation of standing waves during length-mode oscillations in the crystal.

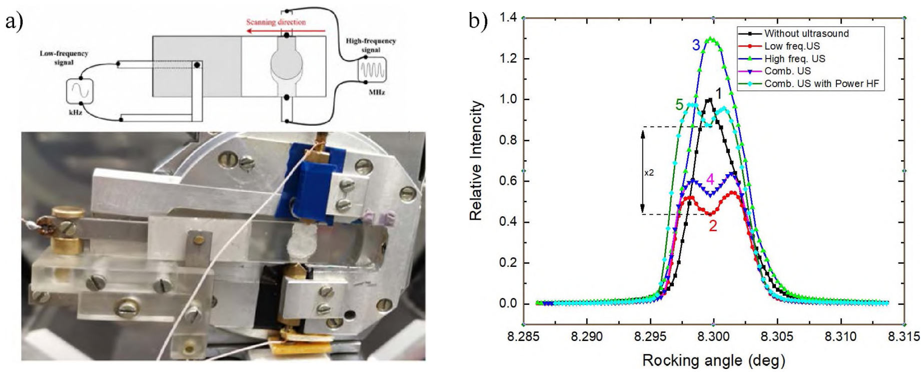

Fig. 4. (a) Crystal-resonator for exciting acoustic oscillations in mutually perpendicular directions, and (b) rocking curves of X-ray reflection from $(10\bar{1}1)$ atomic planes of a quartz single crystal: 1) without oscillations, 2) only with length-mode oscillations (oscillation frequency 132.1 kHz, voltage 45V), 3) only with thickness-mode oscillations (oscillation frequency 2.7744 MHz, voltage 35V), 4) with orthogonal oscillations (signals with a frequency of 2.7744 MHz at a voltage of 35V and a frequency of 132.1 kHz at a voltage of 45 V), and 5) with orthogonal oscillations but a larger amplitude of thickness-mode oscillations (signals with a frequency of 2.7744 MHz at a voltage of 100V and a frequency of 132.1 kHz at a voltage of 45V).

As a result, thickness-mode acoustic oscillations allow for control of the intensity of the reflected X-ray beam, while length-mode acoustic oscillations allow for control of the reflection angle of the X-ray beam. Thus, the first working prototypes of combined X-ray optics elements have been developed, fabricated, and proposed.

The third chapter investigates the peculiarities of Laue geometry diffraction in quartz single crystals of different cuts under the influence of an external temperature gradient, as well as the development of methods for determining the spectral decomposition of reflected X-ray beams and deformations induced in the crystal.

In the first paragraph, the bending behavior of $(10\bar{1}0)$ atomic planes in rectangular X-cut (t=5.72mm) and Z-cut (t=6.7mm) quartz single-crystal samples under a temperature gradient were studied using X-ray diffractometric methods. The goal of the research was to determine which quartz crystal cut should be selected, based on the anisotropy of thermal conductivity and thermal expansion coefficients, to achieve greater deformations at lower temperature gradient values. The experiment was performed using an X-Ray tube with an Ag-anode, operating at a voltage of 38keV and an anode current of 22mA.

The experiments were performed in Laue symmetric geometry of Bragg diffraction, using a collimated polychromatic X-ray beam as the primary beam. Figure 5 illustrates the experimental setup and a schematic view of the prepared samples. The experimental results showed that, due to thermal conductivity anisotropy in quartz samples of different crystallographic cuts, the deformation field parameters (the radius of curvature of reflecting atomic planes and the difference in interplanar distances) differ significantly at the same temperature distribution on the heated surfaces parallel to the reflecting $(10\bar{1}0)$ planes.

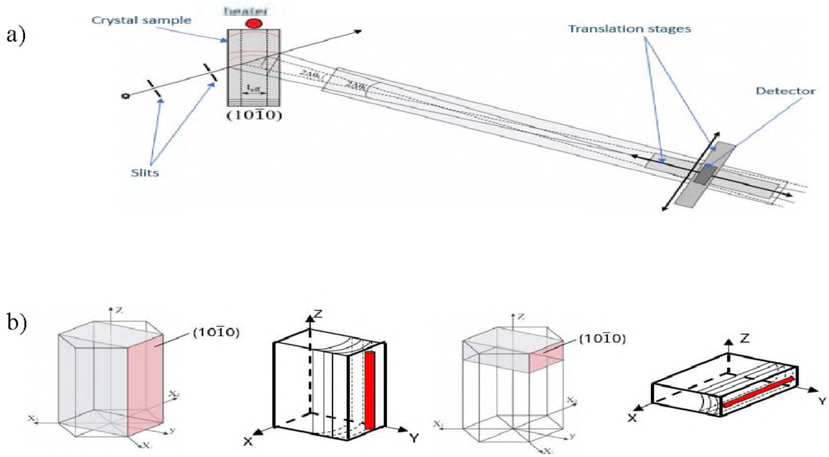

Fig. 5. a) Experimental scheme; b) Schematic representation of the prepared samples.

Specifically, the radius of curvature of the $(10\bar{1}0)$ atomic planes in the X-cut crystal is significantly smaller than that in the Z-cut crystal (Fig. 6). The focal lengths of the polychromatic X-ray radiation ($AgK\alpha_1$, $AgK\alpha_2$) diffracted from X-cut and Z-cut samples differ: focal lengths for the X-cut are shorter than those for the Z-cut. These focal lengths depend not only on the radius of curvature of the reflecting atomic planes but also on the difference in interplanar distances in the formation region of the AgKα_1 and AgKα_2 beams.

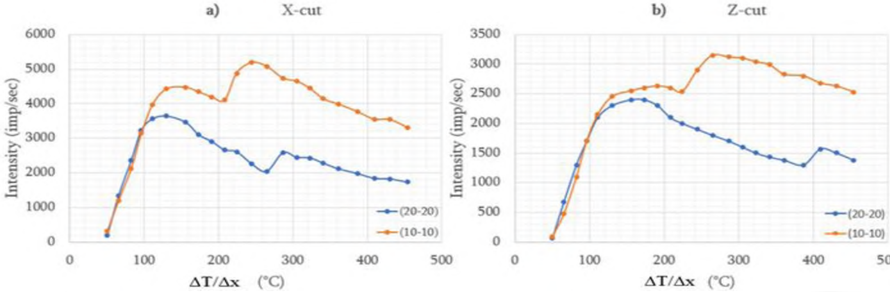

Fig. 6. Dependence of the integral intensity of X-ray radiation reflected from the $(10\bar{1}0)$ and $(20\bar{2}0)$ atomic planes of X-cut (a) and Z-cut (b) quartz crystals on the temperature gradient.

In the second paragraph, the diffraction peculiarities of a narrowly collimated X-ray beam in a quartz single crystal under a temperature gradient were studied in detail. For the X-cut quartz single crystal, the greater bending of $(10\bar{1}0)$ atomic planes at smaller temperature gradient values, combined with the possibility of reflecting different wavelengths (AgKα_1 and AgKα_2) in Laue geometry for a narrow-collimated beam, provide a foundation for developing a new type of X-ray spectrometer with controllable parameters (resolution, luminosity). For this purpose, an X-cut quartz single-crystal ($35\times32\times6.77$ mm^3) sample was studied. The temperature gradient was applied perpendicular to the mentioned planes using a nichrome coil (up to 700°C). The experiments were carried out in Laue symmetric geometry using a collimated polychromatic X-ray beam.

The intensity distribution of the diffracted beams was recorded using a coordinate detector. Fig. 7 shows the intensity distributions in cross-sections of the X-ray beam for the $(10\bar{1}0)$ reflections from a quartz single crystal for different values of the thermal gradient at distances of 134 cm and 180 cm from the crystal exit surfaces.

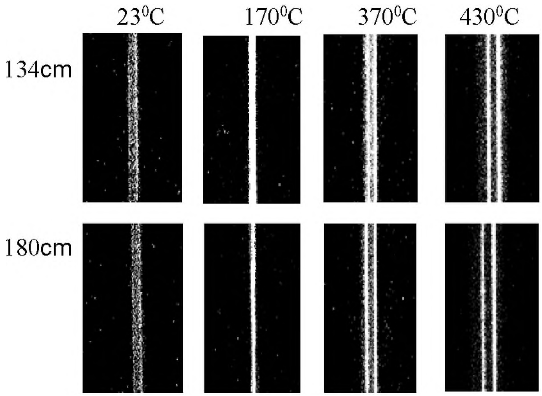

Fig. 7. Topograms of the X-ray beam reflected from the atomic planes of a quartz single crystal $(10\bar{1}0)$ for different values of the temperature gradient and different distances.

The presence of the temperature gradient in the crystal leads to bending of the $(10\bar{1}0)$ planes and it’s increases leads to decrease of the radius of the curvature, which leads to the satisfaction of the Bragg condition for $AgK\alpha_2$ radiation as well. A significant narrowing of the transverse cross-section of the reflected beam was observed, indicating a limitation of the diffraction region. This allows for the extraction of specific wavelength beams from the X-ray spectrum from different regions of the beam propagation direction inside the crystal.

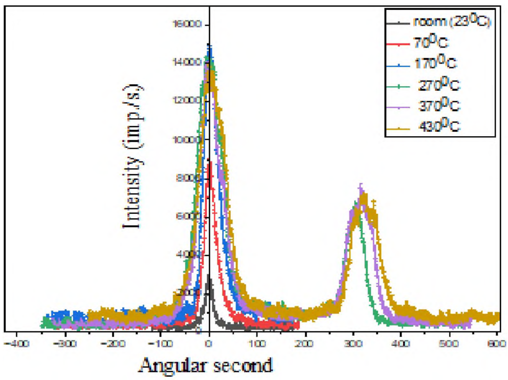

Fig. 8. X-ray the rocking curves obtained from the crystal analyzer for different values of crystal edge temperature (room temperature (23⁰C), 70⁰C, 170⁰C, 270⁰C, 370⁰C և 430⁰C)

For a more detailed analysis of spectral decomposition, an X-cut 0.29 mm thick quartz crystal analyzer was used (in a two-crystal (n, n) scheme) at a distance of 55cm from the crystal sample. Rocking curves were recorded using a rotating stepping platform with an accuracy of

0.7″. Figure 8 shows the rocking curves obtained for different values of the temperature gradient in the crystal, from which the angular divergence and angular distances between characteristic lines reflected from the crystal sample (the first single crystal) were measured for different gradient values. Expressions for the spectral width ($\frac{\Delta\lambda}{\lambda} \approx \frac{t\,\mathrm{ctg}\theta_0}{R}$), linear dispersion ($\frac{\Delta\ell}{\Delta\lambda} = \frac{2R\tan^2\theta}{\lambda}$), and angular dispersion ($\frac{\Delta\theta}{\Delta\lambda} = \frac{2\tan\theta}{\lambda}$) of the resolved beam were derived. It was shown that the spectral width of the resolved beam significantly depends on the sample thickness (t) and the radius of curvature (R) of the reflecting atomic planes. Linear dispersion depends directly on the deformation parameter, while angular dispersion is independent of deformation. Based on the obtained results, a new type of X-ray spectrometer with controllable characteristics (resolution, luminosity) was developed, enabling an increase in resolution by up to 2 times compared to other spectrometers.

The fourth chapter is dedicated to theoretical research concerning the problems of dynamical diffraction of thermal neutrons and X-rays. Paragraphs one through four of the fourth chapter present the results of research dedicated to the problem of dynamical X-ray diffraction from a point source in a crystal lattice with a continuous and weak deformation field. These results are based on the integral formulation of solutions represented via the Green-Riemann function for hyperbolic differential equations, which describe the propagation of scattered X-ray wave amplitudes within the crystal lattice. The conditions for the diffraction focusing of one of the wave modes both inside the crystal and in the vacuum outside the crystal have been examined.

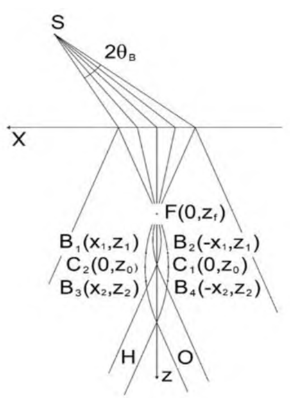

Fig. 9. Schematic representation of the diffraction field of a crystal lattice and the corresponding characteristic points: $F(0,z_f)$ - focal point; $B_1(x_1, z_1)$ and $B_2(-x_1, z_1)$ are the points of approach to the Bragg condition of the corresponding wave components; $B_3(x_2, z_2)$ and $B_4(-x_2, z_2)$) are the points of departure from the Bragg condition of the corresponding wave components, $C_1(0, C_2(0, z_0)$ are the points satisfying the exact Bragg condition.

The principles of formation of the dynamical X-ray diffraction field from a point source in a crystal lattice with a continuous and slowly varying deformation field were examined, and several characteristic parameters of this field were calculated (Fig. 9).

Specifically, the depth of focusing within the lattice is $z_f = \frac{L_{ef}}{\gamma}$, where $\gamma = \frac{\pi k \sin\theta_B \sin 2\theta_B}{|\sigma|}$, $L_{ef} = \frac{\pi l_1 k \sin^2 2\theta_B}{\pi k \sin^2 2\theta_B - l_1 |q|}$, $q = \frac{\pi h}{R}$. The depth Δz_0 at which a beam with an angular deviation of $\Delta\theta$ from the Bragg condition in the initial beam will appear at an angular position exactly satisfying the Bragg condition is $\Delta z_0 = 2Rcos^2\theta_B \Delta\theta_B$. The difference in depths Δz at which a beam with a given angular deviation $\Delta\theta$ enters and exits the angular range of Bragg reflection is $\Delta z = \frac{|\chi_{hr}|\, R\, cos\theta_B}{2}$. As $R \to 0$ (strong deformations), both parameters approach zero.

This indicates that the turning points of the trajectories move toward the entrance surface of the crystal, and the spatial displacements of beams with different energies are determined by the condition $\delta x = \frac{l\, tan\theta_B}{\lambda\, cos^2\theta_B} \delta\lambda$.

Within the framework of Takagi's equations, which describe the propagation of transmitted and reflected wave amplitudes in the lattice, analytical solutions are provided for the dependence of the diffraction field amplitudes on deformation parameters. The angular width of the reflected X-ray radiation and its dependence on the single-crystal thickness were studied. It was shown that as the deformation increases, the crystal rocking curves gradually broaden, and their maximum intensity increases, reaching unity (the case of complete transfer). With further increases in the deformation of the reflecting planes, the rocking curves continue to broaden, and their maximum slowly decreases. It was also shown that in the case of complete transfer, the angular width of the X-ray beams is directly proportional to the thickness of the crystal sample. A theoretical interpretation for all observed phenomena was provided, based on Takagi's equations and the eikonal approximation. Figs. 10 and 11 present the spatial distributions of relative intensity in the reflected beam in the lattice and vacuum at focal planes, at different depths within the lattice, and at different recording distances in vacuum. The problem of wave-field formation in the dynamical diffraction of X-rays in a crystal lattice with continuous, weak deformations was considered when the diffraction vector is parallel or antiparallel to the temperature-gradient vector.

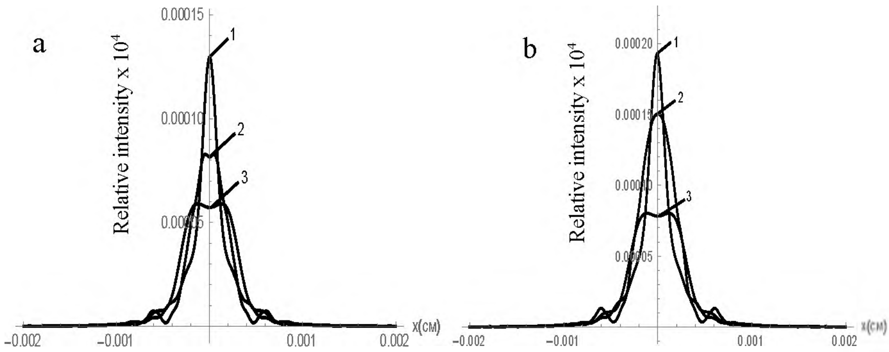

Fig. 10. The spatial distribution of the relative intensity of reflected radiation within the crystal at different depths: a. q=0. 1) z=0.0137 cm, 2) z=0.02 cm, 3) z=0.01cm; b. $q=10m^{-1}$. 1) z=0.0137 cm, 2) z=0.02 cm, 3) z=0.01 cm.

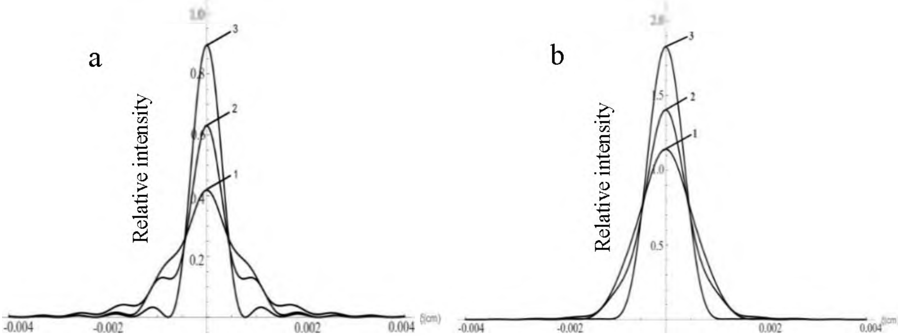

Fig. 11. The spatial distribution of the relative intensity of the reflected beam at different distances from the crystal in the recording plane: a. q=0. 1) L=5,29m, 2)L=3,29m, 3)L=8,29m; b. $q=10m^{-1}$. 1)L=5,29m, 2)L=3,29m, 3)L=8,29m.

The final three paragraphs address the problem of dynamical diffraction of thermal neutrons from a point source in a crystal lattice with a weak deformation field. The study is based on the asymptotic representation of the Green-Riemann function for hyperbolic Hamilton-type equations, which describe the propagation of quasi-amplitudes of scattered thermal neutrons within the crystal lattice. The conditions for the focusing of one of the wave modes in the crystal lattice are examined. The fundamental parameters of the focal spots within the lattice were studied as a function of the distance between the thermal neutron source and the crystal. The behavior of these focal spot parameters was also analyzed in detail, depending on the deformation field parameter. Figure 12 displays simulated computer images of the formation of wave diffraction fields within the lattice

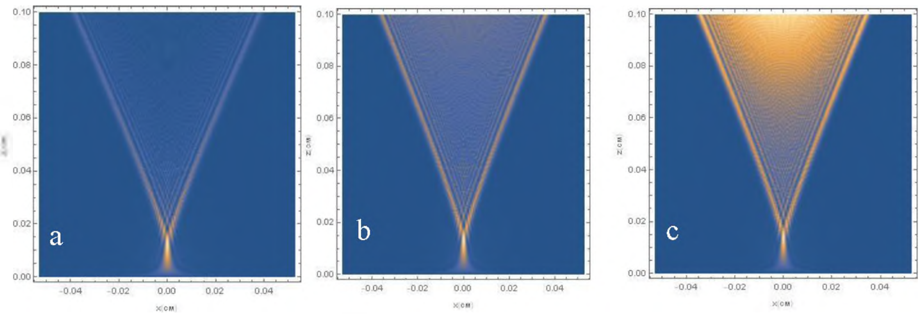

Fig. 12. Energy density distribution of the scattered thermal neutron field in the crystal. Source-crystal distance 10 m. a) $R \rightarrow \infty$ perfect lattice b) R=130m, c) R=80m

The interference fringes of the 'Pendellösung' solution are presented as V-shaped lines, resulting from the interference of the two modes of the reflected wave field. The vertices of these fringes point in opposite directions before and after focusing; that is, the interference fringes undergo inversion upon crossing the focal plane. Before the focal plane, converging neutron beams interfere, whereas after this plane, diverging beams interfere.

The mapping of the thermal neutron diffraction field in vacuum was performed using the first-Born approximation, which describes the formation of the field in vacuum based on the corresponding formulas for the diffraction field of the crystal lattice:

$$U_h^v(r) = -ik \iint_{-\infty}^{\infty} U_h^c(r') \frac{e^{ik|r-r'|}}{|r-r'|} dx'dy'$$

Integral formulations for the quasi-amplitudes of wave fields formed in vacuum were derived. Based on these formulas, further calculations were performed numerically, depending on various factors determining this distribution, particularly the distance L from the crystal plate to the registration plane and the radius of curvature R of the reflecting atomic planes. Figure 13 describes the dependence of the focal point shift, the diffraction compression of the beam wave front, and the broadening of the focal spot in the beam propagation direction on the radius of curvature R of the reflecting planes, at a given registration plane. The broadening of the focal spot is explained by the fact that a decrease in the radius R narrows the angular aperture of the reflected beam, which in turn leads to a spatial blurring of the focal point along the direction of wave propagation.

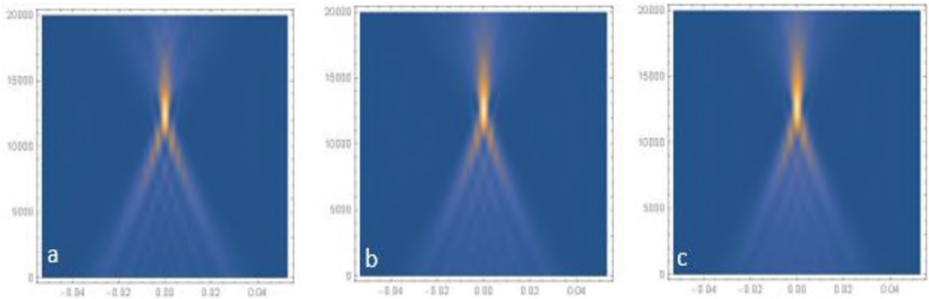

Fig. 13. Distribution of the energy density of the scattered thermal neutron field in vacuum. The source-to-crystal distance is 10 m. a) $R \to \infty$ perfect lattice b) R=130m, c) R=80m

CONCLUSION

- For the first time, the behavior of diffracted X-ray beams depending on the amplitude of the acoustic wave was investigated in single crystals of the biphthalate family under the conditions of Laue diffraction geometry, and it was shown that these crystals can be used as controllable X-ray optics elements, in particular, to obtain intensity-modulated X-ray radiation.
- For the first time, the peculiarities of the pumped diffracted X-ray beam and the crystal rocking curve in the presence of simultaneous kHz and MHz acoustic waves in a quartz single crystal have been investigated. The studies were carried out in Laue geometry for different atomic planes of X-cut and AT-cut crystals, and it was shown that by exciting transverse and longitudinal acoustic waves in a single crystal, the intensity and propagation direction of the reflected beam can be controlled independently of each other. In particular, by changing the amplitude of transverse (MHz) acoustic waves, the intensity and monochromaticity of the reflected beam can be controlled, and by changing the amplitude of longitudinal (kHz) acoustic waves, the direction of the reflected beam can be controlled.
- The characteristics of the reflected X-ray beam and the deformation field generated in the single crystal as a result of a temperature gradient applied perpendicular to the same atomic planes in X-cut and Z-cut quartz single crystal plates were investigated. It was shown that in the case of the X-cut single crystal, the control of the parameters of the reflected X-ray radiation (monochromaticity, focal length, angular aperture, energy width, and intensity) using the temperature gradient is more effective than in the case of the Z-cut crystal.
- A new type of X-ray spectrometer with controllable parameters (resolution and luminosity) has been designed and developed, providing up to 2 times increased resolution compared with conventional spectrometers.
- The diffraction focusing behavior of thermal neutrons and X-rays in weakly deformed single crystals, as well as the dependence of the energy exchange between the two modes of the reflected wave field on the radius of curvature of the reflecting planes, have been theoretically investigated. It has been shown that energy can be pumped from a strong absorbing field to a weak absorbing field depending on the magnitude and sign of the radius of curvature, although the V-shaped layers of the “pendulum solution” continue to be observed in the lattice as a result of the interference of these fields.
- It has also been shown that, in parallel with the increase in the radius of curvature, the focus of thermal neutrons inside the crystal shifts towards the exit surface of the crystal, and outside it shifts in the opposite direction.

LIST OF PUBLICATIONS ON THE TOPIC OF THE THESIS

1. K.G. Trouni, V.R. Kocharyan, D.E. Baghdasaryan, A.V. Shahverdyan. Diffraction Image of a Point Source of Slow Neutrons in a Weakly Deformed Crystal, Journal of Contemporary Physics (Armenian Academy of Sciences), 57 (3), 303-307 (2022) DOI:10.1134/S1068337222030161
2. A.E. Blagov, V.R. Kocharyan, Ya.A. Eliovich, A.V. Targonsky, A.E. Movsisyan, V.A. Korzhov, A.V. Shahverdyan, A.H. Mkrtchyan, M.V. Kovalchuk. X-Rays Diffraction by Excitation of Orthogonal Acoustic Oscillations in a Quartz Crystal, Journal of Contemporary Physics (Armenian Academy of Sciences), 57 (2), 192-197 (2022) DOI:10.3103/S1068337222020086
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4. Ya.A. Eliovich, V.R. Kocharyan, A.E. Blagov, A.V. Targonsky, V.A. Korzhov, A.E. Movsisyan, A.V. Shahverdyan, S.N. Noreyan, A.G. Mkrtchyan, M.V. Kovalchuk. Possibilities of Creating X-Ray Acoustic Elements from Bi-Phthalate Family Crystals with Thickness Vibrations, Journal of Contemporary Physics (Armenian Academy of Sciences), 58(4), 405-409 (2023) DOI:10.1134/S1068337223040096
5. A.V. Shahverdyan. Formation of a Diffraction Field During Dynamic Scattering of Slow Neutrons in a Deformed Crystal, Armenian Journal of Physics, 16, 136-139 (2023) DOI:10.54503/18291171-2023.16.4-136
6. K. Trouni, V. Kocharyan, S. Noreyan, D. Bagdasaryan, M. Mesropyan, V. Margaryan, A. Shahverdyan. Diffraction image of a narrow X-rays beam in crystals with weak deformation, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 1060, 169042 (2024) DOI:10.1016/j.nima.2023.169042
7. A.V. Shahverdyan, K.G. Trouni, V.R. Kocharyan. Dynamic diffraction of thermal neutrons in crystals with continuous deformation field, Journal of Instrumentation, 19 (06), C06014 (2024) DOI:10.1088/1748-0221/19/06/C06014
8. V.R. Kocharyan, T.G. Dovlatyan, V.V. Margaryan, Yu.M. Cherepennikov, A.E. Movsisyan, V.N. Aghabekyan, R.K. Mirzoyan, H.G. Margaryan, A.V. Shahverdyan, M.H. Mesropyan, S.N. Noreyan. X–ray diffraction in different crystal cuts under a temperature gradient, Radiation Physics and Chemistry, 243, 113654, (2026) DOI:10.1016/j.radphyschem.2026.113654

ԱՄՓՈՓԱԳԻՐ

- Առաջին անգամ դիֆրակցիայի Լաուէ երկրաչափության պայմաններում բիֆտալատի ընտանիքի միաբյուրեղներում ակուստիկ ալիքների առկայությամբ հետազոտվել է արդրադարձած ռենտգենյան փնջերի վարքը կախված ակուստիկ ալիքի ամպլիտուդից և ցույց է տրվել, որ այդ բյուրեղները կարող են կիրառվել որպես կառավարելի ռենտգենյան օպտիկայի տարրեր, մասնավորապես ստանալ ըստ ինտենսիվության մոդուլացված ռետգենյան ճառագայթում:
- Առաջին անգամ հետազոտվել է քվարցի միաբյուրեղում միաժամանակ կՀց-ային և ՄՀց-ային ակուստիկ ալիքների առկայության պայմաններում դիֆրակցված ռենտգենյան ճառագայթման վերամղման և բյուրեղի ճռման կորի առանձնահատկությունները: Հետազոտությունները իրականացվել են Լաուե երկրաչափության պայմաններում X-կտրվածքով և AT-կտրվածքով բյուրեղների տարբեր ատոմական հարթությունների համար և ցույց է տրվել, որ միաբյուրեղում գրգռելով լայնական և երկայնական ակուստիկ ալիքներ կարելի է միմյանցից անկախ կառավարել անդրադարձած փնջի ինտեսիվությունը և տարածման ուղղությունը: Մասնավորապես, լայնական (ՄՀց-ային) ակուստիկ ալիքների ամպլիտուդի փոփոխմամբ կարելի է կառավարել անդրադարձած փնջի ինտեսիվությունն ու մոնոքրոմատիկությունը, իսկ երկայնական (կՀց-ային) ակուստիկական ալիքների ամպլիտուդի փոփոխմամբ՝ անդրադարձած փնջի ուղղությունը:
- Հետազոտվել են X-կտրվածքով և Z-կտրվածքով քվարցի միաբյուրեղական թիթեղներում՝ նույն ատոմական հարթություններին ուղղահայաց կիրառված ջերմային գրադիենտի արդյունքում միաբյուրեղում առաջացած դեֆորմացիոն դաշտի և անդրադարձած ռենտգենյան ճառագայթման առանձնահատկությունները: Ցույց է տրվել, որ X-կտրվածքով միաբյուրեղի դեպքում անդրադարձած ռենտգենյան ճառագայթման պարամետրերի (մոնոքրոմատիկություն, ֆոկուսային հեռավորություն, անկյունային բացվածք, էներգետիկ լայնություն և ինտեսիվություն) կառավարումը ջերմային գրադիենտի օգնությամբ ավելի էֆեկտիվ է, քան Z-կտրվածքով բյուրեղի դեպքում:
- Մշակվել և ստեղծվել է կառավարելի պարամետրերով (լուծաչափ, լուսաուժ) ռենտգենյան սպեկտրոմետրի նոր տիպ, որը հնարավորություն է տալիս այլ սպեկտրոմետրերի նկատմամբ լուծաչափը մեծացնել մինչև 2 անգամ:
- Տեսականորեն հետազոտվել է թույլ դեֆորմացված միաբյուրեղներում ջերմային նեյտրոնների և ռենտգենյան ճառագայթման դիֆրակցիոն կիզակետման երևույթը: Հիմնվելով այն փաստի վրա, որ անդրադարձած և անցած ալիքային դաշտերի երկու մոդերի միջև էներգիայի փոխանակումը կախված է անդրադարձնող հարթությունների կորության շառավղից, ցույց է տրվել, որ կորության շառավղի մեծությունից և նշանից կախված ուժեղ կլանող դաշտից էներգիան կարող է փոխանցվել թույլ կլանող դաշտին, չնայած դրան ցանցում այդ դաշտերի ինտերֆերենցիայի արդյունքում շարունակվում են դիտվել «ճոճանակային լուծման» V-աձև շերտերը:
- Ցույց է տրվել նաև, որ բյուրեղի ներսում ջերմային նեյտրոնների ֆոկուսի տարածական դիրքը կախված է կորության շառավղից, որի մեծացմանը զուգահեռ այդ դիրքը տեղաշարժվում է դեպի բյուրեղի ելքի մակերևույթ, իսկ դրսում ֆոկուսը տեղաշարժվում է հակառակ ուղղությամբ:

ЗАКЛЮЧЕНИЕ

- Впервые в условиях дифракции в геометрии Лауэ в монокристаллах семейства бифталата исследовано поведение отражённых рентгеновских пучков в зависимости от амплитуды акустической волны. Показано, что эти кристаллы могут применяться в качестве элементов управляемой рентгеновской оптики, в частности, для получения рентгеновского модулированного по интенсивности излучения.
- Впервые исследованы особенности переброски дифрагированного рентгеновского излучения и кривой качания монокристалла кварца при одновременном воздействии акустических волн кГц-ого и МГц-ого диапазонов. Исследования проведены в условиях геометрии Лауэ для X-среза и AT-среза кристаллов, для различных атомных плоскостей, и показано, что при одновременном возбуждения в монокристалле поперечных и продольных акустических волн можно независимо друг от друга управлять интенсивностью и направлением распространения отражённого пучка. В частности, изменением амплитуды поперечных акустических волн можно управлять интенсивностью и монохроматичностью, а изменением амплитуды продольных акустических волн — направлением отражённого пучка.
- Исследованы особенности деформационного поля, возникающего в монокристаллических пластинах кварца X-среза и Z-среза под действием теплового градиента, приложенного перпендикулярно тем же атомным плоскостям, а также характеристики отражённого рентгеновского излучения. Показано, что для монокристалла X-среза управление параметрами отражённого рентгеновского излучения (степень монохроматичности, фокусное расстояние, угловая апертура, энергетическая ширина и интенсивность) с помощью теплового градиента эффективнее, чем для кристалла Z-среза.
- Разработан и создан новый тип рентгеновского спектрометра с управляемыми параметрами (спектральное разрешение, светосила), позволяющего увеличить спектральное разрешение в 2 раза по сравнению с другими спектрометрами.
- Теоретически рассмотрена задача о формировании дифракционного поля в слабо деформированном монокристалле. Анализированы условия дифракционной фокусировки тепловых нейтронов и рентгеновского излучения. Дана интерпретация явлению переброски энергии между волновыми модами и влияние обмена энергии между двумя модами при формировании дифракционного волнового поля. Показано, что в зависимости от величины и знака радиуса кривизны энергия от проходящего поля может передаваться к отраженному полю и наоборот. При этом в результате интерференции этих полей в решетке по-прежнему наблюдаются V-образные полосы «маятникового решения».
- Показано, что с увеличением радиуса кривизны атомных плоскостей фокусное пятно тепловых нейтронов внутри кристалла смещается к выходной поверхности кристалла, а изображение этого пятна вне кристалла — смещается в противоположном направлении.