

Federal Scientific Research Center "Crystallography and Photonics" Russian Academy of Science

(FSRC «Crystallography and Photonics» RAS)

Olga Alekseeva, *Director*

Moscow, Russia



Crystallography: stages of development

Starting as the mineralogical science, crystallography became an interdisciplinary science, where the achievements of chemistry, biology, physics, and geology are mixed and complementary.



Crystallography: stages of development

Shubnikov Institute of Crystallography – research ideology that is based on the "growth– structure–properties" triad with a deep relationship between these concepts. During 75 years our institute went the same way as the science of crystallography and now our research fields are including mineralogy, chemistry, chemical analysis, crystal growth, Xray diffraction analysis, physical materials science and also biology and protein crystallography.



FSRC «Crystallography and Photonics» RAS

- After the merger of the Institutes the main directions of scientific research has significantly expanded:
- Crystallography, Condensed Matter Physics, Materials Science;
- Physics and Technology of Nanomaterials and Nanostructures;
- Additive Technology;
- Structure and Function of Biomolecules and Supramolecular Complexes;
- Structural Diagnostics Methods with the use of X-ray and Synchrotron Radiation, Electrons, Neutrons, and Atomic Force Microscopy;
- Space Materials Science;
- Photonics, Photochemistry;
- Laser-Information Systems and Technologies;
- Products and Technology for Medical Application, Intelligent Systems for Medicine;
- Computer Optics, Adaptive Intelligent Vision Systems;
- Radio-, Acousto-, Optoelectronics, Optical and Microwave Communication systems;
- Pharmacology: Pharmaceutical Chemistry, Biopharmacy.

For most of these scientific areas the use of synchrotron radiation source is very important and gives new unique research opportunities.



Scientific research

 Methods for diagnostics of inorganic, organic and bioorganic materials, nanostructures using X-ray, synchrotron radiation and electrons: Development and Application







Scientific research

- 2. Studies of the structure and properties of nanomaterials using electrons and atomic force microscopy.
- 3. Processes of formation of crystalline materials, their defective structure and properties, including that at the extreme conditions of low and high temperatures; high and ultrahigh pressures.









S Kat A

FSRC "Crystallography and Photonics" RAS Shubnikov Institute of Crystallography IC RAS

Crystallization in space man-controlled or automatic – since 1976 till now

From inorganic crystals to proteins





«Crystallization micro-vat» program

Development of the equipment for crystal growth in space





Unit-3

here somhel Dryktission DJAXA



Design and manufacturing of Stations for Kurchatov synchrotron radiation source

for:

- Protein Crystallography "Belok"(Protein)
- Liquid/air Interfaces (Langmuir)
- X-ray crystallography and material science (XCMS)
- X-ray topography and tomography (X-TOM)
- X-ray diffraction analysis (XDA)



Under the scientific leadership of Prof. M. Kovalchuk







Development of X-ray diagnostics of inorganic, organic, bioorganic materials

X-ray diagnostics of multilayer systems Reflectivity and grazing angle diffraction



Small angle scattering Methods & Soft for data management



X-ray optics based upon crystals with acoustic vibrations Focusing, I scanning, stroboscopy



X-ray micro topo-tomo-graphy Equipment and methods



Epiphysis: a – normal, b– alcohol dependent.





Ultra fast X-ray imaging of scientific processes with on-line assessment and data-driven process control

Each full scan per 30 мsec.

In collaboration with: Prof. Marc Weber, Prof. T. Baumbach, V. Altapova, D. Hänschke,





FSRC "Crystallography and Photonics" RAS Image Processing Systems Institute IPSI RAS

Scientific research

- 1. Computer optics, nanophotonics, optical information technologies
- 2. Systems for image analysis and pattern recognition
- 3. Geoinformation technologies



Creation of nanophotonics components for light control



Processing of medical images and analysis of Big Data





FSRC "Crystallography and Photonics" RAS Institute of Photon Technologies IPT RAS

Scientific research

- Additive technologies for medicine.
- Optical data communication for supercomputers.
- Upconversion nanoparticles for medicine and photonics applications.
- Smart laser system for cardiosurgery.
- Supercritical fluid technologies.

Equipment developed at the IPT RAS

Smart laser cardiosurgery system



Spectroscopic refractometer for the refractive index measurements of liquids and solids.



Universal mini laboratory for the physical and chemical process study in supercritical fluids.



Systems for the biocompatible and bioactive bulk structure synthesis.

Laser system for 3D polymer micro- and nanostructures formation.

FSRC "Crystallography and Photonics" RAS Institute on Laser and Information Technologies ILIT RAS

Scientific research

- 1. Development of equipment and technologies for 3D synthesis of complete details from different materials.
- 2. Development of technologies for laser synthesis of new nanomaterials and nanostructures for nanophotonic and electronic.
- 3. Development and production of high power laser systems and new laser technologies for production and medicine.
- 4. Development of methods for computer modelling of different process in laser technologies.



Last model of laser system for cardio surgery



Created in ILIT RAS equipment for laser stereolitography production

FSRC "Crystallography and Photonics" RAS Photochemistry Centre PC RAS

Scientific research

- Development of materials and devices of photonics based on supramolecular architectures.
- 2. Investigation of self-organization principles of molecules and nanoparticles.
- 3. Photonics and photochemistry of supramolecular architectures.
- 4. Design of molecules able to create the composite supramolecular architectures by the selforganization.



Supramolecular architectures





Single crystal and powder X-ray diffraction, including conditions of external fields, high pressures, high and low temperatures

Beamline requirements:

- Energy range 6.0 90.0 keV
- Monochromatic beam (Δ*E*/*E*~10⁻⁴)
- beam size min/max: 5-1000 µm

Sample enviroments:

- Cryo/heating
- Temperature range 5 K to 1000 K
- Magnetic and electric fields
 - application system
- High pressure up to 500 Gpa







Macromolecular crystallography ultra-high resolution structure analysis and microcrystallography

Study of structural aspects, interaction and functioning of various proteins and their complexes

X-ray diffraction, time resolving protein crystallography

Beamline requirements:

- energies 5-20 keV
- monochromator
- beam size: 4.0 × 5.0 μm²
- Detector with readout time ~0.3sec
- X-ray fluorescence detector

Infrastructure - user laboratories:

- Samples preparation room
- Samples cryostorage
- Crystallization plates storage

Sample enviroments:

- Cryocooler
- Automatic sample changer

Software:

for semi-automatic data collection (automatic crystal centering, data autoprocessing_



Real crystal structure dynamics under external influences

Time-resolved studies of real structure behavior in functional crystals (piezoelectrics) under external electric field

Time-resolved double- and triple-axis diffraction and spectroscopy

Sample enviroments:

- Cryo/heating
- Magnetic field application system
- High pressure

Infrastructure - user laboratories:

- Sample preparation equipment

Beamline requirements:

- energies 3-20 keV;
- monochromatic beam ($\Delta E/E \sim 10^{-4}$);
- fast (ultrasonic resonators or bending crystals) X-Ray optics
- beam size min/max: 20-1000 µm
- detectors: point, linear, 2D;
- multichannel analyzer
- sample holder with possibility of applying electric field





Small-angle X-ray scattering for nanotechnology, molecular biology, biomedical applications

Study of structural aspects, interaction and functioning of various proteins; structural nanodiagnostic of the nanomaterials.

SAXS; in-line size-exclusion chromatography (SEC)-SAXS; the invacuum and in-air setups; anomalous SAXS; time-resolved SAXS environments.

Beamline requirements:

-energies 4-20keV

-monochromator Si 111, multilayer for high flux

-beam size: $0.2 \times 0.1 \text{ mm}^2$

```
-fast pixel detectors (Dectris)
```

Infrastructure - user laboratories:

- -sample preparation and characterization (SPC)
- -sample storage
- -user laboratory

Sample enviroments:

- -temperature control
- measurement cells for in-vacuum and inair measurements
- -automatic sample changer
- -the in-air setup

Software:

- automation of SAXS experiment
- automated data processing and analysis





Polymer capsules for entrapment of hydrophobic and hydrophilic bioactive substances

Biocompatibility and biodegradability Low toxicity and immunogenesity High stability within a broad pH range

Layer-by-Layer technique Ultrasound treatment Emulsification

SAXS, WAXS

Infrastructure - user laboratories:

- -Shaker
- -Centrifuge
- -Ultrasonic device
- -Microscopy

Sample enviroments:

-In-air setup -Automatic sample changer -Cryo



Soft condensed matter on liquid/air interfaces

Study of organic and bioorganic layered systems formation on the liquids surface, biomembrane modeling - protein interactions with lipids ets.

- Grazing incidence X-ray diffraction (GIXD)
- Grazing-Incidence Small-Angle Xray Scattering (GISAXS)
- X-ray reflectometry (XRR)
- X-ray Fluorescence at Total Reflection (TXRF)
- X-ray standing wave under total external reflection conditions (XSW)

Infrastructure - user laboratories:

- Samples preparation room, including Langmuir trough
- Chemical room with cryostorage

Sample enviroments:

- Langmuir trough for liquids and films (with cover)
- Gas-flow equipment

Beamline requirements:

- energies 5-25 keV
- monochromator
- Optical scheme ride X-ray at water surface
- beam size: 4.0 × 5.0 μ m²
- 1D and 2D Detectors
- X-ray fluorescence detector



µ-X-ray fluorescence analysis: qualitative/quantitative analysis, mapping and tomography



Study of element composition in inorganic, organic and bioorganic objects and elements distribution in bulk or near surface

X-ray diffraction, time resolving protein crystallography

Beamline requirements:

- energies 5-40 keV
- monochromator
- beam size min/max: 0.5*0.5/500*500 μm²
- 1D/2D detectors
- X-ray fluorescence detectors

Infrastructure - user laboratories:

- Samples preparation room

Sample enviroments:

- Sample chamber for air/low vacuum

- Sample holder with 3D moving and rotating

Software:

for semi-automatic data collection (spectra collection point-by-point during mapping and tomography)

Nuclear Resonance Methods under the High Pressures and Low Temperatures in Magnetic Field

Search for new materials and study of their properties for the power engineering and conversion, high-temperature superconductivity, electronics and spintronics, geophysics and etc

NFS – Nuclear Forward Scattering (hyperfine interactions)

SMS – Synchrotron Mossbauer Spectroscopy (hyperfine interactions)

NIS – Nuclear Inelastic Scattering (local phonon DOS)

Beamline requirements:

- Energy range 7.0 80.0 keV
- Temperature range 2 K to 650 K
- Magnetic field to 9 T





Thank you for attention