Synchrotron and Free electron laser Radiation: generation and application (SFR-2022)

June 27 – 30, 2022

Book of Abstracts

300 Лет
Российская Академия Наук

Organized by Budker INP

BUDKER INSTITUTE OF NUCLEAR PHYSICS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCE

Sponsored by SPE Group

НАУЧНОЕ ОБОРУДОВАНИЕ
ГРУППА КОМПАНИЙ

Synchrotron and Free electron laser Radiation: generation and application (SFR-2022)

Book of Abstracts

Novosibirsk
2022

УДК 535.33/.34; 538.97-405

ББК 22.344; 22.386

Book of abstracts of International Conference "Synchrotron and Free Electron Laser Radiation: Generation and Application".

Книга абстрактов Международной конференции по генерации и использованию синхротронного и терагерцового излучения.

ISBN 978-5-904968-08-3

Настоящий сборник абстрактов является рабочим документом Международной конференции по генерации и использованию синхротронного и терагерцового излучения SFR-2022, организованной ИЯФ СО РАН, г. Новосибирск, с 27 по 30 июня 2022 г. Книга предназначена для научных сотрудников и инженеров, занимающихся исследованиями на синхротронном, терагерцовом излучении, разработкой элементов ускорителей заряженных частиц, а также может быть полезной студентам и аспирантам соответствующих специальностей.

ISBN 978-5-904968-08-3

Contents

RADIOLUMINESCENCE AND OPTICAL PROPERTIES OF NON-RADIOACTIVE SYNTHESIZED POLYMETHYLMETHACRYLATE #1

Submitted by **Gleb Lyubas**
For track: X-ray spectroscopy
Authors:

- Gleb Lyubas (Institute of Solid State Chemistry and Mechanochemistry of Siberian Branch Russian Academy of Sciences, Kutateladze 18, Novosibirsk, 630090 Russian Federation)
- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
- Vladimir Nazmov (Budker INP, Novosibirsk, Russia)

High-energy physics requires new luminescent materials with nanosecond flash times or less. The study of luminescent structures based on porous aluminum oxide was carried out in works [1-3]. The use of polymethylmethacrylate as a luminophore has not been practically investigated. This work is a logical continuation of the works [1-3]. The first aim of this study was to determine the effect of the molecular weight on the spectral characteristics of the radioluminescence of non-radioactive synthesized polymethylmethacrylate. The second aim of this study was to determine the effect of the molecular weight on the optical properties of non-radioactive synthesized polymethylmethacrylate.

This work was supported by the Ministry of Science and Education of Russia (project № FWUS-2021-0004).

References:

1. G.A.Lyubas, J. Mater. Sci. 53, 15204 (2018).
2. G.A.Lyubas, Nanotechnologies in Russia 12, 276 (2017).
3. G.A.Lyubas, Nanosystems: Physics, Chemistry, Mathematics 8, 793 (2017).

ВХОДНОЙ КОНТРОЛЬ ВОЛЬТАМПЕРНЫХ ХАРАКТЕРИСТИК КОМПОЗИЦЫОННЫХ ПРОВОДНИКОВ НА ОСНОВЕ Nb-Ti СПЛАВОВ ПРИ ТЕМПЕРАТУРЕ ЖИДКОГО ГЕЛИЯ #2

Submitted by **Alexandr Brodnikov**
For track: SR and FEL sources and centers
Authors:

- Бродников А.Ф. (Институт ядерной физики им. Г.И. Будкера СО РАН (ИЯФ), г. Новосибирск, Россия)
- Кондратьев В.И. (Институт ядерной физики им. Г.И. Будкера СО РАН (ИЯФ), г. Новосибирск, Россия)

Рассмотрены метод и измерительная установка для определения действительных значений критического тока в сверхпроводниках, при гелиевых температурах, поступающих на рынок от отечественных и зарубежных производителей композиционной проволоки, круглого или прямоугольного сечения, на основе сплава Nb-Ti. Приведены результаты исследования, подтверждающие работоспособность измерительной установки.

В настоящее время композиционные проводники на основе Nb-Ti сплавов преобладают на мировом рынке сверхпроводящих материалов. Ввиду достаточно высокой критической плотности тока, пластичности, а также относительно низкой стоимости, они являются расходным материалом и широко используются в криогенной технике, в продолжение последних нескольких десятилетий. В данный момент федеральные законы «О техническом регулировании» и «О стандартизации» имеют статус «добровольного применения» [1], поэтому отечественные предприятия, включая зарубежные, поставляющие на рынок различные материалы, не имеют обязательств и возможностей осуществлять выходной контроль по колоссальному числу существующих свойств, да ещё и в диапазоне криогенных температур.

Поэтому получая от производителей композиционную проволоку на основе Nb-Ti сплавов выпускаемую серийными партиями или экспериментальные образцы которые представляет собой композит, содержащий Nb-Ti волокна, распределённые в матрице из высокочистой меди или резистивного сплава на базе меди, в состав которого могут входить и другие материалы, используемые в качестве диффузионных и резистивных барьеров такие как Nb, Cu-Ni, Cu-Mn. Мы осуществляем входной контроль композиционной проволоки с целью предотвращения запуска в производство продукции, не соответствующей требованиям конструкторской и нормативно-технической документации.

Операции входного контроля сверхпроводников различной формы реализуется следующим образом, изготавливается оправка в виде плоскопараллельного цилиндра в которой сверлятся отверстия, в которых располагаются образцы исследуемых проводов из разных партий приобретённого сверхпроводящего провода, далее проводники закрепляются в отверстиях, производится шлифовка и вслед за тем оправку располагаем в электронном микроскопе HITACHI S-3400N. По полученной информации сканирования шлифа проводов проводим анализ и делаем заключение о качестве исследуемых образцов, и их дальнейшего применения или забраковываем.

Также при проектировании сверхпроводящих магнитов и других объектов криогенной техники особую роль уделяем характеристикам указанными производителями сверхпроводящих проводов. В связи с этим в ИЯФ было принято решение о создании измерительной установки, предназначенной для определения действительных значений критического тока в сверхпроводниках, поступающих на рынок от отечественных и зарубежных производителей композиционной проволоки, на основе сплава Nb-Ti.

Измерительная установка изготовлена на базе криостата КГ-60/300-1 во внутренней полости которого, в среде жидкого гелия, располагается соленоид, а в его центральной части располагается вставка-держатель с образцом. Питание соленоида и исследуемого образца, по токовводам расположенными в верхней крышке криостата, осуществляется источниками питания фирмы Danfysik – system 8800 при помощи ПК и управляющей программы, разработанной в ИЯФ.

Для опробования установки по определению вольтамперных характеристик (ВАХ) в сверхпроводниках при гелиевых температурах, были проведены испытательные измерения по методике МВИс 400-423/8-2018 разработанной АО «ВНИИНМ» [2]. Измерения проводили на образцах композиционной проволоки, на основе сплава Nb-Ti, длиной равной 0,08 м и диаметрами 0,5 и 0,85 мм, отрезанными от проводов штатных партий, при этом ВАХ были указаны производителями данных сверхпроводников. Каждый образец припаивался к оправке из меди сечением 4×2 мм индий-оловянным низкотемпературным припоем. Оправка с образцом монтируется к токовводам криостата. В центре измеряемого провода припаивали потенциальные провода на расстоянии 1 см между собой, которые подключаются к универсальному прецизионному измерителю В7-99. Весь процесс измерений регистрируется при помощи программного обеспечения, поставляемого с измерителем.

После пайки все технологические канавки обезжириваются и заливаются высокотемпературным силиконовым герметик-прокладкой. После окончательной сборки вставки-держателя в его центральной части устанавливается датчик Холла, для измерения магнитного поля, производства компании «Lake Shore Cryotronics Inc.» (Sensor Model: HGCT-3020, Mean Loaded Sensitivity: 0,773mV/kG) непосредственно вблизи с измеряемым сверхпроводником. Перед проведением испытаний все средства измерений данной установки, были откалиброваны в метрологической службе ИЯФ.

Вслед за проведением всех организационных операций при заливке в криостат жидкого гелия, осуществляя контроль уровня газа в криостате и его температуры 4,2±1К (датчиками температуры DT-670 Silicon Diodes, компании Lake Shore Cryotronics Inc.), а также температуры токовводов. Далее поднимаем магнитное поле в соленоиде до уровня 7 Тл согласно показаниям датчика Холла (54,11±0,01 mV), в качестве опорной точки указанной производителем сверхпроводника.

Запись ВАХ в образцах проводится при увеличении силы тока со скоростью до 0,1 А/с вплоть до появления величины напряженности электрического поля Е равной 0,8 – 1,0 мкВ/см [3]. За критический ток (Ic) принимается значения тока, соответствующее электрическому полю в образце 0,8 – 1,0 мкВ/см, как наклон графика log E - log I в указанном диапазоне электрических полей. Результат измерения критического тока в проводнике в зависимости от индукции магнитного поля представлен на графике ВАХ образца диаметром 0,5 мм при 7 Тл.

Расчетное значение критического тока, указанного изготовителем измеряемых сверхпроводящих проводов при 7 Тл должно составлять 200 А и 372 А. Полученное нами значение составило 212 А и 382 А, что составляет менее 10% [4] и это соответствует пределу допускаемой основной абсолютной погрешности измерителя В7-99 которая составляет ± (1,5·10-3 + 4,5·10-5·|U|) мВ (U - измеренное напряжение, мВ). Как видно работоспособность измерительной установки для определения действительных значений критического тока подтверждена, а дальнейшее повышение точности результата измерений может быть достигнуто путём совершенствования современной прецизионной цифровой измерительной аппаратуры, с не менее допускаемой основной абсолютной погрешностью ±0,0025%+0,02 нВ.

БИБЛИОГРАФИЯ

1. Рыбак Н.И., Черепанов В.Я., Шейнин Э.М., Ямшанов В.А. Правовой статус национальных стандартов единства измерений // Стандарты и качество. — 2015. — № 12. С. 44 – 47.
2. МВИс 400-423/8-2018 // Методика измерения критического тока и определения показателей кривизны вольтамперной характеристики сверхпроводящих проводов на основе сплава Nb-Ti // АО «ВНИИНМ» -2018 г.
3. Н.В. Быковский, В.С. Высоцкий, А.А. Носов, С.С. Фетисов // Установка для исследования температурной зависимости критического тока сверхпроводников на основе диборида магния // Кабели и Провода. – 2016 – №5. С. 20 – 25.
4. Сотников Д. В., // Исследование токонесущих свойств перспективных высокотемпературных сверхпроводящих материалов для электротехнических устройств // ОАО «Всероссийский Научно-Исследовательский Проектно-Конструкторский и Технологический Институт Кабельной Промышленности» - 2016 г.

SOME COMPOSITE MATERIALS BASED ON AN ALUMINUM MATRIX FROM SHOT BLASTING WASTE OF VANADIUM ALLOYS #3

Submitted by **Danil Eselevich**
For track: X-ray structural analysis
Authors:

- Danil Eselevich (Institute of Solid State Chemistry UB RAS)
- Maksim Baklanov (Institute of Solid State Chemistry UB RAS)
- Vladimir Shevchenko (Institute of Solid State Chemistry UB RAS)

Aluminum alloys and composites based on it are widely used in various fields of mechanical engineering for the manufacture of parts with improved performance. JSC "Uralredmet" mastered highly efficient industrial production of ligatures for titanium alloys, which are used in the manufacture of parts for the aerospace industry, defense equipment, shipbuilding and chemical engineering. The alloy VnAl-65 (V = 60-65%, rest. Al) and VnAl-1 (V = 70-75%, rest. Al) is the main product for producing Ti-6Al-4V titanium alloy. Increasing volumes of production of Al-V alloys lead to the accumulation of a large amount of waste at JSC Uralredmet, which has not yet been used.

The products of shot blast cleaning (shot blast dust, SBD) from ingots of Al-V system ligature have been certified. Based on the obtained data on phase and chemical analysis, morphology and size distribution, pressed samples of a mixture of aluminum powders and SBD composition were made: 30 wt. % Al + 70 wt. % SBD and 95 wt. % Al + 5 wt. % SBD. They were annealed in an argon

medium at temperatures of 750 ºC and 1050 ºC, electron microscopic and X-ray phase analysis was carried out. It has been established that after annealing (at 1050°C) tablets with a low SBD content contain only metal phases in their composition: 49.9% Al; 31.9% Al45V7; 14.3% Al3V and 3.9% Fe4Al13, which indicates the prospects of using SBD for testing the modes of obtaining composite materials based on an aluminum matrix.

The work was carried out in accordance with the state order of the Institute of Solid State Chemistry UB RAS № AAAA-A19-119031890028-0

IN-SITU STUDY OF STRUCTURAL CHANGES DURING HEATING OF HAp NANOCOMPOSITES MODIFIED BY TiOy #4

Submitted by **Danil Eselevich**

For track: X-ray structural analysis

Authors:

- Danil Eselevich (Institute of Solid State Chemistry UB RAS)
- Zakhar Vinokurov (Boreskov Institute of Catalysis SB RAN)
- Svetlana Rempel (Institute of Solid State Chemistry UB RAS, Ural Federal University)

As a basis for bioimplants in medicine, calcium phosphates and composites based on them are widely used. Due to its high biocompatibility, special attention is paid to synthetic hydroxyapatite (HAP). In order to significantly improve the mechanical properties (strength, abrasion resistance and crack resistance), it was modified with titanium monoxide (TiOy). The certification was carried out, the morphological properties and structure of the obtained nanocomposites (HAP + 10 and 20 wt. % TiO0.92, HAP + 10 and 20 wt. % TiO1.23) were studied.

The physicochemical properties of the initials and modified HAP were studied in-situ on a synchrotron radiation source when heated from room temperature to 900°C at a rate of 5°C/min. in a stream of dry air. It has been established that the temperature shift of phase transitions and the thermal stability of hydroxyapatite depend on the stoichiometry and the amount of titanium monoxide in the nanocomposite. Thus, the addition of 10 wt. % TiO0.92 increases the decomposition temperature of HAP by approximately 100°C. In the case of a content of 20 wt. % TiO0.92, the decomposition temperature of HAP increases only by 20°C. In nanocomposites, the α-TCP phase appears in the temperature range of 780–840°C, while the β-TCP phase appears at 860–900°C. The range of TiOy phase transitions is 480-600 °C and depends on the initial stoichiometry and the amount of additive.

All phases of nanocomposites are biocompatible after heat treatment up to 900°C. The oxyapatite and TiO2 phases retained the nanostate of their initial components, while α- and β-TCP were microcrystalline.

The reported study was funded by RFBR, project number 20-03-0067

RADIOLUMINESCENT OF CORUNDUM/GARNET STRUCTURES #5

Submitted by **Alexey Zavjalov**

For track: X-ray fluorescent analysis

Author: Gleb Alexandrovich Lyubas (Institute of Solid State Chemistry and Mechanochemistry SB RAS, 630128 Novosibirsk, Russia)

Co-authors:

- Alexey Pavlovich Zavjalov (Institute of Solid State Chemistry and Mechanochemistry SB RAS, 630128 Novosibirsk, Russia)
- Oleg Olegovich Shichalin (Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok 690922, Russia)
- Anastasia Andreevna Vornovskikh (Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok 690922, Russia)

- Denis Yurievich Kosyanov (Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok 690922, Russia)

This work is a logical continuation of the works [1-3]. Al_2O_3−Ce:YAG and Al_2O_3–Ce:(Y,Gd)AG composite ceramics were fabricated by reactive spark plasma sintering (SPS) using high-purity commercial oxides. In brief, α-$_2O_3$ (99.99%, Fenghe Ceramic Co., Ltd, China; d~0.2−0.4 μm), Y_2O_3 (99.999%, Fujian Changting Golden Dragon Co., Ltd, China; d~5 μm), Gd_2O_3 (99.999%, Jining Zhongkai New Materials Co., Ltd, China; d~3−5 μm), CeO_2 (99.99%, Alfa Aesar Chemical Co., Ltd, China; d~2−3 μm) were used as raw materials. For the ceramics, the molar ratio of garnet/Al2O3 was controlled to be ~1.3 (Al_2O_3 content was ~11.5 wt%); the Ce^{3+} and Gd^{3+} concentrations were set to be 0.1 at% and 25 at%, respectively, according to the stoichiometric ratio of (Ce+Y+Gd):Al=3:5 for the YAG phase. Sintering additives were 0.8 wt% tetraethyl orthosilicate and 0.08 wt% MgO. The raw materials were mixed for 12 hours by a planetary ball mill (QM-3SP2, Nanjing Chi Shun Technology Development Co., Ltd., China) with a rotation speed of 279 rpm, using ethanol as a dispersant and alumina balls as grinding media, respectively. Then the obtained homogeneous slurries were dried at 70 °C in an oven, sieved through a 200-mesh screen, and calcined at 600 °C in the air for 4 hours. The prepared powder systems (sample 1.5 g) were loaded into a graphite die with an inner diameter of 15 mm, the internal surface of which was covered with a graphite sheet, subjected to an SPS-515S sintering machine (Dr. Sinter LAB^{TM}, Japan), and pressed. SPS experiments were conducted in a vacuum (~6 Pa) at the temperature 1450 °C and dwell sintering time 15 min (under external pressure 30 MPa). After sintering, the ceramics were annealed in the air at 1000 °C for 10 hours to recover oxygen vacancies and remove residual stress. Finally, samples were mirror polished for further measurements.

To study the spectral and kinetic characteristics, X-ray spectroscopy with time resolution was used when a synchrotron radiation beam was excited at the experimental station “X-ray spectroscopy with time resolution” of Siberian Synchrotron and Terahertz Radiation Center (SSTRC), Budker INP, Novosibirsk. The maximum of the spectrum of the sample $0.75Al_2O_3$–$Y_{2.997}Ce_{0.003}Al_5O_{12}$ lies at ≈533 nm, the maximum $0.75Al_2O_3$–$Y_{2.247}Gd_{0.75}Ce_{0.003}Al_5O_{12}$ lies at ≈542 nm, i.e. the addition of gadolinium leads to a shift in luminescence to the red region of the spectrum (the so-called “redshift”).

Also, the second sample in the red region of the spectrum clearly shows a line associated with the addition of gadolinium (the maximum of the line is approximately at ≈628 nm), which may be interesting, including from the point of view of combining these laser structures with He-Ne lasers operating at a wavelength of 0.63 microns. The intensities of the samples are the same.

Acknowledgments: This work was partially supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. FWUS-2021-0004), and by the Russian Science Foundation (Project No. 20-73-10242; Fabrication of Al_2O_3−RE:YAG (RE=Ce; Ce+Gd) composite ceramic phosphors). D.Yu.K. is grateful to the Council for Grants of the President of the Russian Federation (scholarship no. SP-3221.2022.1).

References:

1. G.A.Lyubas, J. Mater. Sci. **53**, 15204–15212 (2018).
2. G.A.Lyubas, Nanotechnologies in Russia **12**, 276–284 (2017).
3. G.A.Lyubas, Nanosystems: Physics, Chemistry, Mathematics **8**, 793–797 (2017).

THE SECONDARY SYNCHROTRON RADIATION SOURCE AT VEPP-4 #6

Submitted by **Boris Tolochko**
For track: X-ray structural analysis
Author: Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
Co-authors:

- Aleksandr Kosov (Budker INP SB RAS)
- Vladimir Nazmov (Budker Institute of Nuclear Physics)
- Nikolay Razumov (Институт химии твердого тела и механохимии Со РАН)

On the synchrotron radiation beamline of VEPP-4 No. 8, a secondary SR source was formed with dimensions of 25x25 μm (7x7 μm in plans). This made it possible to realize the registration of small-angle X-ray scattering from a minimum angle of 0.2 deg. At VEPP-3, the initial SAXS detection angle is 0.6 deg. This methodological result expands the range of research of nano-objects by 3 times, which is extremely necessary for our users.

A problem has been discovered: the micron slits of the secondary source under the action of SI VEPP-4 due to the arising thermal stresses completely overlap after 10 seconds of operation under the beam.

This work was supported by RFBR grant number 19-29-12045.

INVESTIGATION OF "DUSTING" USING SYNCHROTRON RADIATION #7

Submitted by **Konstantin Ten**
For track: SR technological application and X-ray apparatus
Author: Konstantin Ten (LIH SB RAS)
Co-authors:

- Edward Pruuel (LIH SB RAS)
- Aleksey Kashkarov (LIH SB RAS)
- Iwan Rubtsov (SRF BIC SB RAS)
- Aleksey Studennikov (SRF BIC SB RAS)
- Boris Tolochko (ISSC SB RAS)
- Lev Shekhtman (BINP SB RAS)
- Aleksandr Garmashev (FSUE RFNC VNIITF)
- Dmitriy Petrov (FSUE RFNC VNIITF)
- Evgeniy Smirnov (FSUE RFNC VNIITF)
- Kirill Novoselov (NSU)

The exit of a strong shock wave to the free surface (FS) of a metal sample leads to the ejection of a cloud of particles from the front of the FS (the so-called "dusting"). The destruction of the FS into microparticles occurs due to the presence of small inhomogeneities, in which stress concentration occurs, leading to the detachment of microparticles. Interest in this phenomenon is associated with the influence of the "dust" emission on the results of measurements of the dynamics of the motion of the SP using shadow, electric contact and laser methods of motion registration. Experimental study of these processes is very difficult due to the small size of microparticles (1 - 100 microns) and high speeds of their flight (1-5 km/s). The most commonly used systems are laser systems (PDV) and piezo sensors. Their advantages are multi-channel and the possibility of transportation. And the disadvantages are the low accuracy and complexity of calibrating the measured readings (data). Synchrotron radiation makes it possible to obtain many radiographic images (movies) of the process of generation and dynamics of a cloud of microparticles.

The report presents the results of simultaneous measurements of the dynamics of a dust cloud by three methods - laser PDV, piezo sensors and synchrotron cinema. It is shown that integrally all methods are equivalent, but "fast" measurements of cloud density are visible only with SR radiography.

ON APPLICATIONS OF ULTRASHORT PULSES X-RAY PULSES GENERATED BY THE INVERSE COMPTON SCATTERING #8

Submitted by **Ruslan Feshchenko**
For track: SR and FEL sources and centers
Authors:

- Ruslan Feshchenko (P.N. Lebedev Physical Institute)
- Igor Artyukov (P.N. Lebedev Physical Institute)
- Alexander Vinogradov (P.N. Lebedev Physical Institute)
- Vasiliy Shvedunov (Skobeltsyn Institute of Nuclear Physics)

Ultrashort X-ray pulses with duration in the picosecond range are useful for various applications in such diverse areas as the condensed matter physics, material sciences, inorganic chemistry and molecular biology [1]. This may include, for instance, observing phase transitions in solids in real time, X-ray structural analysis of transient states (including lattice deformations caused by laser heating) as well as studying fast processes such as heat and phonon propagation in solids. Other examples are investigating chemical reactions processes in solutions, solid-state decomposition, and explosion of energetic materials and studying evolution of the structure of complex proteins with a picosecond temporal resolution. Picosecond X-ray pulses can be used to study phase transitions in chalcogenide alloys such as *Ge*2*Sb*2*Te*5 (GST) or similar materials, which may find applications in the so-called Phase Change Memory (PCM) vying as a replacement of both DRAM and FLASH memories [2].

While there exist different ways of generating ultrashort x-ray pulses, which are based on laser plasmas, synchrotron radiation, X-ray lasers and X-ray tubes, these methods do not satisfy the needs of all users. So, in present work a design, X-ray radiation parameters and possible applications of the Picosecond Compton X-ray Sources (PCXSs), which are based on scattering of short and energetic laser pulses by trains of low emittance electron bunches produced by a linear accelerator, are considered. It is demonstrated that creation of such sources is feasible based on the existing accelerator and laser technologies. The design of both the linear accelerator and main laser system of PCXS are considered. A possible design of the X-ray optical system delivering X-ray pulses onto the sample is also discussed.

[1] M. M. Murnane, H. C. Kapteyn, S. P. Gordon, R. W. Falcone, Ultrashort X-ray pulses, Applied Physics B, 58(3), 261--266 (1994).
[2] H. Hayat, K. Kohary, and C. D. Wright, Emerging Nanoscale Phase-Change Memories: A Summary of Device Scaling Studies, (2016).

SPIN-ORBIT INTERACTION IN OSMIUM COMPLEXES #9

Submitted by **Igor Asanov**
For track: X-ray spectroscopy
Author: Igor Asanov (Nikolaev Institute of Inorganic Chemistry)
Co-authors:

- Anastasia Fedorenko (Nikolaev Institute of Inorganic Chemistry)
- Tatiana Asanova (Nikolaev Institute of Inorganic Chemistry)

The discovery of the influence of strong spin-orbit interaction (SOI) on the properties of compounds has revealed a new class of so-called spin-orbit materials. A strong SOI can change the electrical and magnetic properties of materials. The most well-known materials with strong SOI are compounds with unusual electrical and magnetic properties - topological dielectrics, compounds with an SOI-induced metal-dielectric transition, compounds with low-dimensional, exciton and singlet magnetism.

To understand and predict properties in such materials, it is necessary to identify structural factors that affect the parameters of the electronic structure associated with SOI and understand the

mechanism of their influence. The most promising method of study is the use of an X-ray absorption spectroscopy and theoretical calculations of the electronic structure. X-ray absorption spectroscopy provides information about the local geometry, atomic structure, and the electronic structure, including the density of vacant states, charge, orbital and spin state of the system. Theoretical calculations make it possible to determine the SOI value and its effect on the electronic structure and physicochemical properties.

Osmium(IV) octahedral complexes were chosen as objects of study in the work. Osmium compounds are still poorly understood, despite the discovery and prediction of unusual magnetic properties (singlet magnetism, Kitaev magnetism). Measurements of the magnetic susceptibility showed the presence of a magnetic moment, even though the electron configuration of Os atom is d4 in an octahedral environment of halogen atoms, and should correspond to a zero total moment. Measurement of X-ray absorption spectra at Os L2,3 edges during the formation of finely dispersed Pd-Os and Pt-Os bimetallic alloys at the thermal decomposition of double complex salts [Pd(NH3)4][OsCl6] and [Pt(NH3)4][OsCl6] shows an unusually large ratio of the intensities the absorption edge L3/ L2 [1]. This indicates a strong electronic interaction in these complex salts, and a large value of SOI operator L.S, comparable to iridium compounds where metal-insulator transitions were found. Calculations of the electronic structure and spectra made it possible to estimate the value of the SOI constant in the complexes ~0.4 eV, to reveal the character of the SOI influence depending on the composition and geometry of the ligands and noncubic distortions of the [OsCl6]2- cluster. The results of the work are important for the development of materials with new magnetic properties.

References

1. Asanova T.I., Asanov I.P., Yusenko K.V. et al. //Mater.Res.Bull.2021.V.144.P.111511.

The work was financially supported by the Russian Science Foundation, grant 22-22-00683

COMPRESSIBILITY, POLYMORPHISM AND STABILITY OF THE HIGH-PRESSURE K-CA CARBONATES AS PART OF THE DEEP CARBON CYCLE #10

Submitted by **Anna Likhacheva**

For track: X-ray structural analysis

Authors:

- Anna Likhacheva (1Sobolev Institute of Geology and Mineralogy SD RAS, Novosibirsk, Russia 2Budker Institute of Nuclear Physics SD RAS, Novosibirsk, Russia 3Novosibirsk State University, Novosibirsk, Russia)
- Sergey Rashchenko (1Sobolev Institute of Geology and Mineralogy SD RAS, Novosibirsk, Russia 2Budker Institute of Nuclear Physics SD RAS, Novosibirsk, Russia 3Novosibirsk State University, Novosibirsk, Russia)
- Alexandr Romanenko (1Sobolev Institute of Geology and Mineralogy SD RAS, Novosibirsk, Russia 3Novosibirsk State University, Novosibirsk, Russia)
- Ronald Miletich (4University of Vienna, Vienna, Austria)
- Sofija Milos (4University of Vienna, Vienna, Austria)
- Sergey Goryainov (1Sobolev Institute of Geology and Mineralogy SD RAS, Novosibirsk, Russia)
- Alexey Ancharov (Institute of Solid State Chemistry and Mechanochemistry SB RAS)

Alkali carbonates present an essential but still poorly investigated part of the deep carbon cycle related to the formation and evolution of the mantle carbonatite magmas. There is no definite view of the presence of alkali carbonates in the mantle as stable phases or simply as daughter products within the crystallization sequence of alkali melts. The recent discovery of a number of double K-Ca carbonates in the high-pressure experiments [1,2] stimulates a search for the potassium-bearing phases stable in the mantle conditions. Here we present the first results of the in situ X-ray diffraction and Raman spectroscopy studies of the double K-Ca carbonates with different K:Ca stoichiometry in a wide P-T range. New interesting features of the structure compression mechanisms were revealed.

The obtained data suggest a limited occurence of alkali carbonates as crystalline phases at deep Earth conditions.

This work is supported by the Russian Foundation for Basic Research (grant No 21-55-14001). The work was partly done at the shared research center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB RAS. Diffraction experiments were also performed at the ESRF (Grenoble, France) and PETRA III (DESY, Hamburg, Germany).

References:

[1] Shatskiy A., Litasov K.D., Palyanov Y.N., Ohtani E. (2016) Phase relations on the K2CO3–CaCO3–MgCO3 join at 6 GPa and 900–1400 °C: implication for incipient melting in carbonated mantle domains // American Mineralogist 101(2), 437–447.

[2] Arefiev A.V., Shatskiy A., Podborodnikov I.V., Rashchenko S.V., Chanyshev A.D., Litasov K.D. (2019) The system K2CO3–CaCO3 at 3 GPa: link between phase relations and variety of K–Ca double carbonates at ≤ 0.1 and 6 GPa // Physics and Chemistry of Minerals 46, 229–244.

ПРИМЕНЕНИЕ LIGA-РАСТРОВ ДЛЯ ФИЛЬТРАЦИИ РАССЕЯННОГО ИЗЛУЧЕНИЯ В ДЕНТАЛЬНОЙ РЕНТГЕНОГРАФИИ #11

Submitted by **Evgeny Iv. Palchikov**

For track: SR technological application and X-ray apparatus

Authors:

- Vladimir Nazmov (BUdker Institute of Nuclear Physics)
- Boris Sheplev (Dental-Service, LLC)
- Evgeny Iv. Palchikov (Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk State University, Russia)
- Andrey Dolgikh (LiH SB RAS)
- Mikhail Samoylenko (LiH SB RAS)

Методом LIGA-технологий с использованием синхротронного излучения ускорителя ВЭПП-3 созданы экспериментальные экземпляры шестигранных микроструктур никелевых растров толщиной 1200 мкм и диаметром каналов 80 мкм.

Полученный растр был использован в экспериментах по улучшению качества изображений, получаемых на стандартном зубоврачебном визиографическом комплексе SIRONA – ренгтен-аппарат с напряжением на рентгеновской трубке 60 кВ и максимумом в спектре излучения 40 кэВ с матричным ПЗС-детектором.

Биологические ткани, окружающие зуб и стоящие на пути пучка (десна, щека) состоят из элементов с низким номером ядра. При прохождении сквозь них фотонов с энергий 30-50 кэВ значительный вклад приходится на комптоновское рассеяние, что приводит к ухудшению качества рентгенограмм. Рассеянное тканями объекта съемки вторичное излучение попадает на все пиксели ПЗС-детектора, снижая контраст изображения. Для снижения данного эффекта производители визиографических комплексов используют программную фильтрацию изображений с подчеркиванием контуров и частотной фильтрацией, что снижает пространственное разрешение и может приводить к появлению артефактов.

Размещение растра непосредственно перед ПЗС-детектором позволяет отсечь рассеянное излучение и увеличить соотношение сигнал/шум практически без ухудшения яркости снимка. Прямой пучок от рентгеновского источника проходит через растр практически не задерживаясь. Рассеянное излучение, попадающее на растр под большими углами, наоборот, максимально поглощается стенками растра. В отличие от существующих больших одномерных растров, применяемых, например, при рентгеновской съемке легких, данный растр – двумерный, что позволяет лучше фильтровать вторичное излучение.

Сравнение трассировок цифровых снимков показывает лучший контраст пульпы и щели между пломбой и зубом в случае применения растра. Такой же эффект получен при трассировке поперек зубного канала с растром. Таким образом, показана возможность

использования LIGA-растра для улучшения контраста и соотношения сигнал/шум для дентальной съемки. Для дальнейшего развития методики желательно создать новые образцы растров с более высоким номером атомного ядра и каналами, ориентированными на фокус рентгеновской трубки.

THE LUMPED UHV PUMPS ON BASED NON-EVAPORABLE GETTERS #12

Submitted by **Alexey Semenov**
For track: SR and FEL sources and centers
Author: Alexey Semenov (BINP SB RAS)
Co-authors:

- Alexander Krasnov (BINP)
- Vadim Anashin (BINP)

In the time a vacuum obtaining in the modern accelerators is impossible to present without an applicantion a lumped vacuum pumps on based the non-evaporable getters (NEG). These pumps are one of the types using for vacuum obtaining in the synchrotron source of 4th generation SFR “SKIF”. A company named “Polema” (Tula, Russia) is one of the reliable and proved manufactures the NEG in Russia. The results for the NEG prototype investigations (300 l/s, 600 l/s, 900 l/s for Hydrogen) created by BINP are presented here.

References:

[1] A. Krasnov, Conception of vacuum system for SRS «SKIF», Synchrotron and Free electron laser Radiation: generation and application, 13 July - 17 July 2020, Novosibirsk, Russia.
[2] Patent US8287247B2: Combined pumping system comprising a getter pump and an ion pump.
[3] SAES Getters
https://www.saesgetters.com/sites/default/files/CapaciTorr%20UHV%20general%20%2B%20D%20%20pumps.pdf
[4] Saksaganskii G.L., Sverhvisokii vacuum v radiatcionnofizicheskom apparatostroenii, Atomizdat, M., 1976
[5] G.L. Saksaganskii, Getter and Getter-Ion Vacuum Pumps (Harwood Academic Publishers, Chur, 1994), p. 258.

SR X-RAY LUMINESCENCE, XANES AND IN SITU HEATING XRD OF SRTIO3−TIO2 COMPOSITE CERAMICS AS PROMISING THERMOELECTRIC MATERIAL #13

Submitted by **Alexey Zavjalov**
For tracks: X-ray fluorescent analysis, X-ray spectroscopy
Author: Alexey Zavjalov (1SEC “Advanced Ceramic Materials”, Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok 690922, Russian Federation 2Institute of Solid-State Chemistry and Mechanochemistry, Siberian Branch, Russian Academy of Sciences, 18 Kutateladze Street, Novosibirsk 630128, Russian Federation)
Co-authors:

- Gleb Alexandrovich Lyubas (2Institute of Solid-State Chemistry and Mechanochemistry, Siberian Branch, Russian Academy of Sciences, 18 Kutateladze Street, Novosibirsk 630128, Russian Federation)
- Marat Rashidovich Sharafutdinov (2Institute of Solid-State Chemistry and Mechanochemistry, Siberian Branch, Russian Academy of Sciences, 18 Kutateladze Street, Novosibirsk 630128, Russian Federation 3Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, 1 Nikol'skiy Prospekt, Kol'tsovo 630559, Russian Federation)

- Vladimir Vladimirovich Kriventsov (4Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, 5 Acad. Lavrentiev Avenue, Novosibirsk 630090, Russian Federation)
- Denis Yurievich Kosyanov (1SEC "Advanced Ceramic Materials", Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok 690922, Russian Federation 5Institute for Automation and Control Processes, Far Eastern Branch, Russian Academy of Sciences, 5 Radio Street, Vladivostok 690041, Russian Federation)

Earlier the review paper devoted to the possibility of exploiting the spontaneously emerging two-dimensional electron gas (2DEG) state at the SrTiO3–TiO2 interface to influence the thermoelectric characteristics of the material was published [1]. The idea is to construct by relatively simple consolidation methods oxide biphase materials (which was previously demonstrated using the Y2O3–MgO system [2]) with a chessboard grain to saturate materials by 2DEG state to improve thermoelectric effectively for high temperature applications as a part of a comprehensive solution of the tasks of optimizing traditional methods and the development of alternative types of energy production.

Ceramics was obtained by reactive spark plasma sintering of SrCO3 and TiO2. This work is dedicated to results of applications of synchrotron radiation (SR) techniques implemented at the shared research center SSRC on the basis of the VEPP-4–VEPP-2000 complex at the Budker Institute of Nuclear Physics of Siberian Branch of Russian Academy of Sciences [3] on the experimental stations of the VEPP-3 storage ring to study of the dynamics of the reaction between the components (station 5b "Diffraction Cinema" [4]) and to detect quantum size effects by X-ray luminescence spectroscopy (station 6b "X-ray spectroscopy with time resolution") and XANES (station 8 "EXAFS spectroscopy").

In situ heating XRD experiments made it possible to understand the phase transformations specific dynamic. It has been shown that an excess of TiO2 in the mixture intensifies the interaction reaction of the components, which is expressed in an earlier (by ~100 °C) onset of the formation of the SrTiO3 phase. At the same time the reaction between the components is completed by ~1000 °C. In comparison with the dynamics of compaction, this indicates that in the temperature range of 1000-1200 °C, non-reactive sintering processes are activated.

Clear signs of size quantization in biphasic ceramics were detected by the X-ray luminescence method, which is expressed in the blueshift of the biphase ceramics luminescence spectrum by 21±9 meV and its narrowing by 19.9±1.7 % in comparison with the proportional sum of spectra of separate components [5].

XANES also demonstrate the suppression of the pre-edge lines of the biphase ceramics spectrum up to ~20% in comparison with the proportional sum of spectra of separate components. That's should be modeled for a clear interpretation.

This work was supported by the Russian Foundation for Basic Research (Project No. 18-29-11044).

A.P.Z. appreciate the financial support from the Ministry of Science and Higher Education of the Russian Federation within the governmental order for Institute of Solid State Chemistry and Mechanochemistry of SB RAS (Project No. FWUS-2021-0004).

D.Yu.K. is grateful to the Council on grants of the President of the Russian Federation (scholarship No. SP-3221.2022.1) for supporting the studies devoted to obtaining advanced composite ceramics by the reactive sintering technology.

The work was partially done at the shared research center SSTRC on the basis of the VEPP-4–VEPP-2000 complex at Budker Institute of Nuclear Physics of Siberian Branch of Russian Academy of Sciences.

References:

1. A. Zavjalov, Mater. 12, 2895 (2019).
2. N.A. Safronova, Ceram. Int. 46, 6537–6543 (2020).
3. P.A. Piminov, Phys. Procedia 84, 19–26 (2016).

4. O.V. Evdokov, Nucl. Instrum. Methods Phys. Res. A: Accel. Spectrom. Detect. Assoc. Equip. 603, 194–195 (2009).
5. G.A. Lyubas, J. Exp. Theor. Phys. 75, 179–183 (2002).

КОМПЛЕКСНОЕ СТРУКТУРНОЕ IN SITU ИССЛЕДОВАНИЕ $ND_{1.6}CA_{0.4}NI_{1-Y}CU_YO_{4+\Delta}$ (Y = 0.0-0.4) С ПРИМЕНЕНИЕМ ПОРОШКОВОЙ РЕНТГЕНОВСКОЙ И НЕЙТРОННОЙ ДИФРАКЦИИ В СРЕДАХ С РАЗЛИЧНЫМ ПАРЦИАЛЬНЫМ ДАВЛЕНИЕМ КИСЛОРОДА. #14

Submitted by **Denis Mishchenko**
For track: X-ray structural analysis
Authors:

- Denis Mishchenko (SRF «SKIF» BIC SB RAS)
- Alexander Shmakov (SRF «SKIF» BIC SB RAS)

Кристаллическая структура образцов состава $Nd_{1.6}Ca_{0.4}Ni_{1-y}Cu_yO_{4+\delta}$ (y = 0.0-0.4, Δy = 0.1) и ее поведение при высоких температурах в газовых средах с различным парциальным давлением кислорода была изучена методами in situ порошковой рентгеновской дифракции с использованием синхротронного излучения на станции «Прецизионная дифрактометрия - 2» ВЭПП-3, СЦСТИ, ИЯФ СО РАН [1], лабораторного дифрактометра Bruker D8 Advance (Karlsruhe, Germany) и времяпролетной порошковой нейтронной дифракции высокого разрешения на нейтронном дифрактометре высокого разрешения (ФДВР), Лаборатория нейтронной физики им И. М. Франка (Объединенный институт ядерных исследований, г. Дубна) [2].

Изучаемые в данной работе образцы являются перспективными для применения в качестве материалов катодов среднетемпературных твердооксидных топливных элементов (в том числе с протон-проводящими электролитами) [3].

In situ рентгеновской дифракцией были определены температуры фазового перехода *Bmab – I4/mmm* для всех образцов при последовательном нагреве и охлаждении сначала в атмосфере синтетического воздуха (80 % He+ 20 % O2), затем в атмосфере гелия. Температуры фазового перехода оказались выше в атмосфере гелия, что было связано с уменьшением количества высокоподвижного междоузельного кислорода в структуре при нагреве в атмосфере с пониженным парциальным давлением кислорода. Были измерены объемные коэффициенты теплового расширения, обнаружено уменьшение объемных КТР при допировании медью.

Использование нейтронной дифракции позволило установить координаты и заселённость кислородных позиций в структуре до и после высокотемпературной обработки на воздухе и в вакууме (10^{-6} бар). Было обнаружено перераспределение кислорода между апикальной позицией в кислородном октаэдре вокруг переходного металла и позицией кислородного междоузлия в структуре типа K_2NiF_4 после высокотемпературной обработки на воздухе. Дополнительно было определено, что кислородные вакансии для данных образцов образуются в основном в апикальной позиции кислородных октаэдров.

Данная работа выполнена в рамках финансирования проекта государственного задания Министерства науки и высшего образования Российской Федерации для ЦКП «СКИФ» ИК СО РАН.

1. Piminov P.A., Baranov G.N., Bogomyagkov A.V., Berkaev D.E., Borin V.M., Dorokhov V.L., Karnaev S.E., Kiselev V.A., Levichev E.B., Meshkov O.I., Mishnev S.I., Nikitin S.A., Nikolaev I.B., Sinyatkin S.V., Vobly P.D., Zolotarev K.V., Zhuravlev A.N. Synchrotron Radiation Research and Application at VEPP-4//Physics Procedia, 2016, Vol. 84, P. 19-26.
2. Balagurov A., Balagurov D., Bobrikov I., Bogdzel A., Drozdov V., Kirilov A., Kruglov V., Kulikov S., Murashkevich S., Prikhodko V., Shvetsov V., Simkin V., Sirotin A., Zernin N., Zhuravlev V. High-resolution neutron Fourier diffractometer at the IBR-2 pulsed reactor: A new concept//Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with

Materials and Atoms, 2018, Vol. 436, High-resolution neutron Fourier diffractometer at the IBR-2 pulsed reactor, P. 263-271.
3. Tarutin A.P., Lyagaeva J.G., Medvedev D.A., Bi L., Yaremchenko A.A. Recent advances in layered Ln 2 NiO 4+δ nickelates: fundamentals and prospects of their applications in protonic ceramic fuel and electrolysis cells//Journal of Materials Chemistry A, 2021, Vol. 9, Recent advances in layered Ln 2 NiO 4+δ nickelates, No. 1, P. 154-195.

THZ REFRACTOMETRY OF METAL SURFACES VIA SURFACE PLASMON INTERFEROMETRY ON THE NOVOSIBIRSK FREE ELECTRON LASER #15

Submitted by **Vasily Gerasimov**

For track: THz radiation aplication

Authors:

- Vasily Gerasimov (Budker Institute of Nuclear Physics SB RAS)
- Alexey Nikitin (Scientific and Technological Center for Unique Instrumentation of RAS)
- Aleksey Lemzyakov (Budker INP SB RAS)

A novel method is proposed for determining the average permittivity of highly conductive reflecting metal surfaces in the terahertz range from the characteristics of surface plasmon polaritons (SPPs) (propagation length and refractive index) measured with Michelson SPP interferometer using THz radiation of the Novosibirsk free electron laser. This method is reliable and allows avoiding the parasitic effect of SPP radiation losses generated on metal surface inhomogeneities.

CHERENKOV RADIATION BY A CHAIN OF BUNCHES MOVING INSIDE A PARTIALLY DIELECTRIC LOADED WAVEGUIDE #16

Submitted by **Levon Grigoryan**

For track: THz radiation aplication

Authors:

- Levon Grigoryan (professor)
- Artak Mkrtchyan
- Sultan Dabagov
- Aram Saharian (professor)
- Hrant Khachatryan
- Kocharyan Vahan
- Mher Grigoryan
- Kotanjyan Vardazar
- Hayk Harutyunyan

In this report we are going to deliver our recent results on the radiation by a chain of relativistic electron bunches moving along the cylindrical waveguide axis, assuming, that the waveguide is loaded with a dielectric substance. We have output the analytical expression for the spectral distribution of radiation energy flux through the waveguide cross section at large distances from the plate obtained solving Maxwell equations for the motion of a single electron along the waveguide axis. The numerical analyses prove the feasibility of getting a quasi-coherent Cherenkov radiation by a chain at certain waveguide modes. The obtained results are compared with the radiation intensity by a chain moving inside a cylindrical hole of a dielectric-loaded waveguide. We will discuss the phenomenology of this mechanism of radiation amplification as well as, based on this phenomenon, the possibility of developing novel powerful sources in GHz and THz frequency ranges. The work was supported by the Science Committee of RA, in the frames of the research project No 21AG-1C069.

SIMULATION OF AN ACOUSTO-OPTIC DEFLECTOR OF TERAHERTZ RADIATION WITH A FOUR-SECTIONED ULTRASOUND TRANSDUCER #17

Submitted by **Pavel Nikitin**
For track: THz radiation aplication
Author: Pavel Nikitin (Scientific and Technological Center of Unique Instrumentation of RAS)

Commercial acousto-optic (AO) deflectors are characterized by the number of resolvable (according to the Rayleigh criterion) elements close to N=500 in the scanning range. This is possible due to the use of birefringent single crystals (for example, paratellurite TeO2) as the AO interaction medium. In the terahertz (THz) range, the known birefringent AO crystals are opaque. Therefore, AO devices suitable for this range can be based only on the optically isotropic medium. In addition, it is necessary to take into account the strong divergence of long-wave radiation beams in comparison with the visible one. As a result, the characteristics of the AO deflector are significantly worse. For example, an AO deflector based on germanium Ge is characterized by the number of resolvable elements N=10. When the ultrasound frequency F changes, the Bragg synchronism is violated, which leads to a narrowing of the operating frequency bandwidth ΔF and a decrease in N. If, with a change in the ultrasound frequency, a synchronous rotation of the wave front of the sound wave occurred, satisfying the Bragg condition, then it would be possible to significantly increase ΔF and N. This can be realized if a sectioned ultrasound transducer is used. The paper presents the results of modeling an AO deflector with a four-sectioned ultrasound transducer, the phase difference between the sections of which is equal to π. A comparison was made with an AO deflector with a single-section ultrasound transducer of the same size.

This research was funded by the Ministry of Science and Higher Education of the Russian Federation under State contract No. FFNS-2022-0009.

МИКРОМОРФОМЕТРИЧЕСКИЕ ХАРАКТЕРИСТИКИ КАТАЛИЗАТОРОВ МЕТОДОМ МАЛОУГЛОВОГО РЕНТГЕНОВСКОГО РАССЕЯНИЯ НА ЛАБОРАТОРНОМ ПОРОШКОВОМ ДИФРАКТОМЕТРЕ #18

Submitted by **Arsen Bakirov**
For track: X-ray structural analysis
Author: Арсен Бакиров (ФГУП «РФЯЦ-ВНИИТФ им. академ. Е.И. Забабахина»)
Co-authors:

- А. Станкевич (ФГУП «РФЯЦ-ВНИИТФ им. академ. Е.И. Забабахина»)
- К. Чистяков (Институт органического синтеза им. И.Я. Постовского УрО РАН)
- Н. Алехина (Ф«РФЯЦ-ВНИИТФ им. академ. Е.И. Забабахина»)
- Г. Русинов (Институт органического синтеза им. И.Я. Постовского УрО РАН)
- Е. Смирнов (ФГУП «РФЯЦ-ВНИИТФ им. академ. Е.И. Забабахина»)

Катализаторы, как правило, имеют высокую пористость, развитую поверхность и определённый химический состав. Данные характеристики, как известно, снижают энергию активации химических реакций. Микроморфология и структура определяет скорость реакций, а химический состав направление протекания реакций. Одним из методов исследования микроморфологии, надатомной структуры, внутренних неоднородностей веществ является метод малоуглового ренттгеновского рассеяния (МУРР), на что был сделан акцент в данной работе.

На порошковом дифрактометре были получены кривые малоуглового рентгеновского рассеяния, определены корреляционные функции, функции распределения по расстояниям. Выяснили, это образцы имеют пористую структуру. Посчитаны радиусы инерции, максимальный размер частиц и объем частиц.

Установлены взаимосвязи упругого рассеяния рентгеновского излучения с кристаллической структурой и удельной поверхностью медноцинковых катализаторов.

DEVELOPMENT OF A ONE-DIMENSIONAL COUNTING DETECTOR FOR DIFFRACTION EXPERIMENTS AT A SYNCHROTRON RADIATION BEAM #19

Submitted by **Anastasia Glushak**
For track: X-ray structural analysis
Authors:

- Anastasia Glushak (BINP SB RAS)
- Lev Shekhtman (BINP SB RAS)

The Institute of Nuclear Physics is developing coordinate X-ray detectors for conducting diffraction experiments to study structural and phase changes. Currently, two OD3M gas detectors for these purposes are working at the beam lines of the Siberian Synchrotron and Theraherz Radiation Centre (SSTRC). The SOCOD one-dimensional coordinate semiconductor detector under development allows providing a spatial resolution better than 100 microns at photon energy in a wide energy range (3-30 keV) and rate capability up to 1 MHz per channel which significantly exceeds the parameters of previous versions of detectors. A specialized integrated circuit (ASIC) SICOD8A has been developed for such a detector that includes 8 registration channels each containing charge-sensitive and forming amplifier, followed by four comparators with adjustable thresholds and four scalers. This configuration allows counting photons in four energy ranges. The first detector prototype is based on GaAs microstrip sensor with strip pitch of 50 um and strip length of 10 mm. The prototype has 96 recording channels. The first measurements of the parameters of the ASIC and the detector as a whole were carried out, including the dependence of noise on the input capacitance, count rate of the calibration signal as a function of threshold and the measurements of spatial resolution, dependence of count rate on the threshold and rate capability with synchrotron radiation beam.

REACTIVE SPS OF AL_2O_3−CE:(Y,GD)AG COMPOSITE CERAMICS: APPROACH OPTIMIZATION BY SR XRD INVESTIGATIONS #20

Submitted by **Alexey Zavjalov**
For track: X-ray structural analysis
Author: Alexey Pavlovich Zavjalov (1Institute of Solid-State Chemistry and Mechanochemistry, Siberian Branch of RAS, Novosibirsk, 2SEC “Advanced Ceramic Materials”, Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok)
Co-author: Denis Yurievich Kosyanov (2SEC “Advanced Ceramic Materials”, Far Eastern Federal University, 10 Ajax Bay, Russky Island, Vladivostok)

White light-emitting diodes (WLEDs) have attracted increasing attention as the next-generation solid-state lighting source in recent years. Ideal WLEDs must possess many advantageous properties, including high luminous efficacy (LE), adjustable correlated color temperature (CCT), high color-rendering index (CRI), exceptional thermal performance (excellent high-temperature strength, thermal conductivity, and quenching behavior), etc. [1]. To solve the problems mentioned above, a new type of WLEDs using Al_2O_3−Ce:(Y,Gd)AG composite ceramics has been emerging as a hot topic in recent years [2, 3]. Recently, we suggested a new approach to obtain fine-grained RE3+:YAG ceramics via reactive SPS of nanopowders in the Y_2O_3–RE_2O_3–Al_2O_3 oxide systems with controlled particle size distribution [4]. This work is therefore devoted to study formation of structural-phase state of fine-grained Al_2O_3−Ce:(Y,Gd)AG composite ceramics by reactive SPS.

A series of Al_2O_3−Ce:(Y,Gd)AG composite ceramics were prepared by reactive SPS using high purity commercial oxides: muα-Al_2O_3 (99.99%, Fenghe Ceramic Co., Ltd, China; d~0.2−0.4 μm), Y_2O_3 (99.999%, Fujian Changting Golden Dragon Co., Ltd, China; d~5 μm), Gd_2O_3 (99.999%, Jining Zhongkai New Materials Co., Ltd, China; d~3−5 μm), CeO_2 (99.99%, Alfa Aesar Chemical Co., Ltd, China; d~2−3 μm). The powders mixture was prepared for the ceramics expected molar ratio 0.75 mol Al_2O_3 (~11.5 wt%) to 1 mol $(Y_{0.749}Gd_{0.25}Ce_{0.001})_3Al_5O_{12}$. Sintering additives were 0.8 wt% tetraethyl orthosilicate and 0.08 wt% MgO. The raw materials were mixed for 12 h by a planetary

ball mill (QM-3SP2, Nanjing Chi Shun Technology Development Co., Ltd, China) with a rotation speed of 279 rpm, using ethanol as a dispersant and alumina balls as grinding media, respectively. Then the obtained homogeneous slurries were dried at 70 °C in an oven, sieved through a 200 mesh screen, and calcined at 600 °C in the air for 4 hours. The prepared powder systems (1.5 g) were loaded into a graphite die with an inner diameter of 15 mm, the internal surface of which was covered with a graphite sheet, subjected to an SPS-515S sintering machine (Dr. Sinter LABTM, Japan), and pressed. SPS experiments were conducted using a two-step sintering profile: heating up to 1000 °C with a rate 100 °C·min-1, above 1000 °C − 50 °C·min-1. Two experimental series ("Temperature" and "Pressure") was obtained. "Temperature" series regime was: the holding temperature 1350, 1400, 1425 and 1450 °C and dwell sintering time 15 min under external pressure 30 MPa. "Pressure" series regime was: the holding temperature 1425 °C and dwell sintering time 30 min under external pressure 30, 60 and 90 MPa. After sintering, the ceramics were annealed in the air at 1300 °C for 5 hours to recover oxygen vacancies and remove residual stress. Finally, samples were mirror polished for further measurements.

Two synchrotron radiation (SR) techniques implemented at the shared research center SSRC on the basis of the VEPP-4–VEPP-2000 complex at the Budker Institute of Nuclear Physics of Siberian Branch of Russian Academy of Sciences [5] on the experimental stations of the VEPP-3 storage ring (2nd beamline station "Precision diffractometry and anomalous scattering" [6] ana 4th beamline station "Diffractometry in the hard X-ray range and at high pressures" [7]) was applied to study formation of structural-phase state of the ceramic samples.

Precision diffractometry study of the [10 0 4] reflex of YAG-like phase for "Temperature" series demonstrates at least two components for the samples sintered at holding temperature up to 1425 °C which correspond to (Y,Gd)AG:Ce solid solutions of different stoichiometry (the ratio estimated by components intensities are 60:40, 73:27 and 86:14 for the holding temperature 1350, 1400 and 1425 °C, respectively) and clear one component structure for the sample sintered at holding temperature at 1450 °C which demonstrate completeness of (Y,Gd)AG:Ce solid solution formation. At the same time 2D diffractometry study of "Temperature" series demonstrates recrystallization only for the last sample which reason is an eutectic melting closeness. So, for further investigations the holding temperature 1425 °C was chosen as an optimal but the holding time had should be prolonged.

Precision diffractometry study of the [10 0 4] reflex of YAG-like phase for "Pressure" series demonstrates clear one component structure for the samples sintered under external pressure 30 and 60 MPa and at least three components for the sample sintered under external pressure 90 MPa (the ratio estimated by components intensities are 6:49:45). At the same time 2D diffractometry study of "Pressure" series demonstrates no recrystallization for all samples. Additionally, the crystallinity for the sample sintered under external pressure 60 MPa was higher and the sintering regime of this sample was chosen as an optimal.

Acknowledgments: This work was supported by the Russian Science Foundation (Project No. 20-73-10242). A.P.Z. appreciate the financial support from the Ministry of Science and Higher Education of the Russian Federation within the governmental order for Institute of Solid State Chemistry and Mechanochemistry of SB RAS (Project No. FWUS-2021-0004). Also, D.Yu.K. is grateful to the Council on grants of the President of the Russian Federation (scholarship No. SP-3221.2022.1) for supporting the studies devoted to obtaining advanced composite ceramics by the reactive sintering technology.

References:

1. S. Li, Laser Photonics Rev. **12**(12), 1800173 (2018).
2. X. Liu, J. Eur. Ceram. Soc. **39**, 2149–2154 (2019).
3. D.Yu. Kosyanov, Mater. Charact. **172**, 110883 (2021).
4. D.Yu. Kosyanov, Ceram. Int. **44**, 23145–23149 (2018).
5. P.A. Piminov, Phys. Procedia **84**, 19–26 (2016).
6. A.N. Shmakov, J. Struct. Chem. 35, 224-228 (1994).
7. A.I. Ancharov, Nucl. Instrum. Methods Phys. Res. A: Accel. Spectrom. Detect. Assoc. Equip. **470**(1–2), 80-83 (2001).

RADIATION OF A CHARGE MOVING PARAXIALLY INSIDE A DIELECTRIC CYLINDER #21

Submitted by **Vardazar Kotanjyan**
For track: THz radiation aplication
Authors:

- Aram Saharian
- Levon Grigoryan (professor)
- Anna Kotanjyan
- Hrant Khachatryan
- Vardazar Kotanjyan (PhD student)

We investigate the radiation from a charged particle moving inside a dielectric cylinder parallel to its axis. General case is considered when the cylinder is immersed in a homogeneous medium. By using the electromagnetic field Green tensor, expressions are derived for the electric and magnetic fields inside and outside the cylinder without specifying the frequency dispersion of interior and exterior dielectric permittivities. Depending on the charge velocity and on dielectric permittivities, three types of radiations may present: Cherenkov radiation in the exterior medium, radiation on guiding modes of the dielectric cylindrical waveguide and the emission of surface polaritons confined near the cylindrical interface. Closed analytic expressions are provided for the spectral distribution of the intensity for those types of radiations. It is shown that under certain conditions the strong narrow peaks appear in the spectral distribution of the Cherenkov radiation in the exterior medium. The features of different types of radiations are compared with the corresponding results obtained in [1] for a charge moving outside a cylindrical waveguide.

The work was supported by the Science Committee of RA, in the frames of the research project No 21AG-1C069.

THE SMALL-ANGLE SCATTERING BEAMLINE AT THE KURCHATOV SYNCHROTRON RADIATION SOURCE - CURRENT STATUS AND LATEST RESULTS #22

Submitted by **Georgy Peters**
For tracks: SR and FEL sources and centers, SR for medicine and biology application
Author: Georgy Peters (NRC "Kurchatov Institute")
Co-authors:

- Peter Konarev (NRC "Kurchatov Institute")
- Yurii Gaponov (NRC "Kurchatov Institute")
- Margarita Marchenkova (NRC "Kurchatov Institute")
- Kseniia Il'ina (NRC "Kurchatov Institute")
- Vladimir Volkov (FSRC "Crystallography and Photonics")
- Yurii Pisarevskii (FSRC "Crystallography and Photonics")
- Mikhail Kovalchuk (NRC "Kurchatov Institute")

The small-angle scattering beamline "BioMUR" is used for studying partially or fully disordered structures, mostly of the biological origin, in their native state and under different thermal or chemical conditions. The beamline is located at the Kurchatov synchrotron radiation source and is in operation since 2018. It has a single-crystal Si(111) triangular monochromator and a Rh-coated X-ray full reflection mirror, originally from the former X33 beamline from DESY. The beam can be focused in horizontal and vertical directions by bending the monochromator and the mirror, respectively. The minimal beam size on the detector is 480x260 microns. The DECTRIS Pilatus3 1M with 20-bit dynamic range, zero self-noise and photon-counting pixels is used as the detection system.

Some technical and methodological work was done since the start of the beamline operation to improve the user experience. In particular, the new sample holders were designed and constructed,

allowing to place up to 5 liquid samples and up to 20 powder samples for the experiment simultaneously. The sample holder for the liquid samples can be thermostabilized in the range from -50°C to +90°C. The new construction of the vacuum tube, which contains detachable sections of different size, was developed to speed up the process of changing the sample-to-detector distance. Two last blocks of slits, initially with tungsten carbide blades, were replaced by the scatterless slits (JJ X-Ray, Denmark), this resulted in a complete elimination of the scattering on the slit blades. Also the vacuum windows were changed from 15-micron mylar to 40-micron mica after conducting some test experiments to reduce the background scattering. As the result, the beamline signal-to-noise ratio become 3.5 times better, which allowed to conduct experiments on weakly scattering solutions.

Two examples of recent works demonstrating the opportunities of the BioMUR beamline are shown. The first one is the research aiming to determine the process of structural changes before the crystal formation in the KDP solutions - we have shown that mainly octamers of the KDP lead to the further process of crystallization. The second one is the experimental proof that the right aptamer to the RBD-protein of the SARS-CoV-2 forms a stable complex in the solution. We've obtaines the SAXS curves and built the pair distance distribustion functions showing that the size and shape of the complex change significantly, which means that the aptamer binds to the protein.

X-RAY STUDIES OF CONCREMENTS IN THE CHOROID PLEXUS AND PINEAL GLAND OF THE HUMAN BRAIN #23

Submitted by **Denis Zolotov**
For track: SR for medicine and biology application
Authors:

- Denis Zolotov (FSRC “Crystallography and Photonics” RAS)
- Anna Ivanova (FSRC "Crystallography and Photonics" RAS)
- Alexey Buzmakov (FSRC "Crystallography and photonics" RAS)
- Irina Dyachkova (FSRC "Crystallography and Photonics" RAS)
- Yuri Krivonosov (FSRC "Crystallography and photonics" RAS)
- Victor Asadchikov (FSRC "Crystallography and photonics" RAS)
- Michela Fratini (Institute of Nanotechnology- CNR)
- Alessia Cedola (Institute of Nanotechnology- CNR)
- Francesca Palermo (Institute of Nanotechnology- CNR)
- Inna Bukreeva (Institute of Nanotechnology- CNR)
- Olga Junemann (FSBSI Research Institute of Human Morphology)
- Sergey Saveliev (FSSI Research Institute of Human Morphology)

Physiological (cerebral) intracranial calcifications are frequently observed by radiologists. It is generally believed that their formation is associated with aging changes. It is asymptomatic and detected by chance during neuroimaging. Calcification deposits can be localized in different areas of the brain, namely in the pineal gland, chorioid plexuses, etc. Physiological calcification of cerebral structures is clinically insignificant, but the composition and causes of intracranial calcifications remain unstudied. Studies of calcified deposits occurring simultaneously in different brain structures contribute to the understanding of the mechanism of concrements formation. In addition, they can provide a basis for identifying and comparing pathological and physiological changes occurring in brain structures containing calcifications.

In this work, a detailed study of physiological calcifications in the pineal gland and choroid plexus of the human brain was performed using various X-ray methods: micro-CT, high-resolution phase-contrast tomography (XPCT), diffraction (XRD) and topography (XRDT).

The XRDT experiment revealed the presence of crystalline mineral grains and subgrains in the concrements. The XRD results show that pineal gland concrements consist mainly of crystalline hydroxyapatite with traces of other minerals, whereas calcified choroid plexus concrements have both organic and inorganic composition with a lamination of alternating materials rich in organics and

minerals (hydroxyapatite with a low degree of crystallinity). It was found that the most common morphological structure of calcification in the choroid plexus is the alternation of calcified and non-calcified layers. Analysis of XPCT-images showed that the concrements have different characteristics for each brain structure, i.e., the formation of calcified deposits in different brain structures should be considered structurally specific. In addition, XPCT studies have revealed that once calcification begins, layers are deposited around the primary center, forming individual concrements that may subsequently aggregate together to form larger conglomerates. The XRD method showed that individual concrements can reach hundreds of microns in size, and aggregated conglomerates resembling a mulberry berry are up to several mm in size. Calcospherites in the choroid plexus are mostly regular spherical in shape with a concentric lamination structure developing from a single primary center of their formation. The concrements in the pineal gland are lobed and more irregularly shaped. In addition, irregularly shaped microgranules scattered in the pineal gland parenchyma were found.

The work was supported by the Ministry of Science and Higher Education within the State assignment FSRC "Crystallography and Photonics" RAS in part of "interpretation of tomographic data", The bilateral project CNR/RFBR (2018- 2020) - accordo CNR-RFBR delle Relazioni Internazionali (CUP B86C17000210005 & Russian number 18-52-7819), in part of "absorption, diffraction, and phase-contrast X-ray microtomography".

FLAT-FIELD CORRECTION ON X-RAY TOMOGRAPHIC IMAGES USING DEEP CONVOLUTIONAL NEURAL NETWORKS. #24

Submitted by **Artem Grigorev**
For track: X-ray structural analysis
Authors:

- Artem Grigorev (FSRC "Crystallography and Photonics" RAS)
- Alexey Buzmakov (FSRC "Crystallography and photonics" RAS)

X-ray microtomography allows restoring the internal structure of an object from a set of its projection images. The quality of the projections also depends on the quality of the tomographic reconstruction. One of the main stages of processing X-ray projection images is normalization (flat-field correction) to an empty beam, i.e. to a beam that does not contain an object. Usually, empty beams are registered at the beginning or at the end of the measurement and then the object is no longer removed from the beam. However, the intensity and profile of the direct beam vary greatly during the tomographic measurement. This can happen both on laboratory X-ray microtomography setups, and on free-electron lasers, where each X-ray pulse can be very different from the subsequent ones, and on synchrotron radiation sources. To improve the results of such studies, it is necessary either to measure an empty beam several times when measuring an object, which significantly increases the study time of one sample, which is limited on synchrotron installations and free-electron lasers. For example, using a dynamic normalization method, which requires much more computing power and does not allow tracking changes in real-time.

We propose to use neural networks to solve the problem of normalization to an empty beam. The article describes the process of selecting deep convolutional neural network parameters to solve the normalization problem with the instability of an empty beam. It describes the training of this network and checks its operability on the generated data. The developed method was tested on X-ray laboratory and synchrotron microtomography measurements. The comparison of the quality of flat field corrections with the three methods (classical normalization, dynamic normalization, and normalization using a neural network) is presented.

The work was supported by the Ministry of Science and Higher Education within the State assignment FSRC "Crystallography and Photonics" RAS in part of "interpretation of tomographic data"

HIGH-RESOLUTION SYNCHROTRON X-RAY PHASE-CONTRAST TOMOGRAPHY STUDIES OF THE POST MORTEM HUMAN PINEAL GLAND #25

Submitted by **Yuri Krivonosov**

For track: SR for medicine and biology application

Authors:

- Victor Asadchikov (FSRC "Crystallography and photonics" RAS)
- Inna Bukreeva (Institute of Nanotechnology- CNR)
- Olga Junemann (FSBSI Research Institute of Human Morphology)
- Alessia Cedola (Institute of Nanotechnology- CNR)
- Francesca Palermo (Institute of Nanotechnology- CNR)
- Laura Maugeri (Institute of Nanotechnology- CNR)
- Ginevra Begani Provinciali (Institute of Nanotechnology- CNR)
- Nicola Pieroni (Institute of Nanotechnology- CNR)
- Alessia Sanna (Institute of Nanotechnology- CNR)
- Alexey Buzmakov (FSRC "Crystallography and photonics" RAS)
- Yuri Krivonosov (FSRC "Crystallography and photonics" RAS)
- Irina Dyachkova (FSRC "Crystallography and Photonics" RAS)
- Denis Zolotov (FSRC “Crystallography and Photonics” RAS)
- Marina Chukalina (FSRC “Crystallography and Photonics” RAS)
- Michela Fratini (Institute of Nanotechnology- CNR)
- Sergey Saveliev (FSSI Research Institute of Human Morphology)

In this work, we present the results obtained in the framework of the bilateral project (CNR-RFB) on the study of the limbic system in human brain [1].

In particular, the object of this study were the pineal glands of the human brain. The pineal gland (PG) is located in the hypothalamus, near the center of the brain, and it is the central structure of the circadian system that produces melatonin. PG plays an important role in regulating the circadian rhythm of the body. Calcium deposits are a common occurrence in human PG. They are progressively accumulated in PG tissue with age and are not usually considered pathology. It is expected that the examination of PG by high-resolution X-ray phase-contrast tomography will make it possible to visualize vessels, pinealocytes, neurons, and glial cells in them without using contrast agents. The study of the morphological structure of PG will contribute to further studies of age and sexual changes, as well as individual cytoarchitectonic differences. It can also help in understanding the mechanisms of circadian rhythm disorders in individuals suffering from neurodegenerative diseases.

Here we presented the nondestructive high-resolution 3D investigation of PG morphology at different scales: from the whole organ to the cell. We identified different tissues such as parenchyma, vascular network, calcified tissue, and calcifications. Methods of X-ray microtomography (micro-CT) with a pixel size of 9 microns (FSRC "Crystallography and Photonics" RAS), propagation-based phase-contrast tomography (XPCT) with pixel size of 1.28 microns and 0.64 microns (performed in collaboration with CNR Nanotec @ ESRF and @ Petra III) and histology were used to study the morphological structure of PG. Unlike standard imaging methods such as histology or micro-CT, XPCT enables the high-resolution visualization of both brain tissues conventionally x-ray transparent and x-ray absorbing calcification without destructive sectioning and the need for exogenous contrast agents.

We identified via micro-CT the morphometric parameters of the whole PG, such as the volume of pineal organs, the percentage of calcifications, and their average sizes for all sets of samples under investigation. Using XPCT we displayed in 3D with near-histological quality the PG lobular structure and pinealocytes surrounded by connective tissue spaces, PG vascular network, and calcifications of varying sizes embedded in a PG soft tissue. In addition, we detected PG lesions and visualized the degenerated tissue fine structure invisible in micro-CT. These results were confirmed by histological examinations.

The work was supported by the bilateral project CNR/RFBR (2018- 2020) - accordo CNR-RFBR delle Relazioni Internazionali (CUP B86C17000210005) & the Russian Foundation for Basic Research (Project Nos. 18-52-7819) in part concerning data processing and analysis, the Ministry of Science and Higher Education within the State assignment FSRC "Crystallography and Photonics" RAS in part of micro-CT experiments.
[1] Investigation of the human pineal gland 3D organization by X-ray phase contrast tomography. I Bukreeva, O Junemann, A Cedola, F Palermo, L Maugeri, GB Provinciali et al. // Journal of structural biology 2020, 212(3), 107659

ON THE PHASE CONSTITUTION OF AL - BASED METALLIC-INTERMETALLIC LAMINATE (MIL) COMPOSITES #26

Submitted by **Yulia Emurlaeva**
For track: X-ray structural analysis
Author: Yulia Emurlaeva (Novosibirsk State Technical University)

In recent decades, metallic-intermetallic laminate (MIL) composites based on Al-Ni, Al-Ti, Al-Zr, Al-steel, Al-Cu, Al-Co systems are of great interest in the scientific community. One of the ways to produce MIL composites is annealing of bimetal plates obtained using explosion welding. Intermetallic layer formed during annealing can contain only one phase, as well as two or more layers of different phase constitution. The phases in such interlayers differ significantly from each other both in the crystal structure and in the chemical composition.

In this work, the phase composition and structural features of the intermetallic layer formed during annealing at the interface of Al-Ti, Al-Ni, Al-Zr, Al-stainless steel, Al-Cu, Al-Co explosively-welded plates were studied. The annealing temperature did not exceed the melting temperature of the plates; the annealing duration was in the range from 1 up to 100 hours. The synchrotron X-ray diffraction method was used to determine the phase constitution of the layer. Diffraction patterns were obtained in the German Electron Synchrotron on the high-energy materials science beamline at the PETRA III accelerator. The photon energy was 100 keV, which corresponded to a wavelength of 0.124 Å. The cross-section of the beam was limited by a collimator with a gap of 0.2 mm. The sample was scanned in the direction from the Al to the pair metal with a step of 0.1 mm to assess the change in the phase constitution. Diffraction patterns were recorded using a Perkin Elmer two-dimensional detector with a resolution of 2048 × 2048 pixels2 and a pixel size of 200 × 200 μm2. The sample-to-detector distance was about 1.8 m. Each diffraction pattern was obtained by summing 40 frames with an exposure of 0.1 seconds.

Some studies were also carried out at the Siberian Center for Synchrotron and Terahertz Radiation at the station 8a based on the VEPP-4 accelerator. The photon energy was 69.5 keV and the exposure time was 2 minutes. X-rays passed through the sample with the thickness 0.7 mm, the beam size was 300 × 100 μm2 (vertically×horizontally).

The diffraction ring patterns were azimuthally integrated using the open-source pyFAI package developed for the Python programming language.

It was shown, that annealing of the explosively-welded Al - Ti composite results in two modifications of titanium trialuminide - TiAl3 with the D022 structure type and a Ti8Al24 superstructure. According to X-ray phase analysis, the volume fraction of Ti8Al24 increases as we close to the Ti - intermetallic interface. The Ti8Al24 superstructure can be considered as one of the long-period structures (LPS) in the Ti1+xAl3-x compounds formed at the Ti - intermetallic interface due to the lack of Al for the construction of stoichiometric TiAl3.

During annealing of the explosively-welded Al-Zr composite, only one phase is formed at the interface - ZrAl3 with the D023 structure type.

Annealing of Al - Ni composite at the initial stages shows the formation of a wide NiAl3 layer and much thinner Ni2Al3 layer. Further annealing causes an active growth of the Ni2Al3 intermetallic layer and a decrease in the NiAl3 thickness. Such redistribution of phases in the intermetallic layer is

due to the lack of nickel atoms diffusing to the NiAl3 layer through the Ni2Al3 layer, which leads to gradual depletion of the NiAl3 layer.

After annealing of the Al - stainless steel sample, the intermetallic layer consists of Fe4Al13 (C2/m), Fe2Al5 (Cmcm) and Fe2.024Al5.401 (P21/c) compounds. The intermetallic layer of the Al - Cu sample consists of Cu9Al4 (cubic system, P-43m), CuAl2 (tetragonal system, I4/mcm), Cu4Al3 and CuAl (orthorhombic system) compounds. After annealing the Al - Co sample, the Co2Al9 (P21/c), Co4Al13 (Pmn21) and Co2Al5 (P63/mmc) compounds were found in the intermetallic layer.

The work was carried out according to the project No. C-22-13 of the competition for young scientists on the topic “Features of structural-phase transformations and growth of intermetallic compounds at the boundary of explosively-welded materials” in 2022. Research were conducted at core facility "Structure, mechanical and physical properties of materials" (№ 13.ЦКП.21.0034, 075-15-2021-698).

INVESTIGATION OF THE THIACALIX[4]ARENES ELECTRONIC STRUCTURE AND FEATURES BY RAS, RES, XPS AND QUANTUM CHEMISTRY METHODS AND THEIR SENSORY RESPONSE IN HYBRID MATERIALS WITH CARBON NANOTUBES #27

Submitted by **Svetlana Lavrukhina**

For track: X-ray spectroscopy

Authors:

- Svetlana Lavrukhina (Nikolaev Institute of Inorganic Chemistry)
- Anastasia Fedorenko
- Lev Mazalov
- Vitaly Sysoev
- Anna Makarova
- Galina Semushkina (Nikolaev Institute of Inorganic Chemistry)
- Lubov Bulusheva
- Alexander Okotrub

The development of sensor materials for the detection of toxic, explosive and other dangerous gases and vapors is an actual problem. Various carbon nanotube (CNT) gas sensors for detecting toxic gases with high selectivity, such as NO2, NH3, H2S, organic vapor, etc., can achieve response at room temperature due to fast response, large absorption capacity and stability to the environment [1-4]. At the same time, chemical functionalization or the formation of heterojunctions with other materials improves the sensor properties of CNTs [5–8]. The sensitivity and selectivity of gas sensors can be improved using the principles of molecular recognition and molecular receptor. Calixarenes (CAs) represent an interesting and important class of molecular receptors due to their variable cavity sizes and the presence of two separate hydrophobic and hydrophilic regions, which may play an important role in the early detection of pollutant gases in the air [9-11]. CA and TCA can adopt cone or basket structures, creating voids that can encapsulate ions or small molecules such as gases. An important feature of CA and TCA is the possibility of molecules functionalization by replacing the upper and/or lower rims with various functional groups, as well as by replacing methylene bridges with S, SO, SO2, N, NO–bridges, etc., which makes it possible to change the selective and reactive ability of these compounds. Promising objects for sensor applications are hybrid structures based on thin films of low-dimensional materials (CNTs) acting as carriers with molecular receptors deposited on their surface, such as calixarenes (CA) and thiacalixarenes (TCA).

The receptor and selective properties of materials are related to the features of the electronic structure, which can be described using the methods of X-ray absorption spectroscopy (XAS), emission spectroscopy (XES) and X-ray photoelectron spectroscopy (XPS), in combination with quantum chemical methods.

In this work, the electronic structure of TCA molecules is studied using the experimental methods of XPS, XPS, RSP and quantum chemistry methods. Quantum-chemical calculations of the electronic

structure of TCA molecules were carried out in the ADF software package by the DFT method. XANES calculations of the carbon spectrum were performed in the ground state of molecules and the Z+1 model. The X-ray emission spectra were calculated in the SAOP approximation in the ground state. Fukui calculation In the Orca 4.2.1 program was performed to determine the most preferable sites for electrophilic and nucleophilic attack. Based on the obtained experimental and theoretical data, the composition and energy position of the HOMO and LUMO of molecules were studied, possible donor and acceptor centers were determined, and the receptor and selective properties were compared with the electronic structure of the compounds under study.

1. G.P. Evans, D.J. Buckley, N.T. Skipper, I.P. Parkin, Single-walled carbonnanotube composite inks for printed gas sensors: enhanced detection of NO2,NH3, EtOH and acetone, RSC Adv. 4 (2014) 51395–51403.

2. F. Rigoni, S. Tognolini, P. Borghetti, G. Drera, S. Pagliara, A. Goldoni, L.Sangaletti, Enhancing the sensitivity of chemiresistor gas sensors based onpristine carbon nanotubes to detect low-ppb ammonia concentrations in theenvironment, Analyst 138 (2013) 7392–7399.

3. J. Chaste, A. Eichler, J. Moser, G. Ceballos, R. Rurali, A. Bachtold, Ananomechanical mass sensor with yoctogram resolution, Nat. Nanotechnol. 7(2012) 301–304.

4. P. Vichchulada, Q. Zhang, M.D. Lay, Recent progress in chemical detectionwith single-walled carbon nanotube networks, Analyst 132 (2007) 719–723.

5. Ellis, J. E.; Star, A. Carbon Nanotube Based Gas Sensors toward Breath Analysis. ChemPlusChem 2016, 81 (12), 1248−1265.

6. Dai, M. J.; Zhao, L. P.; Gao, H. Y.; Sun, P.; Liu, F. M.; Zhang, S.; Shimanoe, K.; Yamazoe, N.; Lu, G. Hierarchical Assembly of α-Fe2O3 Nanorods on Multiwall Carbon Nanotubes as a High-Performance Sensing Material for Gas Sensors. ACS Appl. Mater. Interfaces 2017, 9 (10), 8919−8928.

7. Seekaew, Y.; Wisitsoraat, A.; Phokharatkul, D.; Wongchoosuk, C. Room Temperature Toluene Gas Sensor Based on TiO2 Nanoparticles Decorated 3D Graphene-Carbon Nanotube Nanostructures. Sens. Actuators, B 2019, 279, 69−78.

8. Liu, S. F.; Moh, L. C. H.; Swager, T. M. Single-Walled Carbon Nanotube-Metalloporphyrin Chemiresistive Gas Sensor Arrays for Volatile Organic Compounds. Chem. Mater. 2015, 27 (10), 3560−3563.

9. Gutsche, C.D.: Calixarenes, Monographs in Supramolecular Chemistry, vol. 1. Royal Society of Chemistry, Cambridge (1989)

10. Gutsche, C.D.: Calixarenes Revisited. Royal Society of Chemistry, Cambridge (1998)

11. Chawla, H.M., Pant, N., Kumar, S., Kumar, N., Black, D.S.C.: In Chemical Sensors: Fundamentals of Sensing Material. In: Korotcenkov, G. (ed.) Polymers and Other Materials, vol. 3. Momentum Press, New York (2010)

SMART TOMO ENGINE NOVEL TOMOGRAPHY RECONSTRUCTION TOOL #28

Submitted by **Mikhail Shutov**

For tracks: SR for medicine and biology application, SR technological application and X-ray apparatus

Authors:

Mikhail Shutov[1,3], Anastasia Ingacheva[1,2], Danil Kazimirov[1,3], Andrei Yamaev[1,3], MaratGilmanov[1,2], Alexey Buzmakov[1,4], Marina Chukalina[1,2,4], Dmitry Nikolaev[1,2,5], Dmitry Polevoy[1,6,7], Vladimir Arlazarov[1,5,6], Konstantin Bulatov[1,5,6]

[1]Smart Engines LLC, 117312, Russia, Moscow, 60-letiya Oktyabrya Ave, 9

[2]Institute for Information Transmission Problems RAS, 127051, Russia, Moscow, Karetny per. 19, build. 1

[3]Moscow State University, Leninskie Gory, Moscow 119991, Russia

[4]FSRC “Crystallography and Photonics” RAS, 119333, Russia, Moscow, Leninskiy Prospekt, 59

[5]The Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, 141701,

Moscow Region, Russian Federation
[6]Federal Research Center "Computer Science and Control" of the Russian Academy of Sciences, Vavilova str. 44b2 , Moscow, Russia, 119333
[7]National University of Science and Technology MISIS, Moscow, Russia

Computed tomography is spreading into daily life at an incredible speed. Despite the fact that the first commercial scanner came out more than 50 years ago, the technology, that can highlights internal morphology structure with nanometer resolution by nondestructive way, does not stand still and with the development of hardware (advanced sychrotron beamlines and laboratory set-ups), it is required to develop and implement new fast algorithms for reconstruction, for big data loading and saving, and for convenient visualization of reconstruction results.

In our talk we present our novel reconstruction tool the Smart Tomo Engine (STE) developed by Smart Engines Service LLC [1]. STE is a cross-platform software that implements fast [2, 3] and precise reconstruction algorithms, artifacts reduction methods and data 2D and 3D visualization tool. It can be installed on the beamline or on a new laboratory set-up. Typical STE tomography reconstruction workflow consists of the following steps: loading the source data, correcting geometry parameters (like rotation axis position search and correction), tomography reconstruction, artifacts reduction [4, 5], visualization and saving results. The input set of projections can be loaded from different types of format - TIFF (float32, uint16, uint32), PNG (uint16, uint32), DICOM, DICOMDIR, Nexus. The STE supports various CT scanner system geometries that can be combined from beam geometry and scanning scheme, Including any-time approach [6]. Beam geometry is a model of X-ray propagation. Supported geometries: parallel (2D, 3D), fan (2D), cone (3D). Scanning scheme is the relative position of the x-ray tube, the object, and the x-ray detector for all time of the tomographic experiment. Supported schemes in STE: layered circular (layer-by-layer), helical (spiral).

At the first stage of loaded data processing, the flat field correction is performed: the dark current is taken into account if such frames are present in the input dataset; then the images are normalized to frames of the empty beam and, if necessary, the logarithm is taken. Additionally, the STE can automatically search for the axis of object rotation, perform correction of ring artifacts and automatically correct data in order to suppress artifacts caused by polychromatic radiation.

Reconstruction algorithms for layer-by-layer 2D and/or true 3D reconstruction of received data with a circular scan path are also available in the Smart Tomo Engine. In STE we use classical reconstruction algorithms, such as Filtered Back Projection (FBP), Feldkamp, Davis and Kres algorithm (FDK), Direct Fourier Reconstruction method (DFR), Simultaneous Iterative Reconstruction Technique (SIRT), SIRT with Total Variation (TV) regularization, the fastest and the most modern algorithm reconstruction algorithm - Hough based Filtered Back Projection (HFBP) and the fastest iterative reconstruction algorithm - Hough based Simultaneous Iterative Reconstruction Technique (HSIRT). The STE contains an iterative algorithm for metal artifact suppression based on bilateral filter. The STE also provides an iterative algorithm for expanding the reconstruction area. It was created for the case when the entire object does not fit into the field of view of the detector. STE implements x64 compatible CPU, ARM processors, and GPU accelerators (CUDA).

The result of the reconstruction can be viewed layer by layer in different color palettes or in a 3D visualizer. The 3D visualizer presents three types of visualization of the reconstructed volume: monochrome, translucent color and solid visualization. A monochrome rendering type is a grayscale rendering of an image. Type translucent color displays a three-dimensional reconstruction in the form of a translucent volume, according to the laws of light absorption. The solid type renders a 3D continuous isosurface, while the brightness level is set by the user himself in the graphical interface. The reconstruction result can be saved layer by layer in TIFF (float32), PNG (uint8), DICOM formats, as well as in a two-dimensional image of three-dimensional visualization.

This work was partly supported by RFBR 20-07-00934.

[1] Description of the smart tomo engine software. https://smartengines.com/ocr-engines/tomo-engine/, accessed on 3 May 2022.

[2] DOI: http://dx.doi.org/10.14529/mmp200107
[3] DOI: http://dx.doi.org/10.31857/S0235009220010072
[4] DOI: http://dx.doi.org/10.1117/12.2557499
[5] DOI: http://dx.doi.org/10.1155/2019/1405365
[6] DOI: http://dx.doi.org/10.1109/ACCESS.2020.3002019

OPTICAL PROPERTIES OF SPUTTERED THIN ZINC SULFIDE FILMS IN THE MID-INFRARED AND THZ RANGE #29

Submitted by **Vasily Gerasimov**
For track: THz radiation aplication
Authors:
- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)
- Valeriia Kukotenko (Budker Institute of Nuclear Physics)
- Aleksey Lemzyakov (Budker INP SB RAS)
- Ivan Azarov (Rzhanov Institute of Semiconductor Physics SB RAS)
- Nazar Nikolaev (Institute of Automation and Electrometry SB RAS, Novosibirsk, 630090 Russia)

Sputtered thin Zinc sulfide (ZnS) films are dielectrics in the IR and THz ranges. Because of high refractive index and low absorption in the THz range, ZnS films are used as covering dielectric layers of conducting surfaces in the THz plasmonics. To develop plasmonic methods for a surface diagnostics, ZnS films can be used as reference films; therefore, it is important to know their optical properties. The optical constants for bulk ZnS are presented in the reference literature, but there are no data for thin layers. Besides, the structure and homogeneity of films can be significantly depend on sputtering technique, conditions, substrate material and the surface preparation method. In this work mid-infrared and THz optical properties of ZnS sulfide films with about 1-3 mm thick sputtered on different substrates (quartz, silicon, gold layers) with electron beam evaporation were studied using by THz time-domain spectroscopy, ellipsometry and spectrophotometry. Their surface roughness and homogeneity were tested with electron and atomic force microscopy.

COMPARISON CONVERGENCE OF THE RECONSTRUCTION ALGORITHMS FOR MONITORED TOMOGRAPHY ON SYNTHETIC DATASET #30

Submitted by **Anastasia Ingacheva**
For tracks: SR for medicine and biology application, SR technological application and X-ray apparatus
Authors:
- Anastasia Ingacheva (Smart Engines LLC, 117312, Russia, Moscow and Institute for Information Transmission Problems RAS, 127051, Russia, Moscow)
- Konstantin Bulatov (Smart Engines LLC, 117312, Russia, Moscow, Federal Research Center "Computer Science and Control" of the Russian Academy of Sciences, 119333, Russia, Moscow)
- Zhanna Soldatova (Smart Engines LLC, 117312, Russia, Moscow; National University of Science and Technology MISIS,119049, Russia, Moscow)
- Kristina Kutukova (Fraunhofer Institute for Ceramic Technologies and Systems, 01109 Dresden, Germany)
- Marina Chukalina (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow; FSRC “Crystallography and Photonics” RAS, 119333, Russia, Moscow)
- Dmitry Nikolaev (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow)

- Vladimir Arlazarov (Smart Engines LLC, 117312, Russia, Moscow; Federal Research Center "Computer Science and Control" of the Russian Academy of Sciences, 119333, Russia, Moscow)
- Ehrenfried Zschech (deepXscan GmbH, 01109 Dresden, Germany)

X-ray computed tomography (XCT) is a method of non-invasive study of the internal structure of an object using a set of measured transmission images. In recent decades, XCT gained enormous popularity because this type of investigation is nondestructive and reliable. However, an inevitable concomitant phenomenon during a tomographic study is the radiation dose received by the object. This can potentially cause the occurrence of diseases associated with radiation exposure in wildlife objects and damage, up to destruction, of inanimate objects. Therefore, as soon as X-rays were used as a diagnostic tool, the methods for low-dose XCT began to arise. At the moment, it is possible to reduce the dose in several ways: to reduce the exposure time of a single image, to reduce the number of measured images or to apply the method of monitored tomographic reconstruction (MTR). However, to reduce the exposure time leads to the increase of noise in the reconstructed image, which usually leads to a loss of resolution. Reducing the number of projections also leads to a reduced resolution, differently for different reconstruction algorithms. The number of projections (angles sampling) needed to reconstruct a valid image depends on the scanning scheme, the size of the region reconstructed, and the spatial resolution to be achieved. A method that does not depend on the above conditions is the MTR, the study of which is the subject of this work.

The monitored tomographic reconstruction technique is a pioneering method for low-dose X-ray computed tomography that reduces the time of the experiment and the radiation dose. The method was proposed in 2020 by Bulatov et al. [1]. The acquisition of the projections in the monitored reconstruction technique is guided by a scanning protocol built on similar experiments to reach the predetermined quality of the reconstruction. The construction of such a protocol allows to set a threshold for an expectation of the reconstruction quality, which could then be converted to a stopping threshold. In a tomographic study with MRT, the reconstruction process begins from the moment the first projections are obtained and stops when the stopping threshold is achieved. This method allows achieving the same average reconstruction quality as in ordinary tomography while using lower mean numbers of projections. In [1], this approach was demonstrated for the example of real micro-XCT data applying a Filtered Back Projection reconstruction algorithm.

In this paper, we, for the first time, systematically study the MTR technique for several reconstruction algorithms on synthetic data. The phantoms used to obtain synthetic data represent objects with different morphological structures are used to calibrate various parameters of XCT scanners. We use classical reconstruction algorithms, such as Filtered Back Projection (FBP), Direct Fourier Reconstruction method (DFR), Simultaneous Iterative Reconstruction Technique (SIRT), SIRT with Total Variation (TV) regularization, the fastest and the most modern algorithm reconstruction algorithm – Hough-based Filtered Back Projection (HFBP) [2] and the fastest iterative reconstruction algorithm – Hough-based Simultaneous Iterative Reconstruction Technique (HSIRT) [3]. Our goal is to answer the question whether it is possible, under ideal conditions, to obtain a dose reduction for various tomographic reconstruction algorithms using MTR. According to the constructed plots, the dependence of the convergence of reconstruction algorithms on the number of projections selected both in the classical scanning protocol and in the monitoring allow to conclude that the monitored tomographic reconstruction approach is applicable for a broad field of applications. It was shown that the reduction of the mean number of projections with retaining the mean quality when stopping the reconstruction process according to the MTR protocol happens for each evaluated reconstruction algorithm, not only for the FBP as demonstrated previously. While it was shown before that the MTR demonstrates effect if the quality is measured as the distance to a final result achievable with a full protocol, in this paper it is also shown that the effect is demonstrable if a phantom image is considered as a target.

This work was partly supported by RFBR by grant 20-07-00934.

[1] Bulatov, K., et al. "Monitored reconstruction: Computed tomography as an anytime algorithm." IEEE Access 8 (2020): 110759-110774.
[2] Dolmatova, A., Chukalina, M., Nikolaev, D.: Accelerated fbp for computed tomography image reconstruction. In: 2020 IEEE International Conference on Image Processing (ICIP). pp. 3030{3034. IEEE (2020)
[3] Prun, V.E., Buzmakov, A.V., Nikolaev, D.P., Chukalina, M.V., Asadchikov, V.E.: A computationally efficient version of the algebraic method for computer tomography. Automation and remote control 74(10), 1670{1678 (2013)

HIGH-TEMPERATURE IN SITU SYNCHROTRON XRD STUDY OF CR/MO-COATED ZR-1NB ALLOY #31

Submitted by **Maxim Syrtanov**
For track: X-ray structural analysis
Authors:
- Maxim Syrtanov (Tomsk polytechnic university)
- Egor Kashkarov (Tomsk polytechnic university)
- Anastasia Abdulmenova (Tomsk polytechnic university)
- Dmitrii Sidelev (Tomsk polytechnic university)

Currently, many countries with an advanced nuclear industry are developing accident tolerant fuel (ATF) claddings to improve the oxidation resistance and mechanical properties of Zr-based alloys under both normal operation (360 °C, 18.6 MPa) and possible accidental conditions such as loss of coolant accident (LOCA) [1, 2]. One of the promising methods to protect zirconium alloys is Cr-based coating deposition [3, 4]. At high temperature (over 1200 °C) the Cr-Zr interdiffusion at the interface increases significantly, which leads to accelerated oxidation of the Zr-1Nb alloy. One way to solve this problem is to develop a new type of Cr-based protective coating with a barrier sublayer that can prevent Cr-Zr interdiffusion [5].

In this paper, a molybdenum barrier layer is proposed as a sublayer between the Zr-1Nb alloy and Cr coating. Bilayer Cr (8 μm)/Mo (3 μm) and single-layer Cr (8 μm) coatings were oxidized in air at 1100 °C during 15-60 min. In situ XRD measurements were performed to understand the behavior of molybdenum diffusion at linear heating up to 1250 °C in vacuum using synchrotron radiation at the station “Precision diffractometry II” at Siberian Synchrotron and Terahertz Radiation Center of the Budker Institute of Nuclear Physics of the Siberian Branch of Russian Academy of Science. According to SEM, XRD, in situ XRD and optical microscopy it was established that a 3 μm-thick barrier Mo layer can limit Cr-Zr interdiffusion under high-temperature oxidation. The thickness of residual Cr after 60 minutes of oxidation is greater in Cr/Mo-coated Zr alloy (~5 μm) compared to single-layer Cr-coated sample (~3.5 μm). The thickness of Cr2O3 layer after oxidation of Cr- and Cr/Mo-coated samples are similar that indicates insignificant influence of the Mo layers on the outer Cr oxidation resistance. However the diffusion of molybdenum at high temperature leads to the formation of Cr3Mo and Mo2Zr phases at the interfaces (Cr protective layer/Mo layer and Mo layer/Zr-1Nb alloy). The thickness of the Cr-Mo and Mo-Zr interdiffusion layers grows with increasing oxidation time. The thickness of the indicated layers is equal ~2 and 20 μm after 60 min of oxidation in air at 1100 °C.

The research was funded by Russian Science Foundation (grant No. 21-79-00175).
[1] K. Terrani, Journal of Nuclear Materials, 501, 13-30 (2018)
[2] S. Bragg-Sitton, Nuclear News, 57 (3), 83-91 (2014)
[3] J. Yang, M. Steinbrück, C. Tang, M. Große, J. Liu, J. Zhang, D. Yun, S. Wang, Journal of Alloys and Compounds, 895 (162450), 1-23 (2022)
[4] E. Kashkarov, et al., A. Lider, Coatings, 11 (5), 1-31 (2014)
[5] X. Wang, Y. Liao, C. Xu, H. Guan, M. Zhu, C. Gao, X. Jin, P. Pang, J. Du, B. Liao, W. Xue, Journal of Alloys and Compounds, 883 (160798), 1-13 (2021)

NOVEL EXPERIMENTS ON THZ PLASMONICS USING NOVOSIBIRSK FREE ELECTRON LASER #32

Submitted by **Vasily Gerasimov**

For track: THz radiation aplication

Authors:

- Vasily Gerasimov (Budker Institute of Nuclear Physics SB RAS)
- Boris Knyazev (Budker Institute of Nuclear Physics)
- Alexey Nikitin (Scientific and Technological Center for Unique Instrumentation of RAS)
- Ildus Khasanov (Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences)
- Aleksey Lemzyakov (Budker INP SB RAS)
- Oleg Kameshkov (BINP SB RAS)
- Natalya Osintseva (INP SB RAS)
- Valeriia Kukotenko (Budker Institute of Nuclear Physics)
- Vladimir Pavelyev (Samara University)

В докладе будет представлен обзор последних экспериментов, по исследованию терагерцовых поверхностных плазмон-поляритонов (ППП), распространяющихся по плоским, изогнутым и цилиндрическим проводящим поверхностям, а также локализованным состояниям, которые выполнялись на Новосибирском лазере на свободных электронах (НЛСЭ) в последние годы.

Было показано, что эффективность захвата ТГц поверхностных электромагнитных волн методом дифракции на краю составляет десятки процентов, а длины пробега ППП на плоской металл-диэлектрической поверхности достаточно большие (порядка десятка сантиметров), по сравнению с видимым и ИК диапазонами. Продемонстрировано, что ТГц поверхностными волнами можно эффективно управлять с использованием плоских зеркал и диэлектрических делителей, а также направлять по изогнутым поверхностям. Все это позволяет реализовать различные оптические схемы макроскопических масштабов с использованием ТГц ППП. Например, впервые продемонстрирована возможность локации объектов, скрытых за линией горизонта на проводящей искривленной поверхности. С использованием НЛСЭ реализована рефрактометрия проводящей поверхности с использованием плазмонного интерферометра Майкельсона, позволяющая измерять диэлектрические константы металлических поверхностей и пленок толщиной до 100 нм, нанесенных на эти поверхности.

Для рефрактометрии диэлектрических пленок, жидкостей и газовых сред создан НПВО спектрометр (в конфигурации Отто), где за призмой помещается субволновая металлическая одномерная решетка. На решетке в угловом спектре при определенном угле возбуждается плазмонный резонанс. На той же установке продемонстрировано возбуждение широких плазмонных резонансов на беспримесном антимониде индия, который планируется использовать для плазмонной микроскопии объектов.

Впервые продемонстрировано возбуждение плазмонов с орбитальным угловым моментом на осесимметричных односвязных передающих линиях при дифракции на входном торце вихревых радиально поляризованных пучков. Показано, что эти плазмоны распространяются на расстояние до 150 мм по винтовым траекториям, дифрагируют на конце линии и преобразуются в объемные волны с орбитальным угловым моментом, имеющие тот же топологический заряд, который имел возбуждавший плазмоны пучок. Мы полагаем, что, используя комбинации вихревых пучков на входе, можно создать плазмонные мультиплексные коммуникационные линии.

ИССЛЕДОВАНИЕ СПЕКТРОВ ИЗЛУЧЕНИЯ ПЛАЗМЫ, СОЗДАВАЕМОЙ МОЩНЫМИ ПИКОСЕКУНДНЫМИ ЛАЗЕРНЫМИ ИМПУЛЬСАМИ, В ДИАПАЗОНЕ ДЛИН ВОЛН 6-14 Å #33

Submitted by **Dmitry Nosulenko**
For track: X-ray spectroscopy
Author: Дмитрий Носуленко
Co-authors:

- Егор Борисов
- Денис Вихляев
- Дмитрий Гаврилов
- Семен Девятков
- Андрей Емельянов
- Николай Карлыханов
- Петр Лобода
- Антон Овечкин
- Сергей Пахомов
- Анатолий Потапов
- Екатерина Пряхина
- Николай Титаренко

В настоящее время одним из направлений исследований в области физики высоких плотностей энергии является изучение спектральных пробегов рентгеновского излучения в веществе, нагретом до температур в несколько десятков или сотен эВ. Для получения экспериментальных данных по пробегам часто применяется метод зондирования, когда регистрируется изменение спектра источника рентгеновского излучения после прохождения сквозь слой вещества, разогретого до высокой температуры. Для проведения таких экспериментов хорошо подходят мощные лазерные установки с ультракороткой длительностью импульса, которые позволяют создавать как вещество в нужном состоянии, так и источник зондирующего рентгеновского излучения. Основными требованиями к источнику подсветки являются высокая яркость и отсутствие выраженных линий и скачков в интересующем диапазоне энергий. В экспериментах кроме спектра поглощения должны быть измерены плотность и температура плазмы в момент зондирования. Эти параметры могут быть определены по рентгеновским спектрам излучения плазмы из соотношения интенсивностей и формы линий многозарядных ионов.

В работе приведена конструкция спектрографа Иоганна на основе кристалла бифталата калия, а также результаты, полученные с его помощью в экспериментах по облучению различных мишеней лазерными импульсами с интенсивностью 1017−1019Вт/см2. В диапазоне длин волн 7-14 Å измерены спектры излучения мишеней, содержащих церий, самарий и гадолиний, которые могут быть использованы в качестве источника рентгеновской подсветки в экспериментах по исследованию спектральных пробегов излучения в плазме меди и алюминия. Зарегистрировано линейчатое излучения H- и He-подобных ионов алюминия при облучении мишеней толщиной от 1 до 400 мкм. Для мишеней толщиной 1 мкм, облучаемых импульсами с интенсивностью 1017Вт/см2, проведены газодинамические расчёты и расчёты переноса излучения с учётом неравновесности ионного состава плазмы. Получено удовлетворительное согласие расчетных и экспериментальных спектров.

COMPLEX STUDY OF LOOSE CAVE SEDIMENTS OF THE CENTRAL ASIAN REGION USING XRF SR #34

Submitted by **Julia Sholokhova**
For track: X-ray fluorescent analysis
Authors:

- Julia Sholokhova (IGC SB RAS)
- Ekaterina Bazarova (IEC SB RAS)

Loose cave deposits, due to the constancy of temperature, pressure, as well as the lack of light and suppression of biological processes in underground conditions, are able to remain un-changed for a long time and are an attractive object for various kinds of geological and geo-chemical studies.

The presented material is a continuation of the work on the study of the cave-mine Kan-i-Gut [Bazarova et al., 2016], located in Batken district in south-western Kyrgyzstan, in the Sary-Too massif.

We carried out a comprehensive study of 11 samples of loose sediments taken at different points of the cave. The mineral composition of all samples was determined in Irkutsk at the ana-lytical center of the Institute of the Earth Crust of the Siberian Branch of the Russian Academy of Sciences by X-ray phase analysis on the diffractometer DRON-3 on CuKά-radiation. In addi-tion, the mineral composition of the samples (except for the surface soil sample) was determined on a scanning electron microscope VEGA 3 LMH with the system of X-ray energy dispersive microanalysis INCA Energy 350/X-max 20 at the Mining Institute of the UrO RAS in Perm by analyst Korotchenkova O. The elemental composition of the samples was analyzed by X-ray fluorescence analysis with synchrotron radiation at the experimental station "RFA-SR" at Sibe-rian Center for Synchrotron and Terahertz Radiation (BINP SB RAS). The measurement tech-nique and description of the experiment are presented in detail in [Markova et al., 2012].

As a result of the XRF SR study of the sediments, the contents of K, Ca, Ti, V, Mn, Fe, Cu, Zn, Ga, As, Br, Rb, Sr, Y, Zr, Mo, and Ag were determined. The elemental composition of the loose sediments is closely related to the mineral composition of the sample, indicating the pres-ence of certain minerals. Higher concentrations of Mn, Fe, and Zn are noted for samples from the lower and middle parts of the subsurface system. X-ray phase analysis and electron microscopy in these samples were identified minerals such as goethite FeO(OH), hematite Fe2O3, oxides Mn, gypsum CaSO4-2H2O, smithsonite ZnCO3, which is consistent with the elemental composition. Also in these samples increased, relative to the samples from the upper horizon, the content of Ag, As, Mo, and Y was noted. We were not found minerals, the presence of which could cause an increase in concentrations of these elements, but earlier researchers noted the presence of na-tive silver in manganese oxides [Sosedko, 1935], and the increased content of As may be associ-ated with an admixture of this element in marcasite. As for Mo, it is probably also an impurity in sulfides. Increased concentrations of Y may indicate undiscovered Y-bearing minerals associated with Mn- and Fe-oxides; in addition, elevated concentrations of this element may be contained in calcite [Znamensky and Znamenskaya, 2021], since Y and Ca are correlated in the samples. For the sample from the near-entrance grot observed sharply increased K content relative to other samples. X-ray phase analysis did not reveal in this sample K-containing minerals, but the study of the sample on the electron microscope revealed the mineral gergeite K2Ca5(SO4)6-H2O, previ-ously described only for the salt deposits [Tchaikovsky, 2011].

Thus, using three analytical methods, including XRF SR, a comparison of the elemental and mineral composition of the loose sediments of such unusual natural-technogenic object as Kan-i-Gut cave-mine was carried out. As a result, the mineral gergeite was identified for this ob-ject for the first time. The obtained concentrations of Mn, Fe, and Zn agree with the minerals identified in the samples from the middle and lower horizons. Given the increased Y concentra-tions in the loose formations of the studied samples, we can assume the presence of Y- and REE-bearing minerals, which may be the source of the previously noted [Filippov and Mavlyanov, 2013] elevated radioactivity of rocks and ores in the cave.

References

Bazarova E.P., Markova Yu.N., Zolotarev K.V., Rakshun Ya.V., Uschapovskaya Z.F.. First Geochemical Data on Loose Sediments in the Kan-i-Gut Cave Mine (Central Asia) by Synchro-tron Radiation XRF Analysis // Journal of Surface Investigation. X-ray, Synchrotron and Neu-tron Techniques, 2016, Vol. 10, No. 2, pp. 361-364

Markova Y.N., Kerber E.V., Anchutina E.A. et al. //Reference Materials. 2012. № 2. P. 52

Sosedko A.F. Kon-i-Gut // Socialist Science and Technology. Tashkent. 1935. №12. pp. 17 – 24

Znamensky S.E., Znamenskaya N.M. The distribution of rare-earth elements and yttrium in cal-cite Au-Cu-porphyry ores and host rocks of the Kutuev ore occurrence (Southern Urals) // Geo-logical Bulletin. 2021. №1. p. 98-104

Tchaikovsky I.I. Kalistroncite and gergeonite of the Verkhnekamskoye salt deposit // Zapiski RMS. 2011. №3. p. 83-87

Filippov A.G., Mavlyanov G.N. Investigation of radioactivity in the cave-rednik Kan-i-Gut and its surroundings in 1949 - 1950 // Caves: Inter-university. digest of scientific works - Perm: Perm State National University, 2013. Issue. 36. pp. 123 - 136

THE PROJECT OF THE BEAMLINE "X-TECHNO" FOR THE SYNCHROTRON RADIATION SOURCE "SKIF" #35

Submitted by **Vladimir Nazmov**
For track: SR technological application and X-ray apparatus
Authors:

- Vladimir Nazmov (Budker Institute of Nuclear Physics)
- Boris Goldenberg (Budker INP SB RAS, SRF “SKIF”)

A project of the synchrotron radiation station called "X-Techno" at a bend magnet beamline of the "SKIF" SR source is presented. The purposes of the beamline "X-Techno" are study the physicochemical properties of materials under irradiation to X-ray in the spectral range from 2 to 70 keV. The selecting of a narrowed spectral range is supposed to be carried out using metal foils and a grazing-incidence mirror, which provides redirection of the x-ray beam with corresponding radiation spectrum into one of the three experimental chambers. The fourth interchangeable chamber is used for studying samples with low outgassing properties. The objects of study can be like gases, liquids, and solids.

Materials research carried out at the beamline will be the foundation for the development and manufacture of micro parts with a spatial submicron resolution using the above-mentioned devices.

The scheme of the beamline and the station, estimates of the SR power spectra for various applications are resented.

APPROACHES TO THE STUDY OF THE EVANESCENT FIELD OF SURFACE PLASMON POLARITONS AT THE NOVOSIBIRSK FREE ELECTRON LASER #36

Submitted by **Valeriya Kukotenko**
For track: THz radiation aplication
Author: Valeriya Kukotenko (Budker Institute of Nuclear Physics)
Co-author: Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)

Waveguide surface refractometry is one of the applications of terahertz surface plasmon polaritons (SPP) propagating along the conductor-insulator interface. The conductor can be a metal, a dielectric in the absorption line, or a doped semiconductor. Measuring of characteristics of SPP (propagation length along the interface, phase velocity and depth of penetration of the SPP field into the dielectric) allowed restoration of the optical properties of the conductor, which is important for the problems of diagnosing the quality of surfaces and thin films, sensorics, etc. In contrast to the visible range, all noble metals have high conductivity in the THz frequency range. As a result, the

SPP's field in the dielectric is weakly coupled to the surface. There are large radiative losses of plasmon intensity even on small roughness and inhomogeneities [1]. This imposes certain difficulties for the practical implementation of plasmon refractometry, in particular, for measuring the evanescent SPP field above the conductor surface.

In this work, we consider experimental approaches to measuring the attenuation of the intensity of the SPP evanescent field: the probe method with external modulation and modulation by the oscillations of the probe itself, as well as the registration of the field arising after SPP diffraction at the edge of the conducting surface.

1. Vasily V. Gerasimov, Boris A. Knyazev, Alexey G. Lemzyakov, Alexey K. Nikitin, and Guerman N. Zhizhin. Growth of terahertz surface plasmon propagation length due to thin-layer dielectric coating // Journal of Optical Society of America B. V. 33, Is. 11, P. 2196-2203 (2016).

PTYCHOGRAPHY FOR IMAGING RELIEF OF INCLINED SURFACES #37

Submitted by **Nikolay Popov**

For tracks: SR and FEL sources and centers, X-ray structural analysis

Author: Nikolay Popov (P.N. Lebedev Physical Institute of the Russian Academy of Sciences)

Ptychography is a method of obtaining an image by computer processing of overlapping field intensities (scans). When scanning an object, it is assumed that the illuminating beam and the position of the detector remain unchanged. It is used in a wide range of wavelengths from infrared to X-ray and can do without optical elements. In this paper, the possibility of obtaining an image of the relief of the surface of an object inclined to the incident beam at a critical angle is investigated. The wavelength is 0.134 nm, the sliding angle is 0.170. It is shown that ptychography can be useful for controlling the shape of extended objects, such as X-ray mirrors.

FINE CRYSTAL STRUCTURE, SPECTRAL PROPERTIES AND MICROMORPHOLOGY OF FILMS OF ENERGY-INTENSIVE COMPOUNDS OBTAINED BY CRYSTALLIZATION FROM THE GAS PHASE ON VARIOUS SUBSTRATES #38

Submitted by **Aleksandr Stankevich**

For tracks: THz radiation aplication, X-ray spectroscopy, X-ray structural analysis

Authors:

- Aleksandr Stankevich (Federal State Unitary Enterprise «Russian Federal Nuclear Center — Zababakhin All—Russia Research Institute of technical Physics»)
- Anna Sobolevskaya (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)
- Marina Streltsova (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)
- Anastasia Gretsova (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)
- Olga Frolova (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)

In this work, we studied the structure of thin films of various thicknesses from benzotrifuroxan, cyclotrimethylenetrinitramine, cyclotetramethylenetetranitramine, triaminotrinitrobenzene, dinitroanisole, pentaerythritol tetranitrate, diaminodinitroethylene, obtained by crystallization from the gas phase on various substrates: polyethylene terephthalate, parchment, aluminum, quartz glass, polymer resin, silicon and sapphire. Preliminary preparation of gaseous products, which were obtained by the method of thermal vacuum sublimation, was carried out. It has been established that the obtained thin films have a molecular structure corresponding to the studied substances. The texture of the obtained films was determined. In the bulk, the micromorphology of films are determined by particles having a columnar shape, nonequilibrium faceting, and a developed surface. The measurements were carried out by x-ray polycrystalline diffraction, Raman spectroscopy, IR spectroscopy, UV-Vis spectrophotometry, optical and electron microscopy.

In addition, studies of the surface topology and electronic properties of the obtained textured films were carried out.

MICROSTRIP SILICON DETECTOR FOR STUDY OF ULTRA-FAST PROCESSES AT THE SYNCHROTRON RADIATION BEAM #39

Submitted by **Lev Shekhtman**
For track: X-ray structural analysis
Author: Lev Shekhtman (Budker Institute of Nuclear Physics)

Present status of the development of the prototype of the Detector for imaging of explosions (DIMEX) based on silicon microtrip sensor is discussed. The prototype includes silicon p-in-n sensor with metal strips in direct contact with p-implants. Strips are 30 mm long and have 50 um pitch. Signals from the strips are read out with specially developed ASICs DMXS6A, that include 6 channels with DC compensation circuit at the input, four integrators, 32 analogue memory cells and output analogue shift register. The prototype detector has 96 registration channels provided with 16 DMXS6A ASICs. Each strip of the sensor is connected to the guard-ring through a 400 Ohm resistor and through 100 kOhm resistor to the input of the front-end ASIC. This resistive divider allows to adapt the dynamic range of the integrator of the ASIC to the full flux range of the beam line 8 at the VEPP-4M storage ring that includes 9-pole wiggler with 1.9 T B-field as SR source. The measurements of the dynamic range of the DIMEX-Si prototype demonstrate that maximum photon flux from one bunch that can be measured by this detector exceeds 100000 photons per channel. For these measurements the sensor was inclined at an angle of 1.7 degrees with respect to the beam plane in order to increase quantum efficiency. The possibility to work in multi-bunch mode with bunches following in 55 ns is demonstrated, that proves that this detector can be successfully exploited at new SR-source SKIF that is under construction in Novosibirsk region.

EXCITATIONS OF SURFACE PLASMON RESONANCE ON INSB BY ATTENUATED TOTAL REFLECTION PRISM WITH TUNABLE AIR-GAP USING THZ RADIATION OF NOVOSIBIRSK FREE ELECTRON LASER #40

Submitted by **Ildus Khasanov**
For track: THz radiation aplication
Authors:

- Ildus Khasanov (Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences)
- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)
- Oleg Kameshkov (BINP SB RAS)
- Alexey Nikitin (Scientific and Technological Center for Unique Instrumentation of RAS)

We have created a setup for measuring the reflection coefficient from an attenuated total reflection prism in the Otto configuration using a terahertz free electron laser (THz FEL) as a quasi-monochromatic radiation source. The goniometric system of the setup allows to carrying out precision angular measurements in the range from 10 to 70 degrees. The Novosibirsk FEL is a tunable radiation source with many generation lines from 8 to 300 μm, which makes it possible to carry out multispectral measurements in the THz range. The used Otto configuration allows scanning by the size of the air gap, which reaches tens of micrometers in the THz range. The presence of an air gap makes it possible to apply this method as a non-destructive testing for thin and flat samples, such as semiconductor wafers. In the THz range lie plasma frequencies for many semiconductors, which causes to excite a strong surface plasmon resonance and therefore with high sensitivity to determine the concentration of carriers on the surface of the semiconductor. We have carried out a series of angular measurements of the reflection coefficient from a cylindrical prism made of high resistivity float zone silicon separated from an undoped InSb wafer by variuos values of the air gap (up to 320 μm) at a radiation wavelength of 141 μm. We have registered surface plasmon resonance near the critical angle of the prism.

SYNCHROTRON BASED X-RAY FLUORESCENCE MICROSCOPY FOR STUDYING SODIUM DEPOSITS IN CARDIAC AND STRIATED MUSCLES #41

Submitted by **Igor Artyukov**
For tracks: SR for medicine and biology application, X-ray fluorescent analysis
Author: Igor Artyukov (Lebedev Physical Institute RAS)
Co-authors:

- Grigoriy Arutyunov (Pirogov Russian National Research Medical University)
- Dmitry Dragunov (Pirogov Russian National Research Medical University)
- Alessandra Gianoncelli (ELETTRA)
- David Paneke Aguilera (Lebedev Physical Institute RAS)
- Simone Pollastri (ELETTRA)
- Aleksander Vinogradov (Lebedev Physical Institute RAS)

This presentation reports the results of a co-ordinated investigation aiming at validating hypothetical sodium accumulation in the intercellular space of myocardial and striated tissues. In these accumulations the sodium cations are assumed to be in a bound state, which prevents their active participation in the usual osmotic and biochemical processes. The existence of such sodium deposits in the heart muscle leads to a noticeable deterioration in muscle elasticity and, consequently, to dysfunction of the contractile activity.

Sodium accumulation was detected with the help of X-ray fluorescence using both TwinMic STXM/XRF microscope and micro-XRF IAEA beamline workstations of the ELETTRA synchrotron (Italy). The high spatial resolution and spectral sensitivity of the TwinMic X-ray microscope made it possible to obtain composite X-ray images at the cellular level while revealing the chemical composition of myocardial and striated tissue samples, which were taken from laboratory animals from two groups differentiated by the level of salt diet.

The presented finding and study of previously unknown non-osmotic sodium deposits in the intercellular space of the myocardium marks a fundamentally new direction in the diagnosis, prevention and treatment of heart diseases.

NEURAL NETWORK RECONSTRUCTION ALGORITHM FOR WIDE RANGE OF ANGLE COUNT AND NOISE LEVEL #42

Submitted by **Andrey Yamaev**
For track: X-ray structural analysis
Authors:

- Andrey Yamaev
- Marina Chukalina (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow; FSRC “Crystallography and Photonics” RAS, 119333, Russia, Moscow)
- Dmitry Nikolaev (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow)
- Alex Chulichkov (Mr.)

Computed tomography, which allows reconstructing a digital image of an object from a set of measured projections, is currently finding novelties in various important ways of life. This is due to new technological solutions that develop the hardware and software of the method, allowing it to increase its spatial and temporal resolution. New applications also impose new restrictions on the methods of measurements, for example, in medical applications [6], the X-ray dose load is limited; in the dynamic processes research there are restrictions on the exposure time, etc.

With these new restrictions, along with the development of classical approaches to working with measured data, neural network approaches are increasingly used in solving the reconstruction

problem. In this work, we proposed a new complex algorithm, consisting of solutions to three problems that were solved using neural network models.

The first problem was the projection noise, which is caused, in particular, by X-ray probe instability. In the paper [1] there was used our residual convolutional network for noise reduction on projections. It is shown that the proposed approach is computationally efficient in terms of the ratio of quality to running time compared to previously proposed algorithms.

The second issue under consideration is to increase the speed of reconstruction. A time-efficient image reconstruction algorithm from low noise projections was proposed [2]. It is a modification of the FBP algorithm [5], in which the frequency filter is selected by the machine learning method in accordance with the dependency to the projection measurement geometry. This allows us to get the same reprojection error as in computationally complex iterative algorithms, such as, for example, SIRT [4].

The third alleged problem is the regularization of solutions with zero reprojection error in the case of a small number of projections. In this case, there is more than one image, which is conditioned to the measured projections. To select the correct image from all possible, we proposed [3] the residual convolutional network to SIRT reconstruction with interpolation and normalization in the Fourier surface.It is shown that the proposed approach for solving the third problem demonstrates state-of-the-art reconstruction accuracy among existing neural network regularizers.

The paper showed that algorithms for solving these three problems can be used both as independent modules and as a complex reconstruction algorithm. On synthetic and real data sets, it is shown that the proposed complex algorithm has a high reconstruction accuracy when working with highly noisy projections, and in the case of a small number of projections, and in the case of a small number of highly noisy projections. The results obtained by the proposed complex algorithm are also compared with the results obtained using classical approaches and other neural network approaches.

This work was partly supported by RFBR (grant) 19-29-09044.

[1] Yamaev A. et al. Lightweight denoising filtering neural network for FBP algorithm //Thirteenth International Conference on Machine Vision. – International Society for Optics and Photonics, 2021. – T. 11605. – C. 116050L.

[2] Yamaev A. et al. Algorithm of exact frequency flter fnding for few view tomography problem //MMRO-2021. - C. 434-435

[3] Yamaev A. et al. Neural network regularization in the problem of few-view computed tomography //Computer Optics. - T. 46(3)

[4] Trampert J., Leveque J. J. Simultaneous iterative reconstruction technique: physical interpretation based on the generalized least squares solution //Journal of Geophysical Research: Solid Earth. – 1990. – T. 95. – №. B8. – C. 12553-12559.

[5] Pan X., Sidky E. Y., Vannier M. Why do commercial CT scanners still employ traditional, filtered back-projection for image reconstruction? //Inverse problems. – 2009. – T. 25. – №. 12. – C. 123009.

[6] Kalender W. A. Dose in x-ray computed tomography //Physics in Medicine & Biology. – 2014. – T. 59. – №. 3. – C. R129.

ANALYSIS OF THE EVOLUTION OF DISLOCATION STRUCTURE OF POLYCRYSTALLINE MATERIALS BY USING SYNCHROTRON X-RAY DIFFRACTION #43

Submitted by **Ivan Ivanov**
For track: X-ray structural analysis
Author: Ivan Ivanov

Analysis of the dislocation structure is an important but not trivial task. Often, for investigation of dislocation parameters, methods based on microscopy are used. However, the use of such methods is extremely limited by the nature of the object under study. Thus, the determination of

the structure and properties of the dislocations of strongly deformed metal alloys is a difficult task. This thesis presents the possibilities of a method based on the profile analysis of diffraction results for estimating the dislocation structure of metal alloys during the cold plastic deformation and heating. The presented results testify to the internal rearrangements of the dislocation structure in the process of external action and are confirmed by the simulation results.

АТОМАРНАЯ СТРУКТУРА АКТИВНЫХ ЦЕНТРОВ CU/ZSM-5 КАТАЛИЗАТОРОВ СЕЛЕКТИВНОГО ОКИСЛЕНИЯ МЕТАНА: EXAFS ИССЛЕДОВАНИЕ #44

Submitted by **Egor Aydakov**
For tracks: X-ray spectroscopy, X-ray structural analysis
Author: Egor Aydakov (NSU)
Co-authors:

- Andrey Saraev (Boreskov Institute of Catalysis)
- Alexander Trigub (NRC "Kurchatov Institute")
- Evgeny Khramov (NRC "Kurchatov Institute")
- Svetlana Yashnik (Boreskov Institute of Catalysis SB RAS)

Цеолиты с нанесенными переходными металлами являются одними из перспективных катализаторов селективного окисления метана. Например, ZSM-5 позволяются проводить реакцию селективного окисления метана до метанола, однако селективность по метанолу мала, что снижает коммерческую привлекательность процесса. Модификация медью позволяет подавить побочные реакции и увеличить селективность по метанолу до 97%.

Особенностью подобных систем является то, что маршрут протекания реакции определяется как свойствами носителя (цеолита), так и в виде каких центров присутствуют катионы меди. Действительно, катионы меди могут существовать в виде отдельных металлических или окисленных атомов, в виде двухатомных центров, кластеров, наночастиц или кристаллитов. Несмотря на значительный прогресс в понимании свойств цеолитов, модифицированных медью, вопрос о структуре активных центров до сих пор остается открытым.Спектроскопия рентгеновского поглощения – один из наиболее востребованных методов исследования катализаторов, позволяющий установить структуру активных центров. Важно отметить, что в отличии от рентгеновской дифракции позволяет исследовать рентгеноаморфные структуры (кластеры, отдельные атомы, наночастицы размером < 2 нм).

В качестве объектов исследования были выбраны катализаторы на основе ZSM-5 с содержанием меди 1%. Предполагается, что в зависимости от способа синтеза катализаторы содержат медь в различном состоянии: (1) изолированные катионы Cu2+, (2) плоско-квадратные двуядерные оксо- и гидроксо-комлексы в каналах цеолита, (3) наночастицы CuO на поверхности цеолита. Для уточнения структуры катализаторы исследованы с помощью EXAFS-спектроскопии. Эксперименты проведены в Курчатовском центре синхротронного излучения (КИСИ, г. Москва) на станции «Структурное материаловедение». Моделирование EXAFS показало наличие наночастиц меди, а результат РФЭС показал стабильность катализатора до и после реакции.

Благодарности: Работа выполнена при поддержке Программы Приоритет-2030.

IDENTIFICATION OF THE BESSEL MODE IN GIVEN THZ BEAM #45

Submitted by **Natalya Osintseva**
For track: THz radiation aplication
Authors:

- Natalya Osintseva (INP SB RAS)
- Boris Knyazev (Budker Institute of Nuclear Physics)
- Yulia Choporova (Budker Institute of Nuclear Physics)

- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)

Co-authors:

- Vladimir Pavelyev (Samara University)
- Valeriia Kukotenko (Budker Institute of Nuclear Physics)

Gaussian beams were transformed into Bessel beams with topological charges $l = \pm 1, \ldots, \pm 4$ using silicon binary phase axicons with helical zones. To identify the topological charge of the resulting beam, a combination of one of the axicons and a lens was used. The experiments demonstrated the possibility of identifying a mode by this method in a beam propagating both in free space and through an inhomogeneous medium.

THERMOTROPIC PHASE TRANSITION IN ADSORPTION LAYER ON N-HEXANE/WATER INTERFACE ANALYZED WITH SYNCHROTRON X-RAY SCATTERING #46

Submitted by **Yuriy Volkov**

For track: X-ray structural analysis

Author: Yuriy Volkov (FSRC "Crystallography and Photonics" RAS)

Co-author: Alexey Tikhonov (Kapitza Institute for Physical Problems RAS)

Adsorption layer of a surfactant on the oil/water interface can be described in terms of a two-dimensional thermodynamic system with parameters (p, T, c), which can exhibit both isotropic and anisotropic behavior [1]. In particular, increase in temperature T over the critical temperature Tc in the surfactant monolayer leads to phase transition from two-dimensional crystal mesophase to liquid Gibbs monolayer, while subsequent decrease in T leads to multilayered adsorption effects on the interface [2].

We present systematic data on the thermotropic phase transition in a layer of triacontanoic acid $C30H60O2$ on the interface n-hexane $C6H14$ / water solution of KOH (pH ≈ 10), based on the measurements of X-ray reflectivity (XRR) and grazing-incidence diffuse scattering (XDS). Data were obtained at the synchrotron station X19C, NSLS-II, Brookhaven [3] with peak intensity $I \approx 1010\ s^{-1}$ at photon energy E = 15 keV (wavelength $\lambda \approx 0.825$ Å). Liquid/liquid samples have been prepared in a sealed cell with transparent polyester windows [4] kept in a two-step thermostate with temperature precision up to 0.1 °C. Series of experimental reflection and scattering curves were measured within range 43°C to 60°C, with critical phase transition temperature $Tc \approx 50$°C.

Simultaneous analysis of XRR and XDS data has been performed according to self-consistent model-independent method [5] which allowed us to extract depth-graded distributions of electron concentration $\rho(z)$ as well as roughness power spectral density distributions $C(\nu)$. It has been found that during crystallization of Gibbs monolayer, additional planar smectic-type structure forms at the interface, with its roughness spectrum differing from the classical statistics of capillary waves.

Theoretical part of the present work has been supported by the Russian Science Foundation (project #18-12-00108).

[1] T. Takiue, T. Matsuo, N. Ikeda, K. Motomura, M. Aratono, *J. Phys. Chem. B* 102, 4906 (1998).

[2] A.M. Tikhonov, *JETP Lett.* 104, 318 (2016).

[3] M. L. Schlossman, D. Synal, Y. Guan et al., *Rev. Sci. Instrum.* 68, 4372 (1997).

[4] A.M. Tikhonov, *J. Chem. Phys.* 130, 024512 (2009).

[5] I.V. Kozhevnikov, L. Peverini, E. Ziegler, *Phys. Rev. B* 85, 125439 (2012).

STRUCTURAL-PHASE TRANSFORMATIONS AT THE INTERFACE OF METALS UPON FRICTIONAL LOADING: OBSERVATIONS USING SYNCHROTRON X-RAY DIFFRACTION #47

Submitted by **Kemal Emurlaev**
For track: X-ray structural analysis
Author: Kemal Emurlaev (Novosibirsk State Technical University)

An *operando* approach to analyze the structural transformations occurring under dry sliding was recently proposed in [1, 2]. It was found that using of synchrotron X-ray radiation coupled with diffraction models [3] provides an opportunity to analyze the dynamics of the phase constitution as well as microstructure parameters such as the size of coherent scattering regions, density and type of dislocations, etc. directly under frictional loading. Another one method to analyze structural and phase transformations close to the interface of an element of a rubbing pair will be presented during the report. It consists in mapping of the friction surface by a beam of synchrotron radiation. The high brilliance of the radiation provides a high spatio-temporal resolution of maps and gives an opportunity to study surface layer of metals at different stages of wear test in order to identify friction-induced structural changes.

The reported study was funded by RFBR, project number 20-32-90119.

1 A.A. Bataev, V.G. Burov, A.A. Nikulina, I.A. Bataev, D. V. Lazurenko, A.I. Popelukh, D.A. Ivanov, A Novel Device for Quasi In Situ Studies of Materials Microstructure during Friction, Mater. Perform. Charact. 7 (2018) 20170065. https://doi.org/10.1520/MPC20170065.
2 I.A. Bataev, D.V. Lazurenko, A.A. Bataev, V.G. Burov, I.V. Ivanov, K.I. Emurlaev, A.I. Smirnov, M. Rosenthal, M. Burghammer, D.A. Ivanov, K. Georgarakis, A.A. Ruktuev, T.S. Ogneva, A.M.J. Jorge, A novel operando approach to analyze the structural evolution of metallic materials during friction with application of synchrotron radiation, Acta Mater. 196 (2020) 355–369. https://doi.org/10.1016/j.actamat.2020.06.049.
3 T. Ungár, I. Dragomir, Á. Révész, A. Borbély, The contrast factors of dislocations in cubic crystals: the dislocation model of strain anisotropy in practice, J. Appl. Crystallogr. 32 (1999) 992–1002. https://doi.org/10.1107/S0021889899009334.

X-RAY TRANSFOCATORS: TUNABLE X-RAY FOCUSING DEVICES BASED ON COMPOUND REFRACTIVE LENSES #48

Submitted by **Anton Narikovich**
For track: SR technological application and X-ray apparatus
Authors:

- Anton Narikovich (IKBFU)
- Aleksandr Barannikov (Immanuel Kant Baltic Federal University)
- Anatoly Lushnikov (IKBFU)
- Nataliya Klimova (Immanuel Kant Baltic Federal University(IKBFU))
- Ivan Lyatun (X-Ray Coherent Optics Laboratory (IKBFU))
- Igor Panormov (IKBFU)
- Alexander Sinitsyn (IKBFU)
- Dmitrii Zverev (IKBFU)
- Anatoly Snigirev (Immanuel Kant Baltic Federal University)

Compound refractive lenses (CRL) with rotationally parabolic profiles and CRL-based systems are widely used to manipulate synchrotron radiation (SR) beams. These effective and simple optical elements, easy to align and operate, have become standard elements in synchrotron beamline instrumentation. By varying the shape, composition, and number of individual lenses, CRL can be adapted to photon energies from 2 to 200 keV, providing flexible adjustment of focal lengths for a wide range of research methods [1,2].

To date, the magnetic systems of storage rings of existing SR sources are being upgraded up to the 4th generation. SR beams with an ultra-low emittance of about 100 pm*rad have already been obtained at the MAX-IV [3] and ESRF [4]. In Russia, work is underway to create centers with Mega-science-class facilities: design and construction of two SR sources with emittance about 75 pm*rad [5]. A new generation of synchrotron radiation sources with significantly increased beam characteristics poses new challenges to refractive lenses and CRL-based systems. Therefore, there is a great demand for the development of devices equipped with a large number of CRLs, since it allows for comprehensive optimization of X-ray beamline designs for particular user experiments.

First systems with a changeable number of lenses, the Transfocators (TFs), were proposed to move and easily adjust the position of the CRL [6]. Typically, the TF consists of several cylindrical cartridges containing a geometric progression of numbers of Al or Be parabolic lenses between two and 254 lenses grouped by powers of two. The use of these devices made it possible to optimize the size and divergence of beams, including the white SR beam [7]. The simplicity and versatility of TFs led to their wide distribution [8], changing the concept of beamlines at the SR sources [9] and X-Ray Free-Electron Laser Facility [10]. They are used for collimating and pre-focusing the SR beam [11] as well as for rapidly changing the beam size, through combinations of horizontal and vertical lenses [12].

Despite the detailed and elaborate design, the cartridge-type lens arrangement inevitably leaves empty spaces between individual cartridges, and these gaps vary in a complicated way when switching from one set of cartridges to another. Hence, the optical properties of the lens system are affected throughout the entire focal length range. A new ultra-compact version of the transfocator (UCTF) was designed and manufactured by us to minimize the gaps between the individual refractive lenses [13]. The main distinctive feature of the UCTF is discrete-type lens switching, referred by us as a single-lens approach, which means that individual parabolic lenses are moving one by one independently. Moreover, in combination with its small overall size and lightweight, allows one to integrate it at various experimental setups, thus being suitable as a short-focal magnifying objective for a wide range of applications even at non-specialized imaging beamlines. Currently, the device is mounted at the second end station of the EMBL P14 beamline, shaping the beam for time-resolved pump-probe serial crystallography experiments.

In this paper, we present our advanced versions of the CRL-based X-ray TFs. The devices can be used in both white and monochromatic beams to focus, pre-focus, or collimate the beam. The TFs can be used with other monochromators and/or other focusing elements, leading to significant increases in flux. Furthermore, the chromatic nature of the focusing means the TF suppresses harmonics and can also be used as an extremely high flux broad-band-pass monochromator. There are three main options for the mechanical design of X-ray TFs:

- Ultra-Compact Transfocator (UCTF) with discrete-type lenses switching
- In-vacuum Transfocator (IVTF) with binary-type lenses switching
- In-vacuum Transfocator with water cooling system (IVTF+)

All basic parameters of the devices can be changed depending on the specific task of their use. For example, Ultra-Compact Transfocator can be manufactured in the In-vacuum version and equipped with a water-cooling system to ensure stable operation when the device is used under vacuum conditions. The number of lenses is customizable and can be configured according to the customer's request. Special Python-based software was designed to provide high-level access to device-control functions with the possibility to create custom commands. The software can be integrated into most modern synchrotron beamline controlling systems such as SPEC or ACTL.

1. Snigirev A., Snigireva I. High energy X-ray micro-optics // Comptes Rendus Phys. 2008. Vol. 9, № 5–6. P. 507–516.
2. Dimper R. et al. ESRF Upgrade Programme Phase II (2015-2022) Technical Design Study. 2014. P. 190.
3. Leemann S.C., Wurtz W.A. Nuclear Inst. and Methods in Physics Research, A Pushing the MAX IV 3 GeV storage ring brightness and coherence towards the limit of its magnetic lattice // Nucl. Inst Methods Phys. Res. A. 2018. Vol. 884, № December 2017. P. 92–96.

4. Chenevier D., Joly A. ESRF–EBS Facility Update: A Pictorial Essay // Synchrotron Radiat. News. Taylor & Francis, 2020. Vol. 33, № 3. P. 37–41.
5. Baranov G., others. Magnet Lattice Optimization for Novosibirsk Fourth Generation Light Source SKIF // Sib. Phys. J. 2020. Vol. 15, № 1. P. 5–23.
6. Snigirev A. et al. High energy X-ray transfocator based on Al parabolic refractive lenses for focusing and collimation // J. Phys. Conf. Ser. 2009. Vol. 186. P. 10–13.
7. Vaughan G.B.M. et al. X-ray transfocators: Focusing devices based on compound refractive lenses: 2 // J. Synchrotron Radiat. 2011. Vol. 18, № 2. P. 125–133.
8. Zozulya A.V. et al. Microfocusing transfocator for 1D and 2D compound refractive lenses // Opt. Express. 2012. Vol. 20, № 17. P. 18967.
9. Fedotenko T. et al. Laser heating setup for diamond anvil cells for in situ synchrotron and in house high and ultra-high-pressure studies // Rev. Sci. Instrum. AIP Publishing LLC, 2019. Vol. 90, № 10. P. 104501.
10. Zozulya A. et al. Beam conditioning CRL transfocator optics at the MID instrument of the European XFEL // X-Ray Lasers and Coherent X-Ray Sources: Development and Applications XIII. International Society for Optics and Photonics, 2019. Vol. 11111. P. 111110H.
11. Buffet A. et al. P03, the microfocus and nanofocus X-ray scattering (MiNaXS) beamline of the PETRA III storage ring: The microfocus endstation // J. Synchrotron Radiat. 2012. Vol. 19, № 4. P. 647–653.
12. Bowler M.W. et al. MASSIF-1: A beamline dedicated to the fully automatic characterization and data collection from crystals of biological macromolecules // J. Synchrotron Radiat. 2015. Vol. 22. P. 1540–1547.
13. Narikovich A. et al. CRL-based ultra-compact transfocator for X-ray focusing and microscopy: 4 // J. Synchrotron Radiat. 2019. Vol. 26, № 4.

GENERATION OF FAST RECONSTRUCTION ALGORITHMS FOR COMPUTED TOMOGRAPHY WITH ARBITRARY GEOMETRY SET-UP #49

Submitted by **Petr Kulagin**
For track: SR technological application and X-ray apparatus
Authors:

- Petr Kulagin (Moscow Institute of Physics and Technology)
- Dmitriy Polevoy (Smart Engines LLC, , Russia, Moscow, 60-letiya Oktyabrya Ave, 9)
- Anastasia Ingacheva (IITP RAS)
- Marat Gilmanov (Smart Engines LLC, , Russia, Moscow, 60-letiya Oktyabrya Ave, 9)
- Marina Chukalina (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow; FSRC “Crystallography and Photonics” RAS, 119333, Russia, Moscow)
- Dmitry Nikolaev (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow)

In this work, we present a general method for obtaining fast backprojection operators in the tomographic reconstruction problem, based on the transformation of summing algorithms for fast calculation of direct projection operators. This method allows us to reduce the calculation time for reconstruction and do real-time reconstruction.Computed tomography is an X-ray method of non-destructive evaluation of the internal structure of an object. The method is widely used in medicine, industry, security, scientific research related to the study of the morphological structure of advanced functional materials [1].

The task of tomographic reconstruction is the accurate estimation of the internal structure of the object according to the available tomographic projections. Tomographic reconstruction algorithms have been developing for more than 80 years. One of the main directions of optimization of algorithms today is to increase their computational efficiency. This is due to the fact that the user is

expected from the method of increasing the spatial resolution of the digital image of the object under study. This leads to an increase in the amount of data that reconstruction algorithms have to work with.

Analytical, iterative, neural network methods are used to solve the problem of tomographic reconstruction. Linear direct projection operators A and backprojection operators A^T form their basis.

The main contribution of the article is the method of obtaining a fast version of the calculation of the backprojection operator from the accelerated algorithm for calculating the direct projection operator. An effective algorithm for calculating the direct projection operator is implemented using the Brady-Young method in combination with the method of Four Russians. A variant of the fast calculation of the direct projection operator for a circular scanning scheme when probing with a cone beam is proposed and considered in detail in [2]. With this approach, the algorithm is divided into 2 phases: pre-counting with stopping the main summation algorithm at some iteration and further counting. Then the matrix decomposition into the product of binary matrices is valid for this algorithm, and the algorithm for calculating the transpose(backprojection) operator can be obtained by transposing the product of matrices. In total, the algorithm for calculating the transpose operator will look like a sequential application of the transposed operators from the product in reverse order.

In this work we analyze the method on the example of two-dimensional and three-dimensional operators, presents the results of reconstruction using traditional and accelerated calculations of operators.

1. Topal, E., Liao, Z., Löffler, M. et al. Multi-scale X-ray tomography and machine learning algorithms to study MoNi4 electrocatalysts anchored on MoO2 cuboids aligned on Ni foam. BMC Mat 2, 5 (2020). https://doi.org/10.1186/s42833-020-00011-0
2. К. Булатов, М. Чукалина, Д. Николаев. Fast X-Ray Sum Calculation Algorithm for Computed Tomography Problem. Вестник ЮУрГУ. Серия “Математическое моделирование и программирование” (Вестник ЮУрГУ ММП) 2020. 13(1) 95-106. DOI 10.14529/mmp200107

SPOOF SURFACE PLASMON RESONANCES ON SUBWAVELENGTH GRATINGS EXCITED WITH THZ RADIATION OF NOVOSIBIRSK FREE ELECTRON LASER #50

Submitted by **Oleg Kameshkov**

For track: THz radiation aplication

Authors:

- Oleg Kameshkov (BINP SB RAS)
- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)

The classical approach to the detection of tiny molecules with surface plasmon resonances (SPR) on thin metal films is limited in the terahertz frequency range. In the THz range metals behave like perfect electric conductors and have high values of dielectric permittivity as opposed to the optical frequency range. As a consequence, an electromagnetic field cannot penetrate the metal and the air-metal interface cannot support SPR. To overcome this a surface of metals is structured with subwavelength gratings. If the period of such structure is subwavelength the structured region at the metal surface behaves like an effective medium layer, whose dielectric function mixes both air and metal responses and is lower than simple metals. Spoof surface plasmon resonances (SSPRs) can be excited on such structures that are similar to SPR. It enables to detect tiny concentrations and observe small changes in the boundary dielectric medium in the THz range. In this paper, a silicon prism coupled THz SSPR on flat 1D metal subwavelength grating is studied. The grating sample was tested using THz radiation of the Novosibirsk free electron laser. Experimental results are compared with simulation results obtained with COMSOL Multiphysics.

STRETCHED WIRE SAG MINIMIZATION FOR DIRECT CURRENT MAGNETIC MEASUREMENTS METHOD FOR SUPERCONDUCTING INSERTION DEVICES #51

Submitted by **Artem Zorin**
For track: SR and FEL sources and centers
Authors:

- Artem Zorin (Budker INP SB RAS, SRF "SKIF")
- Nikolay Mezentsev (Budker INP SB RAS, SRF "SKIF")
- Vitaliy Shkaruba (Budker INP SB RAS, SRF "SKIF")
- Valeriy Tsukanov (Budker INP SB RAS, SRF "SKIF")
- Askold Volkov (Budker INP SB RAS, SRF "SKIF")
- Olga Tarasenko (BINP)
- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Fedor Kazantsev (Novosibirsk State University)

Stretched wire with direct current magnetic measurements method is widely used for producing insertion devices, especially multipole superconducting insertion devices like wigglers and undulators. This method allows to measure and minimize the first and second field integrals along an orbit trajectory in an accelerator on certain field (like Holl probe method) as well as during ramping up and down. The main problem of the stretched wire method is the relation between sag, current and tension (thus sensitivity and accuracy). To increase sensitivity, one has to increase current and use wire of bigger cross-sectional area, thus increase sag. To decrease sag, one has to increase tension, thus decrease sensitivity. The article proposes method of stretching copper wire with the help of Kevlar sleeve. The method was tested at Budker INP during superconducting undulator measurements.

SOME PROBLEMS IN A PROPOSED PRELIMINARY PROCEDURE FOR THE CALIBRATION OF SAMPLE'S SIMULATION MODEL UNDER THE REALIZATION OF A QUANTITATIVE MICRO-XRF TECHNIQUE BASED ON THE FUNDAMENTAL PARAMETERS MEANS #52

Submitted by **Dmitry Sorokoletov**
For track: X-ray fluorescent analysis
Authors:

- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)

Quantitative x-ray fluorescence microanalysis technique (micro-XRF) is a relatively simple and informative non-destructive method for exploring the elemental composition within inner (sub-surface and deepened) layers of samples of various nature (geological, biological, cosmic, archeological, forensic, medical, etc.) with a ten-micron typical spatial resolution. It may be actual in different applications [1-2]. However, a series of additional approaches (such as quantitative x-ray fluorescence absorption tomography [3], techniques of accounting for the scattered exposed and secondary x-rays as well as the conjoint processing data from two or more detecting devices [4]) was needed early to be developed in order to determinate the elements' mass concentration with a sufficiently high accuracy. It also becomes clear that there exists a range of actual problem those are individual for each type of explored samples.

The simulation models which micro-XRF inverse problem based on are sensitive significantly to any errors in setting values of its inner parameters. For example, lack of knowledge of the mass density and the elemental composition for lightest chemical elements (H, O, C, Si, P, Al, etc.) which cannot be determined by any XRF techniques results potentially in a significant resulting error for calculated mass concentrations. In addition, the thickness of the explored layers of the sample as well

as all some crucial preferences of detector (including the thickness of working and dead layers) should be well known before its defining to the initial simulation model.

On two concrete examples considering to analyzing two standard samples with principally various chemical composition, we have shown in detail that some problem from above mentioned ones is actual in a calibration procedure being developed by us to be follow by quantitative XRF experiments. This procedure includes using the fundamental parameters means. We also have proposed ways to eliminate or fairly minimize some arising errors.

The work have been carried out in the framework of RFBR project no. 19-05-50046. The work was done at the shared research center SSTRC (on the basis of the VEPP-3M/VEPP-4 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022). Some parts of the work were done at the shared research center "Kurchatov Center of Synchrotron and Neutron Radiation (KISI-Kurchatov)" (on the basis of the Kurchatov Specialized Source of Radiation at NRC Kurchatov Institute, using equipment supported by project RFMEFI61914X0002).

[1] Majumdara S., Peralta-Videa J. R., Castillo-Michel H., et al., Anal. Chim. Acta. 755 (2012) 1-16.
[2] Fittschen U. E. A., Falkenberg G., Spectrochim. Acta Part B 66 (2011) 567–580.
[3] Bleuet P., Lemelle L., Tucoulou R., et al., Trends Anal. Chem., 29 (6), 2010.
[4] Spanier M., Herzog C., Grotzsch D., et al., Rev. Sci. Instrum., 87 (3), 2016.

ANALYSIS OF RESULTS OF TWO EARLY PROPOSED APPROACHES DIRECTED TO SUPPRESS THE INFLUENCE OF SEVERAL SYSTEMATICAL ERROR COMPONENTS IN SOLVING ONE- AND TWO-DIMENSIONAL INVERSE DECONVOLUTION PROBLEMS #53

Submitted by **Dmitry Sorokoletov**

For tracks: X-ray fluorescent analysis, X-ray spectroscopy

Authors:

- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)

The one- and two-dimensional convolution equations are strongly ill-posed by Hadamar (i.e., unstable in calculating) inverse problems. These problems widely occur in processing optical (photographic, astronomic, medical, etc.) images [1] and signals of several specific types (in photoelectronic spectroscopy, x-ray fluorescence microanalysis [2], etc.).

So-called regularizing algorithms [3, p. 47-48] only must solve any ill-posed problems. Their working principle consists in "controllable" suppression of the influence of a stochastic component of errors of the left and right parts of the problem to their result (approximate solution) by one or the other means. A crucial limitation of that "controllability" consists in the ability of guarantying only the convergence (under reducing the errors) of one or the other types to the exact solution (that is a-priory unknown) for the resulting approximate one [3, p. 19, 47-48]. However, on the other hand, it is actual under any character of distribution of all problem's terms (or such their behavior that follow some fixed specification being sufficiently general). For example, the working principle of Tikhonov algorithm [3, p. p. 66-68, 118-119; 4, p. 72] as well as the "physical" principle of the obtained result for its most widely applied modification is described most clearly in [5, p. 52-55].

In any cases, regularizing algorithms can "controllable" suppress the influence of only such types of errors that are originally intended only. For example, for Tikhonov algorithm in the modification above mentioned the errors to be handled must by stochastic (e.g., instrumental) noise for the right part of the inverse problem. The law of normal distribution must describe this error only. If any significant systematic component of the errors exists in terms of the problem, the working principle breaks down and, consistently, big additional errors in proposed solution will take place. We developed early two effective approaches [6] whose application yields effective suppressing two type of systematic errors: originated from principally finite level of discretization of the one-dimensional

convolution equation and originated from limited field of observation for the one- and two-dimensional convolution equations. They were the means of subpixel interpolation for all equation's terms (by series of Lagrange polynoms of high degrees for a signal to be found and exactly determined apparatus function from its a-priory known distribution) and the mean of modification of widely applied computation scheme [4, p. 37-38] aimed at the minimization of the bound effects of several types. Certain effectivity of proposed approaches was tested successfully, the RMS for the accuracy of restoring a series of simulated signals was about 15 percent for the first means and more than 75 percent for the second one [6]. In the work we have followed the mentioned investigation by significally increasing a number of types of testing signals to be restored and by following analysing the reasons of some specifics of results in detail.

The work have been carried out in the framework of RFBR project no. 19-05-50046. The work was done at the shared research center SSTRC (on the basis of the VEPP-3M/VEPP-4 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022).

[1] J. B. Sibarita. Deconvolution Microscopy. // Adv Biochem Engin/Biotechnol. 2005. 95. P. 201
[2] P. Wrobel and M. Czyzycki. Direct deconvolution approach for depth profiling of element concentrations in multi-layered materials by confocal micro-beam x-ray fluorescence spectrometry. // Talanta , 62–67 (2013).
[3] A. S. Leonov, Otcherky teorii, prakticheshie algoritmy i demonstraciy v MATLAB (in russian). (Lybrokom, Moskow, 2013, 2nd ed.). P. 336.
[4] Hansen P. C., Nagy J. G., O'Leary D. P. Deblurring Images, Matrices, Spectra, and Filtering. SIAM, Philadelphia, 2006
[5] S. I. Kabanikhin, Obratnye i nekorrectnye zadachi (in russian) (Sibirskoe nauchnoe izdatelstvo, Novosibirsk, Russia, 2009). P. 457.
[6] D. S. Sorokoletov, Ya. V. Rakshun, F. A. Daryin. New Intuitive Regularizating Approaches for Deconvolution Problems. // APMAS 2021. Book of abstracts. 92 p.

TERAHERTZ GHOST IMAGING WITH SPECKLED LIGHT USING NOVOSIBIRSK FREE ELECTRON LASER RADIATION #54

Submitted **Ildus Khasanov**

For track: THz radiation aplication

Authors:

- Ildus Khasanov (Scientific and Technological Center of Unique Instrumentation of the Russian Academy of Sciences)
- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)

Ghost imaging (GI) is a lensless imaging technique with a single-pixel detector that is promising for use in the terahertz (THz) frequency range. Classical GI uses a random light source, for example, spatially modulated by speckle patterns - random interference patterns, the so-called pseudo-thermal source. To create speckle patterns a coherent light source is required, for which we chose a Novosibirsk free-electron laser. THz speckles were obtained by scattering in polypropylene foam. In the experiments we obtained low-quality ghost images. The ghost image reconstruction procedure included post-processing to improve image quality, such as threshold filtering taking into account the autocorrelation function of the speckles. In the report we will discuss the results obtained and ways to improve the technique for THz ghost imaging.

APPLICATION OF HIGH-ENERGY X-RAYS AND ATOMIC PAIR DISTRIBUTION FUNCTION ANALYSIS TO STRUCTURAL DIAGNOSTICS OF CATALYSTS #55

Submitted by**Vera Pakharukova**

For track: X-ray structural analysis

Authors:

- Vera Pakharukova
- Alexander Shmakov (Boreskov Institute of Catalysis SD RAS)

Structural diagnostics is important step in understanding the physicochemical and functional properties of catalytic materials. A majority of heterogeneous catalysts contain highly dispersed nanoparticles of metals or metal oxides, which are supported on support material. There is significant drawback to common XRD methods addressed to well-crystallized materials to probe structure of supported highly dispersed particles. Here we describe the application of high-energy X-rays in combination with atomic pair distribution-function (PDF) analysis to study the structure of supported catalysts. The PDF describes local atomic structure of the material and provides structural information in the form of radial distribution function of inter-atomic distances. The PDFs are obtained by direct Fourier transformation of the total scattering function. Availability of high-energy X-rays at synchrotron sources allows one to obtain PDF data of high resolution.

In this talk, the PDFs calculated from synchrotron radiation data for different catalysts will be presented and types of structural information extracted from the PDFs will be discussed. The possibilities of the method to probe structure of catalysts will be shown for some examples: 1) Ni/Ce1-xZrxO2 catalyst for methanation of carbon oxides; 2) Pt/Ce1-xZrxO2 catalyst for water- gas shift reaction 3) mono- and bimetallic (Pt, Rh)/γ-Al2O3 catalysts for hydrocarbon oxidation.

This work was supported by Russian Science Foundation (project 21-73-20075).

COMBINED ANALYSIS OF CHAIN-MELTING PHASE TRANSITION IN PHOSPHOLIPID LIQUID-CRYSTAL MULTILAYERS WITH THE USE OF SYNCHROTRON X-RAY REFLECTOMETRY, DIFFUSE SCATTERING AND GRAZING-INCIDENCE DIFFRACTION #56

Submitted by **Yuriy Volkov**

For track: X-ray structural analysis

Authors:

- Yuriy Volkov (FSRC "Crystallography and Photonics" RAS)
- Victor Asadchikov (FSRC "Crystallography and photonics" RAS)
- Boris Roshchin (FSRC "Crystallography and photonics" RAS)
- Alexey Tikhonov (Kapitza Institute for Physical Problems RAS)

Co-authors:

- Alexander Nuzhdin (FSRC "Crystallography and photonics" RAS)
- Veijo Honkimäki (European Synchrotron Research Facility)
- Maria Blanco (European Synchrotron Research Facility)
- Florian Russello (European Synchrotron Research Facility)

Colloidal solutions of SiO2 nanoparticles in water (silica hydrosols) exhibit unique boundary conditions at the sol/air interface, in particular strong normally-oriented gradient of surface potential. Previously, an approach to formation of spontaneously-ordered lamellar multilayer structures of phospholipids on a surface of liquid hydrosols has been demonstrated [1], with properties of the multilayer stack depending on the composition of hydrosol substrate.

We present systematic investigations on thermotropic phase transition of multilayers of distearoyl-phosphatidylcholine (DSPC) and dimyristoyl-phosphatidylserine (DMPS) with the combined use of synchrotron X-ray reflectometry(XRR), diffuse scattering (XDS) and grazing-incidence diffraction (GIXRD). Measurements were performed at the synchrotron beamline ID31,

ESRF, Grenoble [2] with peak intensity I ≈ 1019 s−1 at photon energy E = 71 keV (wavelength λ ≈ 0.175 Å). Samples have been prepared in a 100mm fluoroplastic dish kept in a one-step thermostate with temperature precision up to 0.5 °C [3], which allowed us to obtain data within temperature range of 23°C to 40°C. Analysis of experimental data has been performed according to self-consistent model-independent method [4].

Calculated data on depth-graded distribution of electron density, as well as on interface roughness statistic and two-dimensional crystal structure, demonstrated qualitative differences between formation of multilayers of saturated (DMPS) and non-saturated lipids (DSPC), in particular in dynamics of spontaneous ordering and chain melting.

[1] A. M. Tikhonov, *JETP Letters* 92, 394 (2010).
[2] V. Honkimäki, H. Reichert, J. Okasinski, H. Dosch, *J. Synchrotr. Rad.* 13, 426 (2006).
[3] A. M. Tikhonov, V. E. Asadchikov, Y. O. Volkov, A. D. Nuzhdin, B. S. Roshchin, *Instrum. Exper. Techniques* 64(1), 172-176 (2021).
[4] I.V. Kozhevnikov, L. Peverini, E. Ziegler, *Phys. Rev. B* 85, 125439 (2012).

DISTRIBUTION OF CHEMICAL ELEMENTS IN DIFFERENT FRACTIONS OF BOTTOM SEDIMENTS OF THE LAPTEV SEA. #57

Submitted by **Ivan Kirichenko**
For track: X-ray fluorescent analysis
Author: Ivan Kirichenko (V.S. Sobolev Institute of Geology and Mineralogy SB RAS)
Co-author: Kirill Aksentov (V.I.Il'ichev Pacific Oceanological Institute, Far Eastern Branch, Russian Academy of Sciences)

14 samples of the upper layers of bottom sediments of the Laptev Sea were collected in the Lv-83 cruise. As part of the work, separation into fractions of the bottom sediments of the Laptev Sea was carried out. Fractionation was performed using a combination of sieve analysis methods (on 32, 63, and 125 micron sieves) and gravitational sedimentation according to the methods described in [1,2]. We carried out particle size separation of bottom sediment samples into 0-2, 2-10, 10-32, 32-63, 63-125, >125 microns fractions. Sediment fractions of 32-63 and 63-125 microns were further divided into heavy and light components. From the prepared material 30 mg tablets of 5 mm in diameter were pressed [3]. Standards were used as comparison samples: bil-1 and BCR-32. The chemical composition of various bottom sediment fractions was investigated by XRF-SR method on the equipment of "SSTRC " on the basis of "Complex VEPP-3" in the BINP of SB RAS. Energy of primary radiation was 23 keV, additional to this the chemical composition of heavy fractions 32-63 and 63-125 microns was studied at energy of primary radiation 43 keV. Thus the distribution of chemical elements from K to Mo in K-lines and U, Th, Pb in L-series was obtained, for heavy fractions such elements as Ag, Cd, Sn, Sb, I, Cs, Ba, La, Ce, Pr, Nd were also determined. The statistical analysis of the data obtained revealed groups of chemical elements characteristic of each individual fraction. The data obtained will help to identify the source of chemical elements in the bottom sediments of the Laptev Sea, and can be used in paleoclimatic studies.

This work was financially supported by the RSF project. № 18-77-10017. The work was done at the shared research center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB RAS. Some part of work is done on state assignment of IGM SB RAS

1. Ботвинкин О. К., Клюковский Г. И., Мануйлов Л. А. Лабораторный практикум по общей технологии силикатов и техническому анализу строительных материалов //М.: Стройиздат. – 1966.
2. Петелин В. П. Гранулометрический анализ морских донных осадков. – Наука, 1967.
3. Phedorin M. A., Bobrov V. A., Zolotarev K. V. Peat archives from Siberia: Synchrotron beam scanning with X-ray fluorescence measurements //Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. – 2007. – Т. 575. – №. 1. – С. 199-201

MEASUREMENTS OF UNDULATOR AND LASER RADIATION PARAMETERS OF THE NOVOSIBIRSK FEL FACILITY #58

Submitted by **Vladislav Borin**
For track: SR and FEL sources and centers
Authors:

- Vladislav Borin (BINP)
- Yaroslav Getmanov (Budker INP)
- Oleg Meshkov (BINP)
- Oleg Shevchenko (BINP)
- Nikolay Vinokurov (Budker Institute of Nuclear Physics)

Novosibirsk free electron laser (NovoFEL) facility operates with three FELs. The FELs are installed on one-, two- and four- track energy recovery linacs (ERLs) with a common accelerating system. The ERL type of accelerator allows to achieve high average electron current (ordinarily about 10 mA) and to get the high average FEL power (generally more than 100 W). The new diagnostic system was developed to control and study the third FEL's radiation parameters. The new system acquires spontaneous undulator and laser radiation in the middle infrared area 8-14 mkm. The diagnostics is based on the simultaneous application of reflective double-slit interferometer and diffractive monochromator. Using this approach, we can measure spontaneous and laser radiation parameters in time and spectral domain. Spectral data can be obtained directly using a monochromator and can be compared with the measured correlation function. The new station is also used for the laser radiation spatial characteristics measurements. The calculations and the first results obtained with the new diagnostics are presented. Further experiments are discussed.

SAXS-STUDY OF ELECTRON BEAM TREATMENT EFFECT ON HNIW THERMAL TRANSFORMATIONS #59

Submitted by **Mikhail Mikhailenko**
For track: X-ray structural analysis
Authors:

- Mikhail A. MIkhailenko (Institute of Solid State Chemistry and Mechanochemistry SB RAS)
- Marat Sharafutdinov (ISSCM SB RAS, BINP SB RAS)
- Konstantin B. Gerasimov (ISSCM SB RAS)
- Petr I. Kalmykov (Federal Research and Production Center "Altai", Biysk, Russia)
- Eugenia V. Artemova (Federal Research and Production Center "Altai", Biysk, Russia)
- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
- Mikhail V. Korobeynikov (Budker Institute of Nuclear Physics)

Hexanitrohexaazaisowurtzitane, also called HNIW and CL-20, is a nitroamine with the formula C6H6N12O12. It releases 20% more energy than traditional octogen(HMX)-based propellants, and is widely superior to conventional high-energy propellants and explosives.
The crystals of e-phase (that are stable at room temperature) having a size of 40 μm were investigated. Crystals were treate by electron beam gernerated by a pulse accelerator ILU-6 (BINP, Novosibirsk). Electron energy was 2.4 MeV, pulse duration 500 ms, pulse repetition rate 2 Hz. A moving table with the sample crystals passed under a beam window with a speed of 2 cm/s several times with pauses to prevent an overheating of crystals. A total acquired dose was 40 kGy (J/g). A thermal transformation study in situ was carried out by 5b channel a VEPP-3 collider (BINP, Novosibirsk). The heating rate 10 o/min. When heated the e-phase undergoes a polymorphic transformation to a g-phase at a temperature of 150-156 oC and decomposition at 220-225 oC.

Intact samples show no noticeable increase in the scattering intensity up to polymorphic transformation temperature, at which a formation of a pseudomorphosis with numerous interfaces

occurs. An abrupt increase in the scattering intensity occurs at polymorphic transformation temperature.The irradiated samples show linear increase in SAXS intensity at temperatures above 100 oC, that indicates the formation of the internal interfaces. A transition onset in irradiated e-phase crystals at temperature of about 100 °C was not fixed by other methods. SAXS method permits to surely observe it.

PMMA WITH A MOLECULAR WEIGHT OF TEN MILLION GRAMS PER MOLE FOR X-RAY LITHOGRAPHY #60

Submitted by **Vladimir Nazmov**
For track: SR technological application and X-ray apparatus
Author: Vladimir Nazmov (Budker Institute of Nuclear Physics of SB RAS, prosp.Lavrentieva 11, 630090 Novosibirsk, Russia, Institute of Solid State Chemistry and Mechanochemistry of SB RAS, Kutateladze 18, 630128 Novosibirsk, Russia)
Co-authors:

- Alexander Varand (Budker Institute of Nuclear Physics of SB RAS, prosp.Lavrentieva 11, 630090 Novosibirsk, Russia)
- Mikhail Mikhailenko (Institute of Solid State Chemistry and Mechanochemistry of SB RAS, Kutateladze 18, 630128 Novosibirsk, Russia)
- Boris Goldenberg (Budker INP SB RAS, SRF “SKIF”)
- I.Yu. Prosanov (Institute of Solid State Chemistry and Mechanochemistry of SB RAS, Kutateladze 18, 630128 Novosibirsk, Russia)
- K.B. Gerasimov (Institute of Solid State Chemistry and Mechanochemistry of SB RAS, Kutateladze 18, 630128 Novosibirsk, Russia)
- G.A. Lubas (Institute of Solid State Chemistry and Mechanochemistry of SB RAS, Kutateladze 18, 630128 Novosibirsk, Russia)

Widely used in X-ray lithography, polymethyl methacrylate with a molecular weight of one million grams per mole (trademark GS 233) has high consumer characteristics in terms of spatial resolution, stability in acidic environment, glass transition temperature, but low sensitivity to X-rays and relatively low contrast. At the same time, it was shown that with an increase in the molecular weight of the polymer, the ratio of the dissolving rate of the irradiated material to that of the non-irradiated material increases at the same doses of absorbed radiation [1].

In the present work, we studied polymethyl methacrylate, with a molecular weight of ten million grams per mole achieved by ionic polymerization, which differs from its widely used analogue by an approximately tenfold increase in the length of the polymer chain. Based on the obtained absorption spectra in the IR range, data from differential thermal analysis and gel permeation chromatography, the changes caused by the ionizing radiation are studied. During thermal decomposition of the initial polymer, the mass loss dependence can be divided into different sections: low-temperature with a maximum decomposition rate at 260.5-261 °C and a process start point at 207-209 °C and a high-temperature one with a maximum decomposition rate at 379-379 °C with a process start point at 346-348 °C and the end of the process at 398-400 °C.

As the dose is increased, there is a regular decrease in the decomposition start point from 207 (209) to 152 ° C, a decrease in the temperature of the maximum of low-temperature decomposition and its blurring, as well as a shift in the temperature of the end of the process to higher temperatures 398 (400) - 427 (428) °C. At the same time, the position of the maximum of the main decomposition peak is in the range of 376-384 °C. The DTA curves show the disappearance of the pronounced thermal effect of melting even after exposure to minimal ionizing radiation.

The developed polymer has approximately an order of magnitude higher sensitivity to X-rays. The contrast is also slightly higher than that of PMMA with a molecular weight of one million grams per mole. A characteristic feature is a higher development temperature, caused by the large size of the coil molecules, consisting of fragments of the destroyed macromolecule, preventing the

penetration of the developer.The microstructures obtained by deep X-ray lithography have lower internal stresses and curvature at high values of the aspect ratio.1.

Reference

1. W.M. Moreau, Semiconductor lithography: principles, practices, and materials, New York : Plenum Press, 1988.

PERIODICITY IN THE DISTRIBUTION OF CHEMICAL ELEMENTS IN THE BOTTOM SEDIMENTS OF THE CHUKCHI SEA. #61

Submitted by **Ivan Kirichenko**

For track: X-ray fluorescent analysis

Author: Ivan Kirichenko (V.S. Sobolev Institute of Geology and Mineralogy SB RAS)

Co-author: Anatoliy Astakhov (V.I. Il'ichev Pacific Oceanological Institute Far Eastern Branch Russian Academy of Sciences)

As part of the work, a core of bottom sediments of the Chukchi Sea was studied, sampled in 2021 during the LV-95 cruise. To determine the concentrations of chemical elements along the bottom sediment core profile, the non-destructive XRF-SR scanning method using synchrotron radiation was applied. The XRF-SR scanning samples were prepared according to the technique described in [Phedorin and Goldberg, 2005] and represented wet sediment plates with geometric dimensions of 30×1.5×0.5 cm, cut from the central part of the column (core) and placed in aluminum cuvettes. The prepared "slabs" were wrapped in two layers of 10-micron thick polymer film to prevent the integrity of the material under study, as well as to protect the sediment from drying. To take into account the variation of humidity along the length of the studied column, as well as to convert the relative values of chemical element concentrations into absolute values, the method of external standard was applied. For this purpose on various intervals of the studied core of bottom sediments the sites in the size about 0,5-1 cm from which fragments of sediment were selected, which then were dried, rubbed and homogenized From the prepared material 30 mg tablets of 5 mm diameter were pressed [Phedorin, 2007]. Standards were used as comparison samples: bil-1.

"Slabs" were irradiated with a beam of collimated, polarized, monochromatic radiation with a vertical aperture of 1 mm. The following mode of analysis was used: source energy 23 keV, scanning step 1 mm, exposure per point was 45-100 seconds, with a total number of particles hitting the detector per second 5000-10000 Hz. Exposure for tablet studies was 120-300 seconds with a detector load of 12 kHz. Chemical element distributions from K to Mo by K-lines and U,Th, Pb by L-lines were obtained as a result.

Wavelet and Fourier analysis of chemical element distribution data showed significant statistically reliable periodic fluctuations in the chemical element content. The obtained data will help to clarify the climate variability of the Eastern Arctic seas during the last millennia.

This work was financially supported by the RSF project. № 21-17-00081. The work was done at the shared research center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB RAS. Some part of work is done on state assignment of IGM SB RAS

1. . Phedorin M. A., Bobrov V. A., Zolotarev K. V. Peat archives from Siberia: Synchrotron beam scanning with X-ray fluorescence measurements //Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. – 2007. – Т. 575. – №. 1. – С. 199-201

2. Phedorin M. A., Goldberg E. L. Prediction of absolute concentrations of elements from SR XRF scan measurements of natural wet sediments //Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. – 2005. – Т. 543. – №. 1. – С. 274-279.

PRECISE DETERMINATION OF THE CRYSTAL ORIENTATION AND TUNING THE BEAMLINE USING THE MEASURED DIFFRACTION LOSSES #62

Submitted by **Nataliya Klimova**

For tracks: SR technological application and X-ray apparatus, X-ray spectroscopy

Authors:

- Nataliya Klimova (Immanuel Kant Baltic Federal University(IKBFU))
- Anatoly Snigirev (Immanuel Kant Baltic Federal University)

Modern X-ray sources, such as x-ray free-electron lasers (FELs) and the fourth-generation synchrotrons, including the new Megascience facilities that are being built in Russia, have outstanding properties: are fully coherent, can generate a high-energy beam with extremely low emittance and high brightness. To deliver such a beam to the sample X-ray optics, such as monochromators, mirrors, compound refractive lenses (CRLs), attenuators, etc. are needed. To preserve the quality of the beam, the quality of the optics has to match. Therefore, the best materials for optics fabrication are single crystals. Crystalline materials like silicon, germanium, or diamond are robust, very well reproducible and, due to the ideal internal structure, the optics made of such materials produce almost no parasitic background. The last feature of the optics made of single-crystal materials is extremely important for modern x-rays sources. However, there is one drawback of such optics: diffraction losses caused by undesired Bragg/Laue scattering, which is usually termed the "glitch effect" [1].

The glitch effect manifests itself as follows: at some energy of the incident X-rays, the transmitted (or diffracted, in the case of monochromators) beam intensity drops. It happens when Bragg's law is satisfied, and a part of the beam is parasitically diffracted in some direction. Therefore, the main beam (transmitted, or diffracted for monochromators) loses some intensity (the parasitically diffracted part). Such glitches of the intensity are particularly harmful for the measurements that rely on the constant change of x-ray energy, like spectroscopy. But even for the experiments with the fixed X-ray energy, especially for the hard X-rays (E > 10keV), there is a high probability to set the energy close to some glitch. In this case, the intensity of the beam, incident at the sample, would be lower and unstable.

In paper [2] an easy way to simulate and predict the appearance of glitches in single crystals for different energies was demonstrated. Moreover, a way to avoid glitches during the measurements was proposed [3]. It was also found, that the measured glitches can be used constructively [2-4]. For example, one can determine the cell parameters and the orientation of the crystal to the beam [2], its rotation axes [3], and even tune the energy of the X-rays produced by the monochromator by determining the exact pitch angle of the monochromator crystals [4].

In paper [2] the spectrum of glitches from a diamond crystal was corrected by the manually refined pitch angle of the monochromator and then all measured glitches were indexed (attributed to the corresponding Miller indices) and the orientation of the crystal was determined. This procedure might be greatly improved by the simultaneous determination of the exact pitch angle of the monochromator (thus the energies of all measured glitches) and the orientation of the crystalline sample. Such a complex way of solving the problem for the spectroscopy data measured with a systematic error in the pitch angle can increase the precision of the orientation and the cell parameters determination. It would also allow correcting the pitch angle better.

That's exactly what is done in the current work – the spectroscopy data with the systematic error is analyzed in a way, that the error in the pitch angle is determined together with the cell parameters and orientation of the crystalline sample. The data measured at ESRF and used in the papers [1-4] is re-analyzed and better precision is achieved. The whole data processing pipeline is developed as a set of open-source programs deposited at [5].

The proposed method can be automated and routinely used at any beamline for fine-tuning the monochromator to make the energy of the generated X-ray beam more reliable and reproducible. Moreover, a monochromator tuned in this way will produce precise X-ray energy in a wide range of energies. Soon, this method can be successfully applied at the new diffraction-limited synchrotron

radiation source (4th generation facility) for the beam position correction without the need of additional mirrors, which can greatly improve the wavefront of the beam incident at the sample. Such an improvement is relevant and important for the new Megascience facilities that are being built in Russia according to the Federal Scientific and Technical Program for the Development of Synchrotron and Neutron Research and Research Infrastructure during 2019-2027.

Acknowledgments. This research was supported by the Russian Federal Academic Leadership Program Priority 2030 at the Immanuel Kant Baltic Federal University. The author acknowledges great support from Oleksandr Yefanov (CFEL@DESY, Hamburg, Germany)

References:

[1] M. Polikarpov, H. Emerich, N. Klimova. I. Snigireva and A. Snigirev Diffraction losses in monocrystalline X-ray refractive lenses // Proceedings of SPIE – 2017. – Vol.10235, – P. 102350H-2.
[2] N. Klimova, O. Yefanov, I. Snigireva, A. Snigirev, Determination of the exact orientation of single-crystal X-ray optics from its glitch spectrum and modeling of glitches for an arbitrary configuration // Crystals. –2021; - Vol. 11(5):504.
[3] N. Klimova, I. Snigireva, A. Snigirev, O. Yefanov, Suppressing diffraction-related intensity losses in transmissive single-crystal X-ray optics // Crystals. – 2021; - Vol. 11(12), 1561.
[4] N. Klimova, I. Snigireva, A. Snigirev, O. Yefanov, Using diffraction losses in the single-crystal X-ray optics for precise determination of its cell parameters and tuning the monochromator // Journal of Synchrotron Radiation. – 2022, – Vol. 29. – P. 369-376.
[5] Programs to calculate glitches in single-crystal X-ray optics. Online: https://github.com/XrayViz/Glitches

APPLICATION OF SYNCHROTRON RADIATION FOR IN SITU XRD INVESTIGATION OF THERMO-STIMULATED DECAY OF MAGNESIUM HYDRIDES #63

Submitted by **Viktor Kudiiarov**
For track: X-ray structural analysis
Authors:

- Viktor Kudiiarov (Tomsk Polytechnic University)
- Maxim Syrtanov (Tomsk polytechnic university)
- Zakhar Vinokurov (BIC SB RAS)
- Alexander Shmakov (Boreskov Institute of Catalysis SD RAS)
- Roman Elman (TPU)
- Nikita Kurdiumov (TPU)

In this work In situ X-ray diffraction measurements of the process of thermo-stimulated decay of magnesium hydrides were carried out at the station "Precision diffractometry» at Siberian Synchrotron and Terahertz Radiation Center of the Budker Institute of Nuclear Physics. Measurements were performed using SR from the VEPP-3 storage ring.

A MULTISCALE STUDY OF THE STRUCTURE OF POLYLACTIDES USING SYNCHROTRON X-RAY MICROTOMOGRAPHY AND LABORATORY TECHNIQUES #64

Submitted by **Alexey Buzmakov**
For track: SR for medicine and biology application
Author: Alexey Buzmakov (FSRC "Crystallography and photonics" RAS)
Co-authors:

- Andrey Dunaev (Federal Research Center "Crystallography and Photonics" RAS)
- Yuri Krivonosov
- Denis Zolotov (FSRC “Crystallography and Photonics” RAS)

- Irina Dyachkova (FSRC "Crystallography and Photonics" RAS)
- Marina Chukalina (Smart Engines LLC, 117312, Russia, Moscow; Institute for Information Transmission Problems RAS, 127051, Russia, Moscow; FSRC “Crystallography and Photonics” RAS, 119333, Russia, Moscow)
- Larisa Krotova (Federal Research Center "Crystallography and Photonics" RAS)
- Vladimir Volkov (FSRC "Crystallography and Photonics")
- Victor Asadchikov (FSRC "Crystallography and photonics" RAS)
- Vladimir Popov (Federal Research Center "Crystallography and Photonics" RAS)

The regeneration of living tissue (tissue engineering) is one of the most important problems of modern medicine. A possible way of solving this problem is to use bioresorbable porous matrices for this purpose. Such porous matrices can be based, in particular, on polylactides obtained by treating amorphous and partially crystalline polymers with supercritical carbon dioxide (sc-CO2). It is important that matrixes are prepared by this technology without the use of toxic organic solvents or high temperatures.

Comparative analysis of the internal structure and porosity data for poly-lactide scaffolds obtained by treatment with sc-CO2 on the scale of 0.02 μm to 1000 μm was carried out by X-ray small-angle scattering (SAXS), helium pycnometry (HP), mercury intrusion porosimetry (MIP) and laboratory and synchrotron X-ray micro-tomography (micro-CT). This approach opens up possibilities for large-scale evaluation, computer modeling, and prediction of physical and mechanical properties of polylactide scaffolds, as well as their biodegradation behavior in the body. [1]

It was shown that X-ray small-angle scattering can be applied to study pores with a radius less than 0.05 μm, while mercury porosimetry is not suitable for such small pores, as it requires high pressures, which destroys the walls of the polymer under study.

The work was supported by the Ministry of Science and Higher Education within the State assignment FSRC "Crystallography and Photonics" RAS in part of "interpretation of tomographic data" and grant of RFBR №19-29-12045 for synchrotron phase-contrast micro-CT studies.

[1] 1. Buzmakov A.V., Dunaev A.G., Krivonosov Y.S., Zolotov D.A., Dyachkova I.G., Krotova L.I., Volkov V.V., Bodey A.J., Asadchikov V.E., Popov V.K. Wide-Ranging Multitool Study of Structure and Porosity of PLGA Scaffolds for Tissue Engineering // Polymers, 2021, Vol. 13, No. 7, P. 1021.

PHOTOCHEMICAL BEHAVIOR AND EFFECT OF NOX ON FLUORINATED GRAPHITE USING A WHITE-BEAM SYNCHROTRON RADIATION #65

Submitted by **Galina Semushkina**
For track: X-ray spectroscopy
Author: Galina Semushkina (Nikolaev Institute of Inorganic Chemistry)
Co-authors:
- Dmitry Pinakov (Nikolaev Institute of Inorganic Chemistry)
- Galina Chekhova (Nikolaev Institute of Inorganic Chemistry)
- Igor Prosvirin (Boreskov Institute of Catalysis)
- Yuri Shubin (Nikolaev Institute of Inorganic Chemistry)
- Yuliya Fedoseeva (Nikolaev Institute of Inorganic Chemistry)
- Anna Makarova (Physikalische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin)
- Alexander Okotrub (Nikolaev Institute of Inorganic Chemistry)
- Lubov Bulusheva (Nikolaev Institute of Inorganic Chemistry)

The interaction of graphite with inorganic fluorides at room temperature leads to the formation of fluorinated graphites CF0.1-0.5, which are layered carbon materials with high chemical, mechanical and thermal stability. Due to their layered structure and unique amphoteric redox

properties, these compounds can serve as promising carriers of many substances, both donors and acceptors. Of particular research interest are carbon materials as a container for storing poisonous gases. Thus, activated carbon showed high efficiency in the reversible adsorption of NOx molecules, which are common anthropogenic air pollutants. In addition, the carbon carrier can act as a catalyst and, under certain conditions, cause the denitrification of NOx to form non-toxic N2. Denitrification can also take place under the action of ultraviolet radiation. Photolysis of NOx is also of interest from the point of view of studying processes in the Earth's atmosphere under the action of solar radiation, where nitrogen-containing oxides play a key role in redox cycles.

Thereby the aim of the work is to carry out a comparative analysis of the composition of intercalated NOx@CF0.4 before and after annealing at 200ºC using the XPS and NEXAFS methods; study of NOx photoionization, as well as the stability of an intercalated and annealed CF0.4 fluorographite matrix as a result of exposure to a high-intensity polychromatic photon beam (zero-order electromagnetic radiation from the dipole beam of the BESSY II synchrotron radiation facility) for 420 s; using IR spectroscopy to study the functional composition of intercalated fluorinated graphite during heating; when using thermogravimetric analysis, determination of the evaporation temperature of NOx.

In this work, we performed a comprehensive analysis of the functional composition, electronic structure, and stability of the CF0.4 before and after annealing, as well as the photochemical activity of intercalated NOx before and after exposure to a zero-order synchrotron beam in the in situ mode for up to 420 seconds using XPS and NEXAFS spectroscopy. It has been found that exposure to a zero-order synchrotron beam leads to defluorination of the FG system, with possible removal of carbon and the formation of vacancy defects. The graphitic lattice of the annealed sample is more stable than the original sample. The incorporation of liquid N2O4 into CF0.4 causes a number of chemical reactions in the interlayer space of the FG with the dissociation of N2O4 to NO2 and to disproportionation reactions with the formation of NO3 and NO followed by denitrification to N2. Photolysis of NOx in the CF0.4 interlayer space leads to increased denitrification and incorporation of nitrogen atoms into the graphite lattice in the form of pyrrole-like nitrogen atoms. Annealing at ~200°C for 10 minutes promotes the formation of an “empty” fluorographite matrix with traces of HNO3, NO2, N2 and pyrrole-like nitrogen at the NEXAFS probing depth, followed by a decrease in the nitrogen concentration upon irradiation.

GENERATION OF NEAR-INFRARED RADIATION HARMONICS BASED ON REGULAR POLYMER MATRICES WITH CONE AND CYLINDRICAL PORE GEOMETRY AND COATINGS APPLIED ON THEM #66

Submitted by **Irina Dyachkova**

For track: SR technological application and X-ray apparatus

Authors:

- Victor Asadchikov (FSRC "Crystallography and photonics" RAS)
- Vladimir Nazmov (Budker Institute of Nuclear Physics)
- Boris Goldenberg (Budker INP SB RAS, SRF “SKIF”)
- Andrey Konovko (M.V. Lomonosov Moscow State University)
- Alexander Vasiliev (FSRC “Crystallography and fotonics” RAS)
- Yuriy Grigoriev (FSRC “Crystallography and Photonics” RAS)
- Sergey Bedin (FSRC “Crystallography and fotonics” RAS)
- Evgeniy Epifanov (FSRC “Crystal-lography and Photonics” RAS)
- Irina Dyachkova (FSRC "Crystallography and Photonics" RAS)

Thin commercially available films of such material as polyethylene terephthalate are characterized by high values of mechanical strength, high chemical and thermal and radiation resistance, has high transparency in the visible and near-infrared range of the spectrum. Such films

are promising for recording by microlithography methods with high density of information and its long-term storage. Recording of information can be carried out by deep X-ray lithography. For this purpose, the sensitivity of the material with respect to the dose of absorbed radiation and the rate of removal of the irradiated material from the surface of the original film was studied in this work, resulting in a complex dependence of the removal selectivity on the concentration of alkali as a reagent. The resulting relief has the character of a developed regular volumetric microstructure. Thus, regular polymer matrices with cone and cylindrical pore geometry were obtained. Metallic and dielectric cone microstructures were obtained using such matrices. The height of the synthesized microstructures ranged from tens to fractions of microns with a repeatability period of 3 μm. Theoretical and experimental studies of harmonic generation efficiency in the interaction of femtosecond near IR laser radiation with synthesized metallic pointed structures under conditions of plasmon resonance excitation were carried out. It is shown that irradiation by intense femtosecond laser pulses of a periodic in two dimensions microstructured metal target with a thin film metal coating allows the creation of an anisotropic nanostructure on the surface. Formation of the surface nanostructure leads to an increase in the efficiency of radiation generation at the second harmonic frequency in the reflection geometry. An installation for optical study of microstructured materials on the process of the efficiency formation second harmonic from high-frequency femtosecond infrared radiation in the "on reflection" scheme with the possibility of automated framing of the surface and volume of samples was developed and created. A method of diagnosing the morphology of a target based on the study of the second harmonic generation efficiency process in the "backward" geometry in the mode of continuous measurement of spectra has been developed. The developed technique was tested on a high frequency near-infrared femtosecond laser radiation.

The reported study was partially funded by the RFBR research projects 18-29-20090 in terms of obtaining regular membranes and considering the possibility of their applicability for solving photonics problems and by RFBR research projects 18-02-00528 in terms of developing algorithms for solving the diffraction problem on surface nano- and microstructures, writing programs implementing these algorithms and carrying out mathematical modeling.

LIFETIME OF POLYMERIC REFRACTIVE X-RAY LENSES #67

Submitted by **Vladimir Nazmov**
For track: SR technological application and X-ray apparatus
Authors: Vladimir Nazmov, Elena Reznikova (Budker Institute of Nuclear Physics)

The ability to keep the initial properties under irradiation is one of the most important (along with effective aperture) characteristics of X-ray lenses. When irradiated with gamma and X-rays, structural damages are arised in the lens material, called radiation defects, and the temperature in the lens material under the influence of radiation can reach tens and hundreds of degrees. Therefore, it take place radiation-thermal effects in the material. It is known that even refractive lenses made of beryllium undergo destroying in powerful X-ray beams, so it can be expected that the tenure of a polymer lens in the X-ray beam is especially critical both for the lens and for the result of the experiment. The following are the main factors determining the lifetime of a polymer lens in an X-ray beam:

1. Selection of radiation-resistant initial material: polymeric materials are classified according to resistance.
2. Modification of the lens material in order to reduce internal energy of the material.
3. Relaxation of molecules of the material in X-ray beam.
4. Design features: optimized areas of passive material, microsteructure symmetry, supporting beams are outside the area of the lens illuminated by X-rays.
5. The use of high photon energy; low absorbed power of X-rays.
6. Gas environment.

A series of experiments was carried out to study the lifetime of lenses made of SU-8 photoresist. Namely, in X-rays from a bending magnet of the ANKA synchrotron radiation (SR) source, the impact of high power and high temperature induced by X-rays was studied, when the refractive elements were oriented so that the lens optical axis was perpendicular to the direction of the incident radiation. In this orientation, the X-ray power absorbed by each refractive polymer structure is maximum. In other experiments, undulator radiation from ESRF and Spring-8 SR- sources was directed along the optical axis of the lens. The refractive microstructures retained their mechanical and optical properties throughout the experiment. The high resistance of the abovementioned material is based on the radiation-resistant cyclic groups and glycidyl groups in its composition, that provide high thermal stability due to stable bonds with each other.

Secondly, after the lens microstructuring is completed, under the influence of X-rays, up to the accumulation of a dose of about 1 kJ per cubic centimeter, the opening of epoxy cycles continues with the formation of new bonds, which also leads to an increase in the life-time. Third, in the absence of post-curing, the material contains an appreciable amount of water, which leaves the polymer material and carries away some of the absorbed energy.

STUDY OF EXTREME HYDRODYNAMIC PHENOMENA IN LASER PLASMA BY ULTRA-HIGH RESOLUTION COHERENT X-RAY RADIOGRAPHY #68

Submitted by **Sergey Makarov**
For track: X-ray structural analysis
Author: Sergey Makarov (JIHT RAS)
Co-authors:

- Tatiana Pikuz (JIHT RAS)
- Artem Martynenko (JIHT RAS)
- Sergey Dyachkov (1. Dukhov Research Institute of Automatics, Moscow 2. JIHT RAS)
- Vasily Zhakhovsky (1. Dukhov Research Institute of Automatics 2. JIHT RAS)
- Nail Inogamov (Landau Institute for Theoretical Physics of Russian Academy of Sciences)
- Viktor Khokhlov (Landau Institute for Theoretical Physics of Russian Academy of Sciences)
- Gabriel Rigon (Nagoya Univ, Grad Sch Sci)
- Bruno Albertazzi (LULI, CNRS, CEA)
- Paul Mabey (LULI, CNRS, CEA)
- Michel Koenig (1. LULI, CNRS, CEA 2. Graduate School of Engineering, Osaka University)
- Kento Katagiri (Graduate School of Engineering, Osaka University)
- Yuichi Inubushi (1. Graduate School of Engineering, Osaka University 2. RIKEN SPring-8 Center,)
- Kohei Miyanishi (RIKEN SPring-8 Center)
- Keiichi Sueda (RIKEN SPring-8 Center)
- Tadashi Togashi (1. Graduate School of Engineering, Osaka University 2.RIKEN SPring-8 Center)
- Makina Yabashi (1. Graduate School of Engineering, Osaka University 2. RIKEN SPring-8 Center,)
- Toshinori Yabuuchi (1. Graduate School of Engineering, Osaka University 2. RIKEN SPring-8 Center)
- Norimasa Ozaki (1. Graduate School of Engineering, Osaka University 2. Institute of Laser Engineering, Osaka University)
- Sergey Pikuz (JIHT RAS)

In a variety of phenomena that occur in astrophysics and modern nuclear technology, matter is under the influence of high intensity energy. This effect, in turn, leads to a whole complex of complex

hydrodynamic phenomena (various types of instabilities, plasma jets, shock waves), the understanding of which is of interest for both applied and fundamental problems.

With the advent of X-ray free-electron lasers (XFELs), it is possible to solve the problems of studying hydrodynamic phenomena in plasmas with radiographic methods. On the one hand, the femtosecond duration of the pulses of such devices offers a high temporal resolution; on the other hand, monochromaticity, high coherence and brightness enable diffraction-enhanced images of objects with small density gradients. In this way, fundamentally new possibilities arise for the investigation of low-contrast hydrodynamic phenomena in plasmas.

The aim of this work was to investigate with submicron resolution the fast-flow hydrodynamic phenomena such as the evolution of Rayleigh-Taylor instability and paired shock wave structures in nanosecond laser plasmas, taking advantage of X-ray lasers.

CRYSTAL STRUCTURE ANALYSIS OF NICKEL-BASED CATALYSTS #69

Submitted by **Maxim Mikhnenko**
For track: X-ray structural analysis
Author: Maxim Mikhnenko (BIC SB RAS; NSU)
Co-authors:

- Svetlana Cherepanova (Boreskov institute of catalysis SB RAS)
- Alexander Shmakov (Boreskov Institute of Catalysis SB RAS)
- Maria Alekseeva (Boreskov institute of catalysis SB RAS)
- Roman Kukushkin (Boreskov institute of catalysis SB RAS)
- Vera Pakharukova (Boreskov institute of catalysis SB RAS)
- Olga Bulavchenko (Boreskov institute of catalysis SB RAS)

In the last decades the methods of researches on the basis of synchrotron sources (SR) of radiation are actively developed. The use of SR allows to change the wavelength of radiation, which allows using different methods to study the structure of matter. One of such methods is the atomic pair distribution method (pair distribution function, PDF), which uses short wavelengths: 0.1-0.2 Å. Due to this method one can receive information on the coordination environment inside the structure, which is especially relevant. Moreover, the use of SR allows one to apply the methods of in situ X-ray diffraction with an increased, compared to laboratory devices, intensity and improved angular resolution of the obtained data, and thus a more precise study of various processes, due to a shorter accumulation time. This allows a more detailed recording of phase transitions and thus obtain more structural data

In the course of this work, the structural features of NiO-based nanostructured catalysts were investigated. The peculiarity of the systems under study was the stabilization of the oxide in highly dispersed form due to the introduction of silicon additives. X-ray diffraction of the catalyst differed from the "classical" X-ray diffraction of bulk nickel oxide and was characterized by certain features - different broadening of diffraction reflexes - whose interpretation by standard methods did not give satisfactory results. Therefore, the catalyst was investigated by a set of diffraction techniques, which included PDF and X-ray diffraction simulations by the Debye method. The data for the PDF calculation were obtained at the VEPP-4 source using a wavelength of λ=0.1792Å. The following structural models were considered: (1) particle shape effect using cube, sphere, plate, and filament as examples, (2) different models of silicon embedding into nickel oxide structure. It is shown that silicon incorporation is realized due to NiO layer replacement with formation of a fragment following the "spinel" Ni2SiO4 structure fragment. The results of transmission electron microscopy also confirmed this hypothesis and showed that the silicon is evenly distributed on the nickel oxide particles. In addition, the crystallites have a plate-like shape with a thickness of 1.5 nm and a width of 3 nm.

The second task was to carry out in situ X-ray diffraction studies of the reduction process of nickel oxide with the introduction of various additives (W, Si, Cu, Mo). It was shown that depending

on the chemical nature of the modifier, both acceleration and deceleration of the reduction from the oxide state to the metallic state occur.

This work was carried out with the support of Program "Priority 2030" NSU.

STRUCTURAL ANALYSIS OF THROMBIN-BINDING G-QUADRUPLEX APTAMERS BY SAXS METHOD #70

Submitted by **Polina Nikolaeva**
For track: X-ray structural analysis
Author: Polina Nikolaeva (Lomonosov MSU)
Co-authors:
- Vasilisa Raldugina
- Iulia Naumova
- Tatyana Novikova
- Vera Spiridonova

Analyzing 3D structure of G-quadruplex aptamers is not a trivial task as it is not always possible to use the common methods like X-Ray or NMR. However, alternative methods might provide the answer to this question. One of such methods is SAXS method. In this project thrombin-binding G-quadruplex aptamers RE31, NU172 and HD22 have been studied. SAXS method has made it possible to discover structural difference between crystallized and dilluted samples. Moreover the methods has given us the ability to estimate to what extent do different concentration of bivalent ions affect the structure of RE31, NU172 and HD22.

LONG-WAVES REGIME OF TERAHERTZ NOVOFEL WITH HYBRID OPTICAL RESONATOR #71

Submitted by **Vitaly Kubarev**
For track: SR and FEL sources and centers
Author: Vitaly Kubarev (BINP)
Co-authors:
- Oleg Shevchenko (BINP)
- Yaroslav Getmanov (BINP)

Typical regimes of the terahertz NovoFEL assume operation on the modes of an open optical resonator. In recently discovered regimes with anomalously long waves up to 340 μm, intracavity radiation is represented by modes a hollow waveguide inside the undulator and an open cavity modes in the sections between the ends of the undulator and the mirrors.

POINT-LIKE PLASMA-LIMITED HIGH-TEMPERATURE THZ LASER DISCHARGE #72

Submitted by **Vitaly Kubarev**
For track: THz radiation aplication
Author: Vitaly Kubarev (BINP)
Co-authors:
- Alexander Sidorov (IAP)
- Axexander Vodopyanov (IAP)
- Yaroslav Gorbachev (BINP)
- Oleg Shevchenko (BINP)
- Alexey Veselov (IAP)

A continuous equilibrium point laser discharge in the form of a ball 0.8 mm in diameter with a plasma density of 3E17 cm-3 and a temperature inside the ball of 4.2 eV (49 kK) was obtained at the terahertz NovoFEL. The ways of increasing the plasma parameters and its potential application as a source of VUV-radiation are considered.

ОДНОЭЛЕМЕНТНЫЙ ШИРОКОПОЛОСНЫЙ МОНОХРОМАТОР НА ОСНОВЕ ПЛОСКОЙ VLS-РЕШЕТКИ #73

Submitted by **Evgeny Ragozin**
For track: SR technological application and X-ray apparatus
Authors:

- Evgeny Ragozin (P.N. Lebedev Physical Institute)
- Alexey Shatokhin
- Aleksei Kolesnikov (P.N. Lebedev Physical Institute of the Russian Academy of Sciences)

Предложена концепция нового монохроматора на основе плоской VLS-решетки с экспоненциальной зависимостью частоты штрихов от координаты, в котором угол отклонения постоянен, а щели, источник и детектор излучения неподвижны. Сканирование длины волны осуществляется при помощи линейной трансляции решетки вдоль ее поверхности, при этом дифрагированное излучение остается сфокусированным на выходную щель, и аберрации не нарастают. Рассчитана схема прибора для применения на синхротронном источнике в спектральном диапазоне 125 – 4200 Å. Расстояние от источника до решетки составляет 28.55 м, расстояние от решетки до выходной щели – 650 мм, постоянный скользящий угол падения на решетку – 7.0°, постоянный угол отклонения – 19.5°. Разрешающая способность составляет 6000 при ширине выходной щели 8 мкм. Частота штрихов варьируется от ~ 1300 до ~ 35 1/мм. Для покрытия полной ширины диапазона предполагается использование нескольких сменных решеток.

Аналогичный подход оказался применим также к созданию компактного (в частности, менее 1 м) монохроматора высокого разрешения с равными расстояниями входная щель – VLS-решетка и VLS-решетка – выходная щель. Такой монохроматор может использоваться, например, в комбинации с импульсно-периодическим лазерно-плазменным источником излучения в вакуумной области спектра.

ESTIMATION OF THE SPATIAL RESOLUTION VALUE FOR CONTACT PHOTOLITHOGRAPHY AND X-RAY LITHOGRAPHY #74

Submitted by **Aleksandr Gentselev**
For track: SR technological application and X-ray apparatus
Author: александр генцелев

Simple methods for estimating the spatial lithographic resolution during the formation of a resistive mask by means of both X-ray lithography using polymethylmethacrylate (PMMA) as an X-ray resist and synchrotron radiation (SI) as an exposing radiation, and contact photolithography using a negative SU-8 resist (or its analogues) are described. The cases of exposure of thin (~1 microns) and thick (~1 mm) resistive layers are considered. An algorithm for determining the technological window for X-ray lithography based on the formula of the characteristic curve for the used resist and the specified developer composition and development conditions is described. Attention is drawn to the fact that the question of calculating the spatial resolution in the hard X-ray spectral range ($\lambda \approx 0.5 \div 3$ Å), often used in the implementation of deep X-ray lithography (for example, in LIGA technology), remains open and requires further theoretical and experimental research.

RADIATION FROM A METASURFACE AS AN INSTRUMENT FOR ELECTRON BUNCH DIAGNOSTICS #75

Submitted by **Daria Sergeeva**
For track: SR and FEL sources and centers
Authors:

- Daria Sergeeva (National Research Nuclear University "MEPhI")
- Alexey Tishchenko (National Research Nuclear University "MEPhI")

Radiation from electron bunches is usually used for diagnostics of its transverse sizes in accelerators and colliders including FELs and synchrotron injectors. However, the methods of diagnostics continue to improve. There are some ideas on single-short diagnostics, or non-destructive diagnostics, or using new types of targets, among which metamaterials and photonic crystals seem to be attractive. In this report we suggest using incoherent transition radiation from two-periodical targets in order to define transversal sizes of the bunch. Usually the diagnostics is reduced to comparison the measured data to the theoretical one, which take in account the coherent effects. The generally accepted approach to take into account coherence from electron bunches consists in multiplying the radiation intensity from one particle by the bunch form-factor, which takes into account its size, shape, and distribution of electrons. We show that in polarization radiation for a wide class of structures, such as photonic crystals and metasurfaces, this approach is incorrect. We construct a theory of coherent and incoherent Smith-Purcell radiation and transition radiation from such structures and discuss its applicability to relativistic electron bunch diagnostics.
This work was supported by the Russian Science Foundation, grant № 21-72-00113.

PLASMA DISCHARGE IN A NON-UNIFORM GAS FLOW, SUSTAINED BY THE POWERFUL RADIATION OF NOVOSIBIRSK FREE ELECTRON LASER, AS A POINT-LIKE SOURCE OF VACUUM ULTRAVIOLET RADIATION #76

Submitted by **Alexander Sidorov**
For track: THz radiation aplication
Author: Alexander Sidorov (IAP RAS)
Co-authors:

- Alexander Vodopyanov (IAP RAS)
- Alexey Veselov (IAP RAS)
- Vitaly Kubarev (BINP SB RAS)
- Oleg Shevchenko (BINP SB RAS)
- Yaroslav Gorbachev (BINP SB RAS)

In this paper, we consider the prospect of creating a point-like source of vacuum ultraviolet radiation (VUV) based on a plasma discharge, sustained by the terahertz radiation from the Novosibirsk free electron laser.

Investigation of the gas discharge in the quasi-optical beams of high-power electromagnetic radiation of the terahertz frequency range is attractive for a large number of both fundamental and applied research. The study of this discharge became possible only recently due to the development of the unique and reliably working sources of powerful radiation in this range. Namely, terahertz free electron lasers and gyrotrons. The study of localized (point-like) discharge is especially important due to the need to solve the problem of creating a point-like source of extreme ultraviolet (EUV) light for the next-generation projection lithography.

The possibility of creating a point-like (characteristic size 100–500 μm) discharge in an inhomogeneous gas flow sustained by radiation from the terahertz frequency range had been demonstrated for the first time in IAP RAS. The conditions for the existence of such a discharge, the plasma parameters and its luminosity in VUV and EUV ranges were studied. It was experimentally shown that such a discharge radiates very effectively in the region of the vacuum ultraviolet. In

addition, it was demonstrated that an increase in the frequency of the heating field improves the coupling of the radiation with the plasma. It was estimated that the optimal frequency of the heating radiation is in the range of 1-3 THz. Calculations show that for radiation in the vacuum and extreme UV range the optimum plasma density is of 10^16 - 10^17 cm^-3. Thus, the plasma parameters provided by powerful THz radiation turn out to be optimal for the generation of EUV radiation

It is proposed to use high-power free-electron laser radiation to heat heavy noble gases plasma in an inhomogeneous stream as a possible promising source of vacuum and extreme ultraviolet radiation. Experimental studies on the Novosibirsk terahertz FEL with discharges at atmospheric pressure have shown that the terahertz range is optimal for creating dense plasma with a high plasma temperature. The plasma density was of 2·1017 cm-3, the electron temperature was of 2-3 eV, ion temperature in such dense full-ionized plasma can be close to electron temperature.

При этом стоит отметить, что для достижения необходимой степени кратности ионизации (с точки зрения излучения в VUV и EUV диапазонах) многозарядных ионов тяжелых инертных газов необходимо достичь температур электронов в 10-30 эВ. Поэтому основной задачей на данный момент является достижение таких температур в ТГц разряде в неоднородном потоке газа, поддерживаемом излучением Новосибирского ЛСЭ.

It should be noted that in order to achieve the required degree of ionization (in terms of radiation in the VUV and EUV ranges) of multiply charged ions of heavy noble gases, it is necessary to achieve electron temperatures of 10–30 eV. Therefore, the main task at the moment is to achieve such temperatures in a THz discharge in an inhomogeneous gas flow, sustained by radiation from the Novosibirsk FEL.

THE POSSIBILITY OF CONTROL OF THE PHASE OF OPTICAL FID IN MAGNETIC FIELD #77

Submitted by **Evgeniy Chesnokov**
For track: THz radiation aplication
Author: Evgeniy Chesnokov (Istitute of Chemical Kinetics)
Co-authors:

- Pavel Koshlyakov
- Vitaly Kubarev (BINP)

This work demonstrates the possibility of switching the phase of optical free induction (FID) in time-domain experiments. This possibility arises in experiments with paramagnetic molecules (free radicals) in a magnetic field. Changing the direction of the magnetic field alters the direction of rotation of the polarization plane of the FID and inverts the phase of one of the components of FID. This effect will be useful for heterodyne detection the optical FID of the free radicals in the terahertz region.

The spectroscopy of the free radicals in the terahertz region (approximately 1-10 THz or 30-300 μm) could be a useful tool for studying combustion processes. In this region there are rotational transitions of many important free radicals, such as OH, CN, CH, CH2, etc. [1]. Number of works [2–4] demonstrates the application of terahertz spectroscopy for kinetic studies.

The main feature of free radicals is a magnetic moment which is aroused by the presence of unpaired electrons. An external magnetic field affects the energy levels and therefore the absorption and emission spectra of these radicals. Free radicals are usually present in low concentrations, so the task of selective detection of free radicals compared to the absorption of stable molecules is important. In a magnetic field, free radicals can be distinguished because the spectra of stable molecules are insensitive to the magnetic field. Laser magnetic resonance method uses the modulation of the absorption coefficient of the radicals by a magnetic field [5]. It is more convenient to use the effect of a magnetic field on the polarization than on the absorption. This is implemented in the Faraday Rotation Spectroscopy FRS method [6,7].

In the technique of ESR spectroscopy, manipulation of the phases of exciting pulses is widely used [15]. Standard ESR spectrometers operate at around 10 GHz, where phase control can be performed using electronic components. In the simplest case, the alternation of exciting microwave pulses with antiphases and measuring the difference between the corresponding FIDs permits to eliminate all possible instabilities of the receiving system. All modern ESR spectrometers use this technique. Also, special techniques are utilized for exciting the spin echo by a sequence of pulses with a controlled phase shifts, which provide additional information of ESR spectra [16].

Experiments with OH radical. Without magnetic field the FID radiation is linearly polarized with the same direction as the NovoFEL exciting pulse (in our experiments − vertical polarization). Consequently, a horizontally installed polarizer completely blocks the FID signal. When the longitudinal magnetic field was applied, the plane of polarization of the FID rotated and horizontally polarized wave component appeared.

The FID phase was determined relative to the reference optical signal formed from the NovoFEL exciting pulse. The NovoFEL radiation pulse was divided into two parts by a polypropylene beam splitter. The first part excited OH radicals formed in the cell by UV pulse [13]. The horizontal FID component was recorded by a detector with a polarizer in front of it. This polarizer, in combination with the polarization property of the antenna of the Schottky diode detector [21], completely blocked the passage of the powerful FEL pulse to the detector.

When the reference signal was directed to the receiver together with the weak FID signal, the result of their interference was clearly observed. At some points in time, the intensity of the reference signal increased, at others, on the contrary, decreased. When the direction of the magnetic field was changed, the phase of the FID signal was reversed, and the interference pattern was inverted.

The ability to change the phase of the FID will be extremely useful in heterodyne measurement of FID signals. It is well known that methods for heterodyne detection of an electromagnetic wave are much more sensitive than the detection of the radiation intensity. In fact, Fig. 1 demonstrates that a low-intensity FID wave causes a large change in the intensity of the resulting signal as a result of interference with the reference wave.

DEVELOPMENT AND CHARACTERIZATION OF IMPULSE THZ HEATING METHOD USING EPR OF MAGNETOACTIVE COMPOUNDS #78

Submitted by **Sergey Tumanov**
For tracks: SR and FEL sources and centers, THz radiation aplication
Authors:

- Sergey Tumanov (ITC SB RAS)
- N.A. Artiukhova (ITC SB RAS)
- Anatoly Melnikov (International Tomography Center)
- A.S. Bogomyakov
- Oleg Shevchenko (BINP)
- Yaroslav Getmanov (Budker INP)
- V.I. Ovcharenko (ITC SB RAS)
- M.V. Fedin
- Sergey Veber (International Tomography Center SB RAS)

The possibility of a fast temperature change of the sample in a controllable way makes it possible to study related phenomena, such as thermally induced trapping of metastable states in magnetoactive compounds or thermally activated catalytic and biological processes. The Electron Paramagnetic Resonance (EPR) spectroscopy station at the Novosibirsk Free Electron Laser (NovoFEL) makes it possible to study the influence of terahertz radiation on the spin state of paramagnetic systems. Changes in the compound temperature due to radiation absorption are inevitable consequences of such exposure. However, the process of sample heating at the NovoFEL EPR station itself is of great interest because of the record-setting power of THz radiation at NovoFEL along with possibility of

using small compound samples. Together these two factors result in significant heating rate. The magnetoactive complex [Cu(hfac)2LEt] was chosen as a model system for studying the heating process. The advantages of this complex in the scope of the goal are a sharp spin transition and significant differences between the spin states above and below the transition temperature. In current work, the heating process of [Cu(hfac)2LEt] is studied. We have shown the setup ability for pulsed heating with > 60 K amplitude at 7.3 K/ms heating rate. The results are promising for further studying of thermally induced metastable states and other thermally activated processes.

NEW SPIN-POLARIZED ELECTRON SOURCE BASED ON ALKALI-ANTIMONIDE PHOTOCATHODE #79

Submitted by **Oleg Tereshchenko**
For track: SR and FEL sources and centers
Authors:

- Oleg Tereshchenko (A.V. Rzhamov Institute of Semiconductor Physics SB RAS)
- V.S. Rusetsky
- V.A. Golyashov
- S.V. Eremeev
- D.A. Kustov
- I.P. Rusinov
- T.S. Shamirzaev
- A.V. Mironov
- A.Yu. Demin

New spin-dependent photoemission properties of alkali antimonide semiconductor cathodes are predicted based on the detected optical spin orientation effect and DFT band structure calculations. Using these results, the Na2KSb/Cs3Sb heterostructure is designed as a spin-polarized electron source in combination with the Al{0.11}Ga{0.89}As target as a spin-detector with spatial resolution. In the Na2KSb/Cs3Sb photocathode, spin-dependent photoemission properties were established through detection of high degree of photoluminescence polarization and high polarization of the photoemitted electrons. It was found that the multi-alkali photocathode can provide electron beams with emittance very close to the limits imposed by the electron thermal energy. The vacuum tablet-type sources of spin-polarized electrons have been proposed for accelerators, that can exclude the construction of the photocathode growth chambers for photoinjectors.

OPTICAL SCHEMES FOR COHERENT GRAZING INCIDENCE X-RAY IMAGING #80

Submitted by **Igor Artyukov**
For track: SR technological application and X-ray apparatus
Authors:

- Igor Artyukov (Lebedev Physical Institute RAS)
- Aleksander Busarov (Lebedev Physical Institute RAS)
- Nikolay Popov (Lebedev Physica Institute RAS)
- Aleksander Vinogradov (Lebedev Physical Institute RAS)

It is known that X-ray analytical methods and imaging technologies are often used in the reflection mode at grazing incidence. Moreover, such an experimental arrangement is in many cases the most efficient. This paper deals with X-ray imaging. Grazing incidence X-ray imaging is used now both in lens and lens free experimental schemes at SR facilities as well as laboratory set ups [1-3]. In both cases, when operating in the range of 30 eV - 2 keV, the need for oblique illumination of the object is obvious from Fig 1. As can be seen, the reflectivity as well as the transmission of the sample (over 30 μm thick) are extremely low for all the considered elements. In this regard, normal

incidence reflection and transmission imaging are both inefficient and the only way out is grazing incidence reflection imaging.

Fig. 1. Graph of the attenuation length L (solid lines) and the reflectance R (dashed lines) depending on the photon energy for various materials. The figure shows the photon energy range 30 eV - 2 keV where the image can be obtained only by illuminating the sample at small grazing angles for the sample thickness is at least 30 μm.

This work is devoted to modeling X-ray optical schemes with oblique object illumination (Fig 2). To do this, it is desirable to have a theoretical tool similar to the Fresnel diffraction integral, widely used in usual optics from visible to X-rays. Such a tool - tilted object diffraction integral (TOI) was suggested and studied in [4-7]. It has the form:

$$u(x,y,z) = \frac{k}{2\pi i}(x\cos\theta + z\sin\theta)\int_{-\infty}^{+\infty} dy' \int_{-\frac{z}{\cos\theta}}^{\infty} u_0(y',s)\frac{e^{\frac{ik[x-s\sin\theta]^2+(y-y')^2}{2}}}{(z+s\cos\theta)^2}ds$$

where u(x,y,z) - field, k-wave number, θ – angle, u0(y',s) – field on the plane y's.

Using (1), it is possible to show that with oblique illumination of an object, the image is located on an optically conjugate plane (see Fig.2), and also to establish a relationship between the field distributions on the surface of the object and the detector, similar to the known formulas for optical transformations [8].

Fig. 2. Scheme of the optical system: θ, θ' are the angles of inclination of the object and image (detector) planes, respectively, to the z axis; k is the wave vector; The detector is located on a plane optically conjugated to the plane of the object. The proposed theory allows for detailed modeling of images formation, taking into account their quality, to determine the spatial resolution and field of view of a system with grazing incidence object illumination. Some examples will be presented.

References

1. C. Jacobsen, "X-ray microscopy", Cambridge University Press, 2020
2. Motoyoshi Baba, Masaharu Nishikino, Noboru Hasegawa, Takuro Tomita, Yasuo Minami, Ryota Takei, Mitsuru Yamagiwa, Tetsuya Kawachi, and Tohru Suemoto, Submicron scale image observation with a grazing incidence reflection-type single-shot soft X-ray microscope, Japanese Journal of Applied Physics 53, 080302 (2014)
3. Nouamane Laanait, Erika B. R. Callagon, Zhan Zhang, Neil C. Sturchio, Sang Soo Lee, Paul Fenter, X-ray–driven reaction front dynamics at calcite-water interfaces, VOL 349 6254, 2015
4. Artyukov I. A.; Popov A.V.;Vinogradov A.V.: 'Wave field transformation at coherent imaging of a flat reflection mask', Proc. SPIE, 7451, 745114-1 - 745114-3, 2009
5. Artyukov I. A, Mitrofanov A N, Popov A V, Vinogradov A V: "Theory and computation towards coherent reflection imaging of tilted objects", X-ray Lasers 2010: Proceedings of the 12th International Conference on X-ray Lasers (Springer-Verlag, Berlin & Heidelberg, 2010), pp. 329
6. I. A. Artyukov, R. M. Feshchenko, N. L. Popov, A. V. Vinogradov, "Coherent scattering from tilted objects", Journal of Optics, 16 (3), 035703 (2014)
7. I. A. Artyukov, A. V. Vinogradov, N. L. Popov, V. N. Seleznev, "Simulation of grazing-incidence coherent imaging", Quantum Electron., 42:2 (2012), 140–142
8. Athanasios Papoulis, "Systems and Transforms with Applications in Optics", McGraw - Hill Book Company, 1968

COMPARISON OF DIFFERENT APPROACHES FOR DEVELOPMENT OF TERAHERTZ FOCUSING OPTICS #81

Submitted by **Vladimir Pavelyev**
For track: THz radiation aplication
Authors:

- Boris Knyazev (Budker Institute of Nuclear Physics)
- Maxim Komlenok (GPI RAS)
- Vladimir Pavelyev (Samara University)

- Andrey Agafonov (Samara University)
- Sergey Kharitonov (Samara University)
- Yuri Strelkov (Samara University)
- Taras Kononenko (GPI RAS)
- Vasily Gerasimov (Budker Institute of nuclear physics SB RAS)
- V.D. Kukotenko (Budker Institute of nuclear physics SB RAS)
- N.D. Osintseva (Budker Institute of nuclear physics SB RAS)

Different approaches for development of reflective [1] and transmissive silicon [2] and diamond [3] terahertz diffractive optics were presented in before. Results of numerical as well as experimental investigation of silicon subwavelength cylindrical lens will be presented. Results of comparison of different approaches for development of terahertz focusing optical elements will be presented also. All experiments were performed with the application of coherent monochromatic frequency-tunable radiation from the Novosibirsk free electron laser.

The study was supported by the Russian Science Foundation grant No. 19-72-20202.

The experiments were carried out at the Novosibirsk Free Electron Laser Facility, which is part of “the Siberian Synchrotron and Terahertz Radiation Center”.

1. A.N. Agafonov, B.A. Knyazev, V.S. Pavelyev, E.I. Akhmetova, V.I. Platonov, “Elements of the Terahertz Power Reflective Optics with Free-Form Surfaces”, Optoelectronics, Instrumentation and Data Processing, vol. 55(2), pp. 148-153, 2019.
2. T.V. Kononenko, B.A. Knyazev, D.N. Sovyk, V.S. Pavelyev, M.S. Komlenok, G.A. Komandin, V.I. Konov, “Silicon kinoform cylindrical lens with low surface roughness for high-power terahertz radiation”, Optics and Laser Technology, vol. 123, 105953, 2020.
3. M.S. Komlenok, T.V. Kononenko, D.N. Sovyk, V.S. Pavelyev, B.A. Knyazev, Evgeny Ashkinazi, A.S. Reshetnikov, G.A. Komandin, V.P. Pashinin, V.G. Ralchenko, V.I. Konov, "Diamond diffractive lens with a continuous profile for powerful terahertz radiation," Opt. Lett. 46, 340-343 (2021)

ABOUT THE RESULTS OF THE FIRST STAGE OF THE PROJECT «IN SITU METHODS FOR SYNCHROTRON INVESTIGATIONS OF MULTILAYER FUNCTIONAL STRUCTURES WITH UNIQUE PARAMETERS AND PROPERTIES CREATED BY BEAM-PLASMA SURFACE ENGINEERING» #82

Submitted by **Vladimir Denisov**

For tracks: SR technological application and X-ray apparatus, X-ray spectroscopy, X-ray structural analysis

Author: Vladimir Denisov (HCEI SB RAS)
Co-authors:
- Nikolay Ratakhin (HCEI SB RAS)
- Alexandr Schmakov (INP SB RAS)
- Anton Teresov (HCEI SB RAS)
- Nikolay Koval (HCEI SB RAS)

A consortium consisting of such organizations as HCEI SB RAS, INP SB RAS, ISPMS SB RAS, TSC SB RAS, Tomsk universities - TPU, TSU, TUSUR, IEP UD RAS, as well as the Ufa State Aviation Technical University and the industry enterprise "Technopark-AT", since October 2021, have been implementing a project on the topic "In situ methods of synchrotron investigations of multilayer functional structures with unique parameters and properties created by beam-plasma surface engineering" within the framework of the Federal Scientific and Technical program for the development of synchrotron and neutron research and research infrastructure for 2019 - 2027".

The objectives of the project are related to each other and, in accordance with Direction 1 "Synchrotron and neutron research (development) in the field of materials science for the

development of high-tech production technologies", are focused on creating infrastructure and developing methods for synchrotron and neutron research of structural and functional materials.

The report provides information on the progress of the project, including the most important scientific results obtained using synchrotron radiation, a description of the infrastructure facilities being created for synchrotron research, as well as the progress of the educational component of the project.

BEAMLINE FOR STUDYING FAST-FLOWING PROCESSES AT THE SYNCHROTRON RADIATION FACILITY SKIF #83

Submitted by **Ivan Rubtsov**

For tracks: SR and FEL sources and centers, SR technological application and X-ray apparatus

Authors:

- Aleksey Arakcheev (Budker INP)
- Andrey Bukhtiyarov (SRF “SKIF”)
- Aleksandr Garmashev (FSUE Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics)
- Aleksey Kashkarov (Lavrentyev Institute of Hydrodynamics SB RAS)
- Sergey Kazantsev (Budker Institute of Nuclear Physics)
- Anna Konovalova (Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis SB RAS)
- Konstantin Kuper (Budker INP SB RAS, SRF "SKIF")
- Aleksandr Kurepin (JSC Institute of Mechanical Engineering imeni V.V. Bakhireva)
- Anatoliy Mikhailov (FSUE Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics)
- Dmitriy Petrov (FSUE Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics)
- Eduard Pruuel (Lavrentyev Institute of Hydrodynamics SB RAS)
- Ivan Rubtsov (Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis SB RAS)
- Lev Shekhtman (Budker Institute of Nuclear Physics)
- Evgeniy Smirnov (Russian Federal Nuclear Center - VNIITF)
- Ivan Spirin (FSUE Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics)
- Aleksey Studennikov (Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis SB RAS)
- Konstantin Ten (LIH SB RAS)
- Viktoriya Titova (FSUE Russian Federal Nuclear Center—All-Russian Research Institute of Experimental Physics)
- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
- Konstantin Zolotarev (Budker Institute of Nuclear Physics)
- Yan Zubavichus (SRF «SKIF»)

The work is devoted to the concept of an experimental station for studying fast-flowing processes (propagation of shock and detonation waves, interaction of plasma with matter, etc.) on a new source of synchrotron radiation SRF «SKIF».

The beamline for the studying fast-flowing processes consists of two sectors working sequentially: "Dynamic processes" and "Plasma". The main task of the station is to study fast–flowing processes with characteristic scales of process change from picoseconds to milliseconds. In recent years, the direction of the study of fast-flowing processes using synchrotron radiation has begun to develop actively in the world: England, France and Germany have conducted research on the study of shock waves generated by guns and/or lasers, and methods for such research have also begun to develop very actively over the years. And the station in the USA today, in many respects, is a world

leader in the study of fast-flowing processes using synchrotron radiation.Thus, the development of a new experimental station and the improvement of methods for studying fast-flowing processes using synchrotron radiation in the Russian Federation is necessary to maintain a leading position in this field of research.

STUDY OF THE EFFECTS OF SURFACE CRACKS AND TEXTURE ON RESIDUAL STRESSES IN TUNGSTEN #84

Submitted by **Ilya Balash**
For track: X-ray structural analysis
Author: Ilya Balash (Budker INP, ISSC)
Co-authors:

- Aleksey Arakcheev (Budker INP)
- Alexander Shmakov (Boreskov Institute of Catalysis SB RAS)
- Alexander Vasilyev (Budker Institute of Nuclear Physics, Novosibirsk State University)

In a vacuum chamber of a fusion reactor plasma interacts with the divertor walls in the form of periodic heat pulses as well as constant heat load. As a result of these interactions, plastic deformations and mechanical stresses occur causing the destruction of the divertor material. However, these residual deformations and stresses can be relieved by a constant flux of plasma and the consequential high temperature of the material. The goal of this work was to study the influence of different factors, such as pronounced texture and presence of cracks on the sample surface, on the residual stresses in the irradiated material. Residual deformations and stresses were measured using X-ray diffractometry. The measurements were conducted on tungsten samples that were irradiated with an electron beam on the BETA facility with the purpose of modeling plasma heat loads. SR scattering station “Anomalous scattering” on the beam line 2 of VEPP-3 was used to measure diffractograms from which scattering angle – sample tilt angle dependencies were obtained. The experimental data was used for calculation of deformation and stress tensor components. The measurements of the sample with a cracked surface were conducted with spatial resolution and the obtained profile was compared to the profile of the sample without the cracks. Scattering angles were also measured on an ITER-specifications manufactured tungsten sample with a cracked surface. Measurements were conducted on both the irradiated cracked surface and the opposite.

ANALYTICAL MICROSTRATIGRAPHY OF THE BOTTOM SEDIMENTS OF LAKE NIZHNEE MULTINSKOE USING SCANNING MICRO-XRF ON SR BEAMS #85

Submitted by **Andrey Darin**
For track: X-ray fluorescent analysis
Author: Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)
Co-authors:

- Valery Babich (IGM SB RAS)
- Tatiana Markovich (IGM SB RAS)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Natalia Rudaya (IGM SB RAS)

Bottom sediments in mountain lakes archive regional and global environmental changes, including those associated with climate change. Terrigenous material and organics of allochthonous and autochthonous origin are the main sources of bottom sediment for fresh high-mountain lakes of the Altai region. Changes in air temperature and the amount of atmospheric precipitation modulate the elemental composition of bottom sediments, which is determined by the ratio of incoming

terrigenous and organic material. Analysis of variations in the elemental composition along the depth of the core of bottom sediments can provide information on changes in the main climatic parameters of the region over the past millennia with high detail, determined by the spatial (and hence temporal) resolution of the analytical method.

The worldwide development of XRF scanners, providing new geochemical information at the micro level, has provided a standard analytical method for rapidly assessing elemental, density, and textural variations in bottom sediments and other materials with various applications in the study of natural processes. The method of scanning X-ray fluorescence microanalysis with excitation by synchrotron radiation (μXRF-SR), which makes it possible to obtain continuous series of elemental composition over core depth with an annual temporal resolution, was used by us to construct climate reconstructions of high temporal resolution.

The results of the study of bottom sediment cores of Lake Nizhnee Multinskoe (Altai) using analytical microstratigraphy techniques, including scanning μXRF-SR, are presented in the report. A reconstruction of the average annual temperatures in the Altai region for the last two millennia was built with a time resolution of 3 years. The reconstruction is calibrated according to the data of regional instrumental meteorological observations for the time interval 1940–2020. The mathematical analysis of the reconstruction made it possible to reveal the main regularities in the dynamics of climatic processes in the Late Holocene.

The work was supported by grants from the Russian Science Foundation No. 20-17-00110 and RFBR No. 19-05-50046 (micro-XRF).

COMMISSIONING OF THE FIRST FEL WITH VARIABLE-PERIOD UNDULATOR #86

Submitted by **Oleg Shevchenko**

For track: THz radiation aplication

Authors:

- Oleg Shevchenko (BINP SB RAS)
- Nikolay Vinokurov (Budker Institute of Nuclear Physics)
- Yaroslav Getmanov (Budker INP)
- Yaroslav Gorbachev (BINP SB RAS)
- Vitaly Kubarev (BINP)
- Mihail Scheglov (Budker INP SB RAS)
- Stanislav Serednyakov (Budker Institute Of Nuclear Physics)
- Vladimir Tcheskidov (BINP SB RAS)
- Alexander Batrakov (BINP SB RAS)
- Igor Ilyin (BINP SB RAS)
- Konstantin Shtro (BINP SB RAS)

The concept of the variable period undulator (VPU) was proposed several years ago but it has not been implemented in FEL design until recently. The VPUs have some advantages as compared with conventional undulators, e.g., a wider range of radiation wavelength tuning and the option to increase the number of poles for shorter periods. Both these advantages were realized in the VPU developed at Budker INP. The new undulator was recently installed on the second track of the NovoFEL facility instead of the old electromagnetic undulator and the FEL lasing in the wavelength range 15 -120 microns was demonstrated. In this paper we present the new variable period undulator design and the FEL commissioning results.

FIRST RESULTS OF μXRF-SR OF LATE HOLOCENE ERUPTIVE MATERIAL FROM A NUMBER OF KAMCHATKA VOLCANOES #87

Submitted by **Andrey Darin**
For track: X-ray fluorescent analysis
Author: Andrey Darin
Author: Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)
Co-authors:

- Oleg Dirksen (IVS FEB RAS)
- Tatiana Markovich (IGM SB RAS)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Andrey Gogin (NRC «KI»)
- Roman Senin (NRC «KI»)

A collection of eruptive material from the most intense, dated Middle and Late Holocene eruptions of several Kamchatka volcanoes has been collected: Avachinsky (two eruptions), Ksudach (three eruptions), Kurilsky and Shiveluch. The test samples were prepared as a layer of fine powder (200 mesh) applied to a conductive adhesive tape. Such samples without additional sample preparation can be examined using optical and electron microscopes and a confocal X-ray microscope (CX-RM).

2D measurements using a CX-RM unit at energies of 19 and 21 keV were carried out at the Kurchatov Center for Synchrotron Research. The size of the exciting SR beam on the sample was from 100 to 15 μm. The microparticles identified by morphology and elemental composition were delineated and their composition was measured in detail.

The core of the bottom sediments of Lake Myertvoye, containing a layer of visually distinguishable tephra, was scanned to develop a methodology for searching and identifying cryptotephra in the bottom sediments of lakes in the region. As a result of 2D scanning, individual particles of volcanic matter are outlined. Their detailed study allows us to compare the identification with known eruptions.

This work was supported by RFBR grant No. 19-05-50046 (Micromir).

TIO2- AND G-C3N4-BASED PHOTOCATALYSTS FOR CO2 REDUCTION: XAS STUDY #88

Submitted by **Andrey Saraev**
For track: X-ray spectroscopy
Authors:

- Andrey Saraev (Boreskov Institute of Catalysis)
- Ангелина Журенок (ИК СО РАН)
- Анна Куренкова (ИК СО РАН)
- Евгений Герасимов
- Alexander Trigub (NRC "Kurchatov Institute")
- Екатерина Козлова

Растущее энергопотребление современного общества приводит к увеличению выбросов парниковых газов и может привести к глобальным климатическим изменениям, что делает крайне актуальной задачу по поиску технологий утилизации парниковых газов. Как известно, одним из основных компонентов парниковых газов является диоксид углерода – CO2. Перспективным подходом к утилизации CO2 является его конверсия в более реакционноспособные вещества, такие как CO и CH4. Эта технология позволяет снизить количество CO2 в атмосфере и одновременно получать ценные органические соединения,

такие как метан, метанол, этанол и формальдегид, которые затем могут быть использованы в химической промышленности или в качестве топлива. Важным преимуществом данной технологии является доступность как реагентов (CO2 и вода, получаемые из атмосферы), так и источника энергии – солнечного света. Таким образом, процесс фотокаталитического восстановления CO2 является одной из наиболее перспективных технологий утилизации CO2, однако масштабное внедрение этого процесса затруднено вследствие отсутствия эффективных фотокатализаторов. Как известно, для повышения эффективности процесса фотокатализатор подвергают различными модификациям – допирование неметаллами, термическая обработка, нанесение сокатализаторов. Последний способ увеличения эффективности фотокатализаторов является наиболее эффективным, так как нанесение металлов приводит к образованию гетеропереходов и увеличению времени жизни фотогенерированных зарядов (электрон-дырочных пар). Кроме того, в реакции фотокаталитического восстановления CO2 сокатализатор позволяет увеличить селективность по отношению к определенным продуктам реакции. В случае использования сокатализаторов на основе переходных металлов последние могут образовывать различные комплексы с адсорбированными интермедиатами реакции и менять свою степень окисления, что позволяет повышать селективность по тем или иным продуктам. Ранее нами было показано, что модифицирование диоксида титана медью позволяет расширить рабочий диапазон фотокатализатора и увеличить селективность по метану [1]. Исследование фотокатализаторов до и после реакции с помощью метода рентгеновской фотоэлектронной спектроскопии (РФЭС) показало, что катионное распределение меди изменяется в процессе фотокаталитического восстановления CO2. Для того чтобы определить ключевые интермедиаты реакции необходимо проведение in situ исследований, однако метод РФЭС не позволяет проводить исследования в условиях протекания фотокаталитического процесса. В качестве альтернативного метода, позволяющим определить катионное распределение меди в фотокатализаторе, может быть спектроскопия рентгеновского поглощения. Данный метод может быть адаптирован для проведения in situ исследований. В данной работе мы представляем прототип фотокаталитической ячейки для реализации метода спектроскопии рентгеновского поглощения в режиме in situ.

В качестве объектов исследования были выбраны катализаторы на основе TiO2 с содержанием 1 вес.% платины и 5 вес.% меди и на основе g-C3N4 с содержанием 1 вес.% платины. Показано, что под действием облучения УФ и видимым светом происходит изменение катионного распределения меди в реакционный условиях. Исследования проведены в Курчатовском центре синхротронного излучения (КИСИ, г. Москва) на станции «Структурное материаловедение».

Работа выполнена при финансовой поддержке РНФ, проект № 21-73-10235.

[1] Saraev A.A., Kurenkova A.Y., Gerasimov E.Y., Kozlova E.A. // Broadening the Action Spectrum of TiO2-Based Photocatalysts to Visible Region by Substituting Platinum with Copper, Nanomaterials. 2022. V.12. N9. P.1-15. DOI: 10.3390/nano12091584

ФОТОИНЖЕКТОРНЫЙ КОМПЛЕКС ИПФ РАН: РАСЧЕТНЫЕ ПАРАМЕТРЫ И ТЕКУЩАЯ СТАДИЯ РАЗРАБОТКИ #89

Submitted by **Nikolai Peskov**

For track: SR and FEL sources and centers

Authors:

- Н.Ю. Песков (Институт прикладной физики РАН, Нижний Новгород)
- А.В Афанасьев (Институт прикладной физики РАН, Нижний Новгород)
- И.В. Бандуркин (Институт прикладной физики РАН, Нижний Новгород)
- А.А. Вихарев (Институт прикладной физики РАН, Нижний Новгород)
- А.М. Горбачев (Институт прикладной физики РАН, Нижний Новгород)
- К.В. Минеев (Институт прикладной физики РАН, Нижний Новгород)

- Ю.С. Опарина (Институт прикладной физики РАН, Нижний Новгород)
- А.В. Савилов (Институт прикладной физики РАН, Нижний Новгород)

В настоящее время в Институте прикладной физики РАН (ИПФ РАН) разрабатывается фотоинжекторный ускорительный комплекс, рассчитанный на получение электронных сгустков с энергией до 20 МэВ, зарядом ~ 100 пКл и длительностью ~ 10 пс при нормированном поперечном эммитансе на уровне 1 мм•мрад. Первый каскад ускорителя представляет собой классический вариант фотоинжектора с полутораячеечной ускоряющей структурой, которая запитывается 5 МВт / 2.45 ГГц клистроном, и обеспечивает формирование электронного пучка с энергией до 3.5 МэВ. Фотоэмиссию электронного сгустка планируется обеспечить импульсом мощного ультрафиолетового лазера с длиной волны около 260 нм, исследуется возможность создания фотокатода на основе алмазных пленок для фотоинжектора.

Основу электронной оптики фотоинжектора составляет система из основного соленоида с полем до 0.25 Тл и дополнительной закатодной катушки, обеспечивающей нулевое магнитное поле на поверхности фотокатода. Эта система призвана обеспечить режим компенсации эмиттанса, связанного с пространственным зарядом, и фокусировку электронного пучка на длине ~ 1 м. В настоящее время все компоненты ускорительной системы и магнитной системы первого каскада изготовлены и испытаны на малом (в «холодных» тестах) и высоком (при запитке излучением клистрона) уровне мощности. Начата сборка СВЧ - блока ускорителя и совмещение его с лазерной системой для получения электронного пучка.

Первый каскад ускорителя планируется использовать для экспериментального исследования перспективных режимов терагерцового излучения интенсивных электронных сгустков, включая ондуляторный и циклотронный механизмы. Для этого разработана дополнительная магнитная система, обеспечивающая инжекцию электронных сгустков в область взаимодействия с ведущим магнитным полем до 8 Тл, с использованием магнитной линзы ~ 0.4 Тл, расположенной в области фокальной перетяжки электронного пучка. В частности, для реализации режима так называемой отрицательной массы в комбинированном - ондуляторном и околорезонансном ведущем - магнитном поле данная система позволяет поместить электроны на стационарные винтовые баунс-траектории практически без примеси “паразитных” циклотронных колебаний.

Для увеличения энергии частиц до 20 МэВ спроектирован второй каскад ускорителя, состоящий из 3 дополнительных секций и фокусирующих соленоидов. Каждая ускоряющая секция представляет собой последовательность из 6 связанных резонаторов, запитываемых от одного СВЧ - источника и рассчитана на приращение энергии пучка ~ 6 МэВ. После дополнительного ускорения во втором каскаде сгустки с малыми поперечным эмиттансом и скоростным разбросом планируется использовать для комптоновского рассеяния лазерных импульсов, а также для дальнейшей инжекции в систему лазерно-плазменого ускорителя, разрабатываемого в ИПФ РАН, с перспективой создания компактного ЛСЭ рентгеновского диапазона.

Работа поддержана Российским научным фондом (проект № 20-12-00378 в части разработки первого каскада и исследований новых фотокатодов и проект № 21-72-30027 в части разработки второго каскада).

ЭЛЕКТРОДИНАМИЧЕСКАЯ СИСТЕМА МОЩНОГО ТГЦ ЛСЭ НА ОСНОВЕ ЛИНЕЙНОГО ИНДУКЦИОННОГО УСКОРИТЕЛЯ «ЛИУ»: МОДЕЛИРОВАНИЕ И «ХОЛОДНЫЕ» ТЕСТЫ #90

Submitted by **Nikolai Peskov**
For track: SR and FEL sources and centers
Authors:

- Н.Ю. Песков (Институт прикладной физики РАН (Нижний Новгород); Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- А.В. Аржанников (Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- В.И. Белоусов (Институт прикладной физики РАН (Нижний Новгород))
- Н.С. Гинзбург (Институт прикладной физики РАН (Нижний Новгород); Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- В.Ю. Заславский (Институт прикладной физики РАН (Нижний Новгород))
- Д.А. Никифоров (Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- Ю.С. Опарина (Институт прикладной физики РАН (Нижний Новгород); Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- А.В. Савилов (Институт прикладной физики РАН (Нижний Новгород))
- Е.С. Сандалов (Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- С.Л. Синицкий (Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- Д.И. Соболев (Институт прикладной физики РАН (Нижний Новгород))

Создание мощного длинноимпульсного ЛСЭ суб-ТГц/ТГц диапазона ведется в настоящее время в сотрудничестве ИЯФ СО РАН (Новосибирск) и ИПФ РАН (Нижний Новгород). Экспериментальной основой проекта служит новое поколение линейных индукционных ускорителей «ЛИУ» 5 - 20 МэВ / 2 кА / 200 нс, реализованных в настоящее время в ИЯФ СО РАН. Целью проекта является достижение в указанном диапазоне рекордной мощности (от суб-ГВт до ГВт уровня) и энергосодержания в импульсах излучения до 10 - 100 Дж. Одной из ключевых проблем при реализации данного ЛСЭ является разработка электродинамической системы, способной обеспечить стабильную узкополосную генерацию в условиях существенной сверхразмерности.

Для проводки интенсивного релятивистского электронного пучка, формируемого «ЛИУ», через пространство взаимодействия ЛСЭ диаметр системы должен быть $Ø \geq 20$ мм, что на порядки превышает длину волны излучения в обсуждаемых диапазонах. Таким образом, одной из ключевых проблем при реализации этого генератора является разработка электродинамической системы, способной обеспечить стабильный режим узкополосных колебаний в условиях существенной сверхразмерности пространства взаимодействия. Для решения проблемы селекции мод в подобных условиях в рамках развиваемого проекта исследуются два основных типа электродинамических систем: (1) модифицированные брэгговские резонаторы и (2) квазиоптические резонаторы, основанные на эффекте Тальбота.

Отличительной особенностью модифицированных брэгговских резонаторов является включение в цепь обратной связи квазикритических волн, что позволяет существенно улучшить их селективные свойства по сравнению с «традиционными» аналогами. Для работы в диапазоне 0.7 ТГц были разработаны структуры данного типа с указанным диаметром, при этом параметр сверхразмерности составил $Ø/\lambda \sim 45$. Трехмерное моделирование с использованием кода CST Microwave Studio показывает, что даже при таких больших поперечных размерах модифицированные брэгговские структуры позволяют осуществить селективное отражение рабочей волны с эффективностью ~ 80 - 90% по мощности. Проведенные «холодные» электродинамические тесты подтверждают результаты моделирования и демонстрируют наличие эффективного узкополосного отражения в расчетной области частот.

Для «холодных» тестов макет резонатора Тальбо-типа был изготовлен в диапазоне частот около 0.3 ТГц со сверхразмерностью Ø/λ ~ 40. Возбуждение резонатора осуществлялось с входной стороны резонатора, детектирование сигнала проводилось через отверстие связи, выполненное на выходном зеркале. В соответствии с результатами моделирования в проведенных «холодных» тестах наблюдался хорошо различимый пик детектируемой выходной мощности на частоте, соответствующей возбуждению рабочей моды (супермоды) резонатора, что, таким образом, подтверждало его работоспособность.

Работа проводится при частичной поддержке РНФ (грант № 19-12-00212).

ТЕРАГЕРЦОВЫЙ ЛАЗЕР НА СВОБОДНЫХ ЭЛЕКТРОНАХ С ЭЛЕКТРОДИНАМИЧЕСКОЙ СИСТЕМОЙ, ОСНОВАННОЙ НА ВОЗБУЖДЕНИИ СУПЕРМОД ТАЛЬБОТ-ТИПА #91

Submitted by **Andrei Savilov**
For track: SR and FEL sources and centers
Authors:

- Andrei Savilov (Institute of Applied Physics)
- Опарина Юлия (институт прикладной физики РАН)
- Н.Ю. Песков (Институт прикладной физики РАН (Нижний Новгород); Институт ядерной физики им. Г.И.Будкера СО РАН (Новосибирск))
- Щегольков Дмитрий (Институт прикладной физики РАН)

В настоящее время растет интерес к созданию источников, работающих в терагерцевом диапазоне частот с высокой мощностью излучения. Естественный путь реализации такого источника - использование излучения сильноточного релятивистского электронного пучка. Однако существует ряд проблем, связанных с генерацией мощного когерентного ТГц-излучения в мазерах на свободных электронах на основе релятивистских электронных пучков. Прежде всего, применение традиционного подхода (т.е. работа на одной заранее выбранной моде рабочего резонатора) к диапазону частот ТГц сталкивается с естественными трудностями. Очевидно, что рабочий резонатор в этом случае должен быть сверхразмерным; это необходимо по ряду причин, а именно - транспортировка релятивистского сильноточного пучка, проблема пробоя поля мощного излучения внутри резонатора, омический нагрев стенок резонатора мощным излучение и т.д. Однако в этой ситуации спектр поперечных мод микроволновой системы становится очень плотным, что затрудняет обеспечение селективного возбуждения одной рабочей поперечной моды. Вторая проблема заключается в трудности обеспечения селективной одномодовой обратной связи в сверхразмерной системе.

Мы описываем альтернативную концепцию селективного возбуждения рабочего колебания в электронном мазере со сверхразмерной электродинамической системой, запитываемой сильноточным релятивистским электронным пучком. Основная идея состоит в том, чтобы отказаться от возбуждения фиксированной моды резонатора в пользу возбуждения высокодобротной супермоды, формируемой фиксированным набором поперечных мод сверхразмерного волновода. Такая супермода может быть сформирована внутри относительно простого резонатора, представляющего собой отрезок волновода, заканчивающийся двумя зеркалами, в результате эффекта Талбота, а именно периодического воспроизведения поперечной структуры многомодового волнового поля в сверхразмерном волноводе.

Несмотря на сложность многомерных пространственных структур супермод резонаторов типа Талбота, к ним в некоторой степени может быть применена идеология, которая используется при описании мод обычных волноводов и резонаторов, а именно разложение по набору ортогональных мод. Хотя формирование супермод включает большое количество парциальных поперечных мод, количество супермод с высокой добротностью ограничено тем фактом, что дифракционная добротность супермоды резко спадает с увеличением индекса супермоды. Благодаря этому даже в весьма сверхразмерных системах можно добиться того,

чтобы в системе оставался только одна нижшая супермода. По-видимому, это дает нам повод говорить об уникальных селективных свойствах резонаторов типа Талбота.

В качестве примера применения этого подхода мы представлем расчеты лазера на свободных электронах, запитываемого электронным пучком 10 МэВ/2 кА /200 нс и основанного на возбуждении супермоды типа Талбота на частоте, близкой к 2 ТГц. Данная работа направлена на экспериментальную реализацию такого лазера на уникальном сильноточном ускорителе, разработанном в Институте ядерной физики им. Будкера (Новосибирск, Россия). В докладе представлены результаты нашего многоволнового моделирования электронно-волнового взаимодействия в пространственно-временном процессе формирования и усиления супермоды в сверхразмерной микроволновой системе. Расчетный электронный КПД этого лазера на уровне 5% соответствует гигаваттному уровню выходной мощности. Прототип резонатора такого типа разработан и протестирован в холодных экспериментах.

Исследование выполнено за счет гранта Российского научного фонда (проект № 19-12-00212).

CONDUCTION BAND ELECTRONIC STRUCTURE FEATURES OF MANGANESE SULFIDE SOLID SOLUTIONS DOPED WITH LANTHANIDES #92

Submitted by **Mikhail Syrokvashin**
For tracks: SR and FEL sources and centers, X-ray spectroscopy
Authors:

- Mikhail Syrokvashin (NIIC SB RAS)
- Evgeniy Korotaev (Nikolaev Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences)
- Anton Nikolenko (Budker INP SB RAS, SRF "SKIF")

Thermoelectric materials have attracted considerable attention due to their possibility for the direct conversion of waste heat into electrical energy. The thermoelectric generators (TEGs) based on the high-efficient thermoelectric materials could provide an alternative for traditional power generation sources. In recent years, material science is focused on the optimization of existing and development of new high-performance thermoelectric materials based on lanthanide and transition metal chalcogenides. The electrophysical properties of the thermoelectric materials are significantly affected by the electronic structure features. For instance, Seebeck coefficient (S) is one of the main characteristics of the thermoelectric materials and can be represented as follows:

$$S = -\frac{k}{e} \cdot \left(\frac{\left(ln\frac{N_c}{n}+2\right)\cdot n\mu_n - \left(ln\frac{N_v}{p}+2\right)\cdot p\mu_p}{n\mu_n + p\mu_p} \right), \quad (1)$$

where k is the Boltzmann constant, e – the electron charge, Nc and Nv – the effective densities of states (DOS) in the conduction and the valence band, n, p, μn and μp – the concentration and mobility of electrons (n) and holes (p), respectively. As it can be seen from the equation (1), the Seebeck coefficient value is determined by the DOS distribution in the conduction and the valence band. Thus, the electronic structure study is one of the key aspects in the prediction and optimization of the thermoelectric properties of the functional materials. For p-type semiconductors, the thermoelectric properties are determined by the DOS distribution in the valence band, for n-type semiconductors – the distribution in the conduction band.

The cation-substituted solid solutions MxMn1-xS (M – transition metal or lanthanide) based on MnS-matrix are promising functional materials with magnetic and thermoelectric properties. The functional properties of MxMn1-xS could be modified by the type and concentration of the doping atoms (M). The cation-substituted solid solutions LnxMn1-xS with lanthanides have demonstrated the most promising values of Seebeck coefficient (up to 18000 μV/K for Gd0.01Mn0.05S at 900K /1/). This fact allows one to consider the lanthanide-dopes solid solutions as promising functional

materials. Here we report a study of the electronic structure features of the lanthanide-doped solid solutions LnxMn1-xS (Ln = Dy, Tm, Yb; x = 0.01; 0.05). The data on the conduction band structure could be obtained by the X-ray absorption edges near edge structure (XANES) spectroscopy. The local environment and oxidation state of sulfur atoms in LnxMn1-xS was unaffected by cationic substitution. The combination of the experimental data with results of quantum-chemical calculations allowed one to determine the partial contributions of DOS in the absorption edge structure, thereby, to study the features of the conduction band electronic structure formation of LnxMn1-xS.

The authors are grateful for support to the Ministry of Science and Higher Education of the Russian Federation (project No. 121031700313-8).

/1/ Romanova O.B., Ryabinkina L.I., Sokolov V.V., Pichugin A.Y., Velikanov D.A., Balaev D.A., Galyas A.I., Demidenko O.F., Makovetskii G.I., Yanushkevich K.I. Magnetic properties and the metal–insulator transition in GdXMn1−XS solid solutions // Solid State Commun. – 2010. – V. 150. – N. 13–14. – P. 602–604.

CU/TIO2 ФОТОКАТАЛИЗАТОРЫ ПОЛУЧЕНИЯ ВОДОРОДА: РФЭС И XANES ИССЛЕДОВАНИЕ #93

Submitted by **Andrey Saraev**
For track: X-ray spectroscopy
Authors:

- Andrey Saraev (Boreskov Institute of Catalysis)
- Анна Куренкова (ИК СО РАН)
- Анна Кремнева (ИК СО РАН)
- Евгений Герасимов
- Екатерина Козлова
- Василий Каичев (ИК СО РАН)

Растущее энергопотребление современного общества требует развития альтернативных экологически приемлемых источников энергии, одним из которых может стать водород, синтезированный с использованием фотокатализаторов. Действительно, водород можно получать под действием света практически из любых органических соединений. Более того, фотокаталитический синтез водорода решить важные экологические проблемы, в частности, очистка воды от органических загрязнителей. связанные с загрязнением воды. Таким образом, используя фотокаталитические процессы, можно обеспечить и очистку воды, и получение водорода. Основными проблемами на данный момент являются: дороговизна водорода, полученного фото- и электрохимическими методами, и невысокая эффективность получения водорода. В качестве фотокатализаторов обычно используются полупроводниковые материалы, в данной работе изучали диоксид титана с нанесённой на его поверхность медью. Цель данной работы заключается в разработке новых подходов к охарактеризованию фотокатализаторов с нанесенными наночастицами переходных металлов.

Традиционно для получения катионного распределение атомов активного компонента используют метод рентгеновской фотоэлектронной спектроскопии. Было обнаружено, что в процессе записи РФЭС спектров происходит восстановление Cu2+ до состояния Cu1+ и Cu0. Данный факт не позволяет однозначно ответить на вопрос об исходном состоянии меди в исследуемых фотокатализаторах, более того не удается определить долю меди в состоянии Cu1+ и Cu0, вследствие одинаковой энергии связи пика Cu2p3/2 и невозможности измерения Оже-параметра. Более того, было обнаружено, что наночастицы меди до и после реакции имеют различное катионное распределение. С этой точки зрения крайне важно определить катионное распределение меди, так как это напрямую влияет на фотокаталитические свойства. Для решения данной задачи была использована спектроскопия рентгеновского поглощения, измеренная на K-крае поглощения меди. Было установлено, что использование фотонов высокой энергии не приводит к восстановлению меди и позволяет получать важную

информацию не только о катионном распределение атомов меди, но и о фазовом составе медьсодержащих фотокатализаторов. Эксперименты были проведены на УНУ Станция EXAFS спектроскопии. Работа выполнена при финансовой поддержке Министерства науки и высшего образования Российской Федерации (Соглашение № 075-15-2022-263).

ДИФРАКЦИОННЫЙ АНАЛИЗ МНОГОСЛОЙНЫХ МНОГОЭЛЕМЕНТНЫХ НАНОСТРУКТУРИРОВАННЫХ МЕТАЛЛИЧЕСКИХ ПЛЕНОК #94

Submitted by **Юрий Иванов**
For track: X-ray structural analysis
Authors:

- Юрий Иванов (ИСЭ СО РАН)
- Юрий Ахмадеев (ИСЭ СО РАН)

Co-authors:

- Никита Прокопенко (ИСЭ СО РАН)
- Владимир Шугуров (ИСЭ СО РАН)
- Олег Толкачев (ИСЭ СО РАН)
- Елизавета Петрикова (ИСЭ СО РАН)
- Мария Петюкевич (ИСЭ СО РАН)
- Ольга Крысина (ИСЭ СО РАН)
- Александр Шмаков (ИЯФ СО РАН)

Многоэлементные сплавы эквиатомного (близкого к эквиатомному) состава (так называемые высокоэнтропийные сплавы (ВЭС)) являются, как правило, однофазными термодинамически стабильными твердыми растворами замещения, преимущественно, на основе ОЦК или ГЦК кристаллической решетки. В большинстве случаев ВЭС обладают уникальным сочетанием механических, трибологических, физических и т.д. свойств, что позволяет рекомендовать их использование в экстремальных условиях в различных отраслях промышленности.

Целью настоящей работы является анализ результатов, полученных при исследовании элементного и фазового состава, дефектной субструктуры, многослойных многоэлементных наноструктурированных металлических пленок (т.н. высокоэнтропийные сплавы нестехиометрического состава) методами рентгеноструктурного анализа и просвечивающей дифракционной электронной микроскопии (микродифракционный и микро-микродифракционный анализ). Исследуемые ВЭС синтезированы в виде тонких пленок, сформированных в результате осаждения многоэлементной металлической плазмы, созданной электродуговым плазменно ассистированным одновременным независимым распылением катодов выбранных элементов. В качестве элементов, формирующих ВЭС, использованы Nb, Mo, Cr, Ti, Al (далее ВЭС 1) и Ti, Al, Cu, Zr и Nb (далее ВЭС 2). В качестве подложки использованы сталь аустенитного класса 12Х18Н10Т, сплав титана ВТ1-0 и твердый сплав ВК8. Эксперименты по нанесению многоэлементных плёнок металлов проводились на ионно-плазменной установке «КВИНТА», разработанной в лаборатории плазменной эмиссионной электроники ИСЭ СО РАН и входящей в составе комплекса «УНИКУУМ» в перечень уникальных электрофизических установок России (https://ckp-rf.ru/usu/434216/). Элементный и фазовый состав, дефектную субструктуру изучали, используя следующее научно-диагностическое оборудование: просвечивающий дифракционный электронный микроскоп (JEOL JEM-2100 F); растровый электронный микроскоп (Philips SEM-515 с микроанализатором EDAX ECON IV); рентгеновский дифрактометр Shimadzu XRD 6000; источник синхротронного излучения – накопитель электронов ВЭПП-3, ИЯФ СО РАН, высокотемпературная рентгеновская камера Anton Paar HTK-2000, позиционно-чувствительный однокоординатный детектор ОД-3М-350.

Установлено, что сплавы ВЭС 1 и ВЭС 2 являются многослойным нанокристаллическим материалом. Толщина слоев изменяется в пределах (12-23) нм. Размер кристаллитов, формирующих слои, (2-5) нм. Показано (методами рентгенофазового анализа), что пленка ВЭС 1 является однофазным материалом на основе твердого раствора состава MoNbCrTiAl с объемноцентрированной кристаллической решеткой (ОЦК) с параметром 0,3166 нм. Пленка ВЭС 2 является рентгеноаморфным материалом. Методами микродифракционного анализа (просвечивающая электронная микроскопия) установлено, что пленка ВЭС 1 содержит (в малом количестве) дополнительную фазу γ-AlTi. Пленка ВЭС 2 сформирована чередующимися слоями, находящимися в кристаллическом и аморфном состояниях. Аморфные слои обогащены атомами меди.

Исследования образцов ВЭС 1 на термостойкость и жаростойкость методом рентгенофазового анализа с использованием синхротронного излучения показали, что при нагревании на воздухе распад системы начинается при температуре (630-640) °С. При температурах (1070-1080) °С появляются новые рефлексы, предположительно, относящиеся к оксидным соединениям компонентов сплава. Рефлексы ВЭС полностью исчезают при температурах (1260-1270) °С. Далее, покрытие начинает разрушаться, поэтому определить конечное состояние сплава не представляется возможным.

Работа выполнена при финансовой поддержке Российской Федерации в лице Министерства науки и высшего образования (проект № 075-15-2021-1348) в рамках мероприятий № 2.1.5, 2.1.17 и 2.1.20 (исследования сплава ВЭС 1) и за счет гранта Российского научного фонда № 19-19-00183 (исследования сплава ВЭС 2).

SELF-SUPPORTING X-RAY MASKS FOR THE MANUFACTURE OF PLANAR ELEMENTS OF TERAHERTZ OPTICS BY DEEP X-RAY LITHOGRAPHY #95

Submitted by **Aleksandr Gentselev**
For track: SR technological application and X-ray apparatus
Authors:

- Aleksandr Gentselev (Budker INP, Novosibirsk, Russia)
- Sergey Baev (Institute of Automation and Electrometry SB RAS)
- Sergey Kuznetsov (Budker Institute of Nuclear Physics SB RAS)

The design and methods of manufacturing self-supporting perforated (with through holes) metal high-contrast in the X-ray spectral wavelength range $\lambda \approx 0.6 \div 14$ Å X-ray masks are described. They are tools for the formation of high-aspect resistive masks with a thickness of up to 1 mm or more, both positive and negative resists by deep X-ray lithography. Special attention is paid to the method of manufacturing by laser micro-processing (cutting) of foil by focused radiation of a femtosecond pulsed periodic laser. The nature of the interaction of radiation with metals changes fundamentally when the pulse duration decreases to values of ≤ 10 ps. Engraving and cutting of metals occurs as a result of their explosive destruction or ablation in times significantly shorter than the time of thermal conductivity processes in them. In this mode, the zone of thermal influence is practically absent and the resolution is determined by the size of the instrument, i.e. the size of the focused laser beam. By this method, self-supporting X-ray masks were obtained from industrially produced tantalum foil, 30 microns thick, with minimum dimensions of topology elements up to 15 microns. Graphs of the spectral dependence of the contrast of these masks, the SEM-photo fragments of their topology and modes of cutting are given. The samples of X-ray masks made by this method demonstrate reaching a new qualitative level of their manufacture. This will make it possible to obtain samples of planar elements of terahertz optics in the form of metal microstructures using LIGA technology, varying the size of cells, the width of the bridges of structures, and their thickness in a significantly wider range than was previously done. The method of laser cutting using a powerful femtosecond laser is more efficient and requires significantly less technological preparation and fewer operations for its implementation.

PULSED WIRE FIELD MEASUREMENTS OF 128-PERIOD SUPERCONDUCTING UNDULATOR #96

Submitted by **Fedor Kazantsev**

For track: SR and FEL sources and centers

Authors:

- Fedor Kazantsev (Novosibirsk State University)
- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Artem Zorin (Budker INP SB RAS, SRF "SKIF")
- Vitaliy Shkaruba (Budker INP SB RAS, SRF "SKIF")
- Valeriy Tsukanov (Budker INP SB RAS, SRF "SKIF")
- Nikolay Mezentsev (Budker INP SB RAS, SRF "SKIF")
- Olga Tarasenko (BINP)
- Askold Volkov (Budker INP SB RAS, SRF "SKIF")

In this paper, a pulsed wire method (PWM) for magnetic measurements was described. Experimental setup was developed and assembled. A wire position sensor was calibrated. A 128-period 1.2 T superconductive undulator was used for measurements. A series of 1st field integral measurements were carried out for various operating modes of the undulator, including those with local corrective power supplies in various operating configurations. The PWM measurement was also compared with Hall sensor. The results and further works are being discussed.

EXPERIMENTS ON THE SHORT X-RAY PULSE GENERATION AT THE NOVOFEL FACILITY #97

Submitted by **Yaroslav Getmanov**

For track: THz radiation aplication

Authors:

- Yaroslav Getmanov (Budker INP)
- Vladislav Borin (BINP)
- Xiaochao Ma (BINP)
- Yulia Maltseva (BINP)
- Oleg Meshkov (BINP)
- Oleg Shevchenko (BINP)
- Nikolay Vinokurov (Budker Institute of Nuclear Physics)

The Novosibirsk Free Electron Laser (NovoFEL) facility is a laser light source that operates in IR and THz range. The laser radiation is generated by three FELs installed on the one-, two- and four-pass energy recovery linear accelerator (ERL). The energy recovery scheme allows to operate with a high average electron current. The parameters of four-pass ERL are the following: the electron energy is about 40 MeV, the bunch charge is 0.5-1 nC and the bunch duration is 10 ps. The bunch repetition rate used for the FEL lasing is 3.76 MHz which corresponds to the average electron current ~ 4 mA.

Another interesting application of the high current NovoFEL ERL is the generation of the x-ray radiation. This radiation appears as the result bremsstrahlung phenomenon when electron beam interacts with a foil target. In our experiments, we used graphite foil 25 μm thick and aluminum foil 8 μm thick. The advantages of such source are the short pulse duration, high repetition rate and a large number of the x-ray photons. Moreover, there is no need to mount a new radiation output window as photons pass easily through the vacuum chamber. In addition, as the foil target can be fast removed from the electron beam trajectory the facility can quickly return to the ordinary operation mode.

The main challenge for the foil-radiator at the ERL is the electron beam transport. The electron scattering on the target increases beam losses, which is significant for the accelerator with high beam current. The recent results obtained at the NovoFEL and x-ray radiation characteristic are discussed.

THE PERFORMANCE OF THE CONDUCTION COOLED SUPERCONDUCTING SOLENOID FOR THZ SPECTROSCOPY #98

Submitted by **Alexey Bragin**
For track: THz radiation aplication
Author: Alexey Bragin (Budker Institute of Nuclear Physics)
Co-authors:

- Nikolay Mezentsev (Budker INP SB RAS, SRF "SKIF")
- Sergey Khrushchev (Budker INP SB RAS, SRF "SKIF")
- Vitaly Kubarev (BINP)
- Valeriy Tsukanov (Budker INP SB RAS, SRF "SKIF")
- Vitaliy Shkaruba (Budker INP SB RAS, SRF "SKIF")

This presentation reports on test results and performance of the conduction cooled superconducting solenoid to be used in THz spectroscopy experimental station of free-electron laser in BINP. The superconducting solenoid was designed to have 6.5 T in volume having diameter of 102 mm and with length of 0.5 m. The warm bore diameter is 80 mm available for THz spectroscopy experiments. The SC wire with Cu/NbTi = 1.4 was used. The passive quench protection methods were realized in the design. The uniformity of the field of 0.5% was provided by using the iron yoke and by additional side windings. The cryogenics of the solenoid is based on two Sumitomo HI cryocoolers. The solenoid and the iron yoke are conduction cooled by the second stage of the cryocooler via copper links. The manufacturing technology of the SC solenoid was described in details.

The solenoid was tested in LHe bath and its own cryostat, its performance satisfies demands of experimental station. The obtained filed of 7.5 T is more than designed one due to overcooling to 3.6 K. Magnetic field was measured as in bath cryostat as in the design cryostat – the results were according the design calculations. The cool down time of the solenoid is 13 days.

The quench protection was based on passive methods. The quench happened only two times at 5.8 T and 7.5 T of magnetic field.

THE ELECTRONIC STRUCTURE AND SEEBECK COEFFICIENT OF VANADIUM-DOPED COPPER-CHROMIUM DISULFIDES #99

Submitted by **Evgeniy Korotaev**
For track: X-ray spectroscopy
Authors:

- Evgeniy Korotaev (Nikolaev Institute of Inorganic Chemistry of the Siberian Branch of the Russian Academy of Sciences)
- Mikhail Syrokvashin (NIIC SB RAS)
- Irina Filatova (Nikolaev Institute of Inorganic Chemistry Siberian Branch of Russian Academy of Sciences)

The solid solution based on the copper chromium disulfide CuCrS2 are promising functional materials for modern electronics applications. These compounds exhibit the potential properties for practical usage: the thermoelectric properties [1,2], the ionic conductivity [3], the helimagnetic arrangement [4,5], the colossal magnetoresistance and the phase metal-insulator transition [4].

There are several approaches to control the electric and magnetic properties of CuCrS2-based compounds: the cationic substitution of chromium atoms with transition metal atoms (CuCr1-xMxS2, M = V, Fe, Mn), the co-intercalation of the Van der Waals gap with two atom types (Cu1-xAgxCrS2) and the chalcogen substitution (CuCrS2, X = S, Se, Te). It was shown that the low dopant solid solutions CuCr1-xFexS2 exhibit promising thermoelectric properties. In the case of vanadium-doped solid solutions CuCr1-xVxS2, the thermoelectric properties were not investigated yet.

The key aspect to control the electrophysical properties of thermoelectric materials is the understanding the electronic structure features. The corresponding data could be obtained from both the quantum-chemical calculations and the experimental techniques sensitive to the electronic structure. It should be noted that the electronic structure features of CuCrS2-based compounds mainly presented in the published articles are investigated theoretically. That fact indicates the presented study novelty.In this regard, the study of the X-ray absorption edges near edge structure (XANES) features could provide useful information about the conduction band structure. From the other hand, the valence band structure could be investigated using the X-ray emission spectra. Thus, this study involves electronic band structure of the vanadium-doped solid solutions CuCr1-xVxS2 (x=0-0.40). A comprehensive experimental and theoretical study of the X-ray absorption K-edges and valence band X-ray emission lines (Cu(La), Cr(Kb2,5), V(La) and S(Kb1,3)) of the matrix elements and doped-vanadium atoms in the cation-substituted disulfides CuCr1-xVxS2 was carried out. Based on the obtained results, the cationic substitution with vanadium atoms affect to the conduction and valence band structure was studied. The electronic features studied in present investigation were used for the CuCr1-xVxS2 Seebeck coefficient concentration dependence interpretation.

The study was carried out with a funding from the Ministry of Science and Higher Education of the Russian Federation (projects No. 121031700313-8, 121031700315-2)

[1] Korotaev E.V, Syrokvashin M.M., I.Yu. Filatova et al. // Sci. Rep.-2021.- 11-p. 18934
[2] Korotaev E.V, Syrokvashin M.M., I.Yu. Filatova et al. // J. Electron. Mater. -2018.-47. –p. 3392-3397.
[3] Akmanova G.R., Davleshina A.D. // Lett.Mater.-2013.- 3. –p.76-78.
[4] Karmakar A., Dey K., Chatterjee S. et al. // Appl. Phys. Letters. – 2014. –104, N. 5. – P. 052906.
[5] Abramova G.M., Petrakovskii G.A. // Low Temperature Physics. – 2006. – 32, N. 8/9. – p. 954-967.

STATUS OF WORK ON CREATION SUPERCONDUCTING INSERTION DEVICES FOR SYNCHROTRON RADIATION GENERATION ON SKIF SYNCHROTRON LIGHT FACILITY #100

Submitted by **Vitaliy Shkaruba**
For track: SR and FEL sources and centers
Authors:

- Vitaliy Shkaruba (Budker INP SB RAS, SRF “SKIF”)
- Alexey Bragin (Budker Institute of Nuclear Physics)
- Alexandr Erokhin (BINP)
- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Fedor Kazantsev (Novosibirsk State University)
- Sergey Khrushchev (Budker INP SB RAS, SRF “SKIF”)
- Nikolay Mezentsev (Budker INP SB RAS, SRF “SKIF”)
- Alexander Safronov (BINP SB RAS)
- Andrey Sedov (BINP SB RAS)
- Olga Tarasenko (BINP)
- Valeriy Tsukanov (Budker INP SB RAS, SRF “SKIF”)
- Askold Volkov (Budker INP SB RAS, SRF “SKIF”)
- Artem Zorin (Budker INP SB RAS, SRF “SKIF”)

The main devices for generating of synchrotron radiation at the SKIF synchrotron light facility under construction are superconducting insertion devices - wigglers and undulators, created at the BINP SB RAS. This report presents the rationale for the choice of operating parameters, the main characteristics and design features of these devices, as well as the current status of work on their creation.

SUPERCONDUCTING UNDULATOR WITH A PERIOD OF 15.6 MM AND A MAGNETIC FIELD OF 1.2 T #101

Submitted by **Vitaliy Shkaruba**

For track: SR and FEL sources and centers

Authors:

- Vitaliy Shkaruba (Budker INP SB RAS, SRF “SKIF”)
- Alexey Bragin (Budker Institute of Nuclear Physics)
- Alexandr Erokhin (BINP)
- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Fedor Kazantsev (Novosibirsk State University)
- Sergey Khrushchev (Budker INP SB RAS, SRF “SKIF”)
- Nikolay Mezentsev (Budker INP SB RAS, SRF “SKIF”)
- Alexander Safronov (BINP SB RAS)
- Andrey Sedov (BINP SB RAS)
- Olga Tarasenko (BINP)
- Valeriy Tsukanov (Budker INP SB RAS, SRF “SKIF”)
- Askold Volkov (Budker INP SB RAS, SRF “SKIF”)
- Artem Zorin (Budker INP SB RAS, SRF “SKIF”)

A superconducting undulator with a period of 15.6 mm and a mfgnetic field of 1.2 T created at the BINP SB RAS was tested in own cryostat based on indirect cooling with zero helium consumption. The report presents the main characteristics and design features of the magnetic and cryogenic systems of this insertion device. The results of measurements of the magnetic field are presented and the features of the cryogenic system operation in various modes is shown.

RESONANCE EFFECTS IN PHOTOEMISSION SPECTROSCOPY OF RARE-EARTHS IN INTERMETALLIC COMPOUNDS LA1-XTBXMN2SI2 (X = 0, 0.27) #102

Submitted **Ekaterina Ponomareva**

For track: X-ray spectroscopy

Authors:

- Ekaterina Ponomareva (M.N. Miheev Institute of Metal Physics UB RAS)
- Vladimir Grebennikov (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia,Ural State University of Railway Transport, Ekaterinburg, Russia)
- Danil Radzivonchik (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia)
- Yulia Korkh (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia)
- Yurii Yarmoshenko (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia)
- Evgenii Gerasimov (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia, Ural Federal University, Ekaterinburg, Russia)
- Nikolai Mushnikov (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia, Ural Federal University, Ekaterinburg, Russia)
- Tatyana Kuznetsova (M. N. Miheev Institute of Metal Physics UB RAS, Ekaterinburg, Russia, Ural Federal University, Ekaterinburg, Russia)

The rare-earth intermetallic compounds RMn2Si2 (R = rare-earth) with tetragonal ThCr2Si2-type structure have unique magnetic properties, which makes it possible to use them as functional materials. The variety of magnetic structures and magnetic phase transitions in such materials is due to the exchange interaction between manganese and rare earth ions [1–3]. That is why the study of RMn2Si2 electronic structure is closely related to the determination of the magnetic properties. Electronic states in La1-xTbxMn2Si2 (x = 0, 0.27) intermetallic compounds were studied by resonant

photoemission spectroscopy (RPES) using synchrotron radiation. This method makes it possible to investigate the localization of 4f-electrons in the valence band (VB). The main regularities in the formation of the electronic structure upon partial substitution of terbium for lanthanum atoms were established. The dependence of the VB spectra shape on the change in the photon energy near the absorption edges of the internal levels of La, Tb and Mn in the compounds has been studied. The processes of direct and two-stage production of photoelectrons, elastic and inelastic decay channels of these states with the emission of high-energy electrons due to intra-atomic Coulomb interaction have been studied. Atomic-force and magnetic-force microscopy was used to study the features of the surface of compounds at room temperature. The presence of a complex magnetic domain structure in compounds with terbium being partially replaced by lanthanum in LaMn2Si2 is shown.

The research was supported by RFBR project № 20-02-00541.

[1] S. Pandey, V. Siruguri, R. Rawat. Effect of Tb substitution in naturally layered LaMn2Si2: magnetic, magnetocaloric, magnetoresistance and neutron diffraction study // J. Phys. Condens. Matter. 32, 035807 (2020).
[2] E. G. Gerasimov, M. I. Kurkin, A. V. Korolyov, V. S. Gaviko. Magnetic anisotropy and ferro-antiferromagnetic phase transition in LaMn2Si2 // Physica B. 322, 297–305 (2002).
[3] N. V. Mushnikov, E. G. Gerasimov, P. B. Terentev, V. S. Gaviko. Magnetic structures and magnetic phase transitions in RMn2Si2 // AIP Advances. 8, 101411 (2018).

ТЕРАГЕРЦОВЫЕ ГИРОТРОНЫ С ПРИОСЕВЫМИ ЭЛЕКТРОННЫМИ ПУЧКАМИ НА ВЫСОКИХ ЦИКЛОТРОННЫХ ГАРМОНИКАХ ДЛЯ ФИЗИЧЕСКИХ ПРИЛОЖЕНИЙ #103

Submitted by **Andrei Savilov**
For track: THz radiation aplication
Authors:
Юрий Калынов, Иван Ошарин, Andrei Savilov, Дмитрий Щегольков, Илья Бандуркин, Евгений Семенов

В ИПФ РАН в течение многих лет развивается технология создания субтерагерцовых и терагерцовых гиротронов с большими орбитами, позволяющих осуществлять селективную генерацию на более высоких циклотронных гармониках, чем это возможно в традиционных гиротронах. В настоящее время экспериментальные исследования ведутся на двух специализированных установках.

На стенде, позволяющем формировать длинноимпульсные и непрерывные электронные пучки с энергией частиц до 30 кэВ, изучается прототип универсального субтерагерцового источника для магниторезонансной спектроскопии. В этом генераторе получена непрерывная селективная генерация на второй и третьей циклотронных гармониках с частотами 0,267 и 0,394 ТГц при мощности излучения 900 и 370 Вт соответственно. Для получения генерации на четвёртой гармонике на частотах 0,52-0,65 ТГц разработаны новые резонаторы с периодическими фазовыми корректорами. Кроме того, изучается возможность реализации на этом стенде гиротрона с уникально широкой полосой плавной частотной перестройки, основанного на контроле частоты генерации внешним механически перестраиваемым зеркалом. Такой источник был бы весьма востребован в спектроскопических приложениях, где требуются источники, обеспечивающие сочетание стабильности (узкополосности) генерируемого сигнала с возможностью его плавной перестройки в частотной полосе шириной хотя бы несколько процентов, что дало бы возможность получение спектральной картины в относительно широкой полосе.

На стенде с энергией электронов 80-100 кэВ исследуются возможности повышения мощности импульсной генерации на третьей гармонике на частотах, близких к 1 ТГц, для использования в экспериментах по получению газового разряда в сфокусированном терагерцовом волновом пучке и генерации мощного экстремального ультрафиолетового

излучения. Предложена схема реализации испульсного тератерцового гиротрона с мощностью излучения на уровне нескольких киловатт. Отдельным направлением в этих работах стало исследование возможностей использования резонаторов с несимметричным поперечным сечением, которые существенно улучшают селективные свойства генератора.

Исследование выполнено за счет гранта Российского научного фонда (проект № 22-19-00490).

ANALYSIS OF THE LOCAL ATOMIC STRUCTURE OF TIO2 BY SPECTROSCOPY OF EXTENDED ELECTRON ENERGY LOSS FINE STRUCTURE #104

Submitted by **Olga Bakieva**

For track: X-ray spectroscopy

Authors:

- Olga Bakieva (UdmFIC of Ural Branch RAS)
- Rishat Valeev (Physical-Technical Institute of UB RAS)
- Andrew Eliseev (Lomonosov Moscow State University)

The main method of study of the chemical compound and electron structure of surface is spectroscopy based on excitation of inner level of the atom by x-ray or monoenergetic electron beam. The extended fine structure of the electron energy loss spectra EXELFS (Extended Electron Energy Loss Fine Structure) is analogous to the extended fine structure of the X-ray absorption spectra EXAFS (Extended X-ray Absorption Fine Structure) in terms of the nature of formation and the information it contains. Analysis of EXELFS spectra makes it possible to determine partial chemical bond lengths, coordination numbers, and thermal dispersion parameters.

At present, both in EXELFS and EXAFS spectroscopy, there is a problem of analyzing spectra containing superposition of the signal of different chemical elements. In this case, the experimental data are the result of a superposition of the scattering of several wave vectors. For example, in the energy loss spectrum of titanium oxide electrons, there is an L2,3 titanium excitation edge (Eloss=461 eV), behind which there are oscillations, the length of which, according to model calculations, can reach 400-500 eV. Fourier analysis of this oscillating structure can provide information about the parameters of the Ti-Ti and Ti-O bonds. However, in the same energy range, there is the K edge of oxygen excitation (Eloss=532 eV), behind which there are also oscillations containing information about the O-Ti and O-O bonds. As a result, the experimental spectrum is a superposition of excitations of titanium and oxygen atoms. Currently existing software packages (Viper, IFeffit, etc.) for the analysis of both EXAFS and EXELFS spectra are not intended for the analysis of such overlapping structures.

In this work, we propose an algorithm for extracting normalized oscillating parts with a significant area of superposition of experimental signals. Attestation of the proposed method was carried out on titanium dioxide with the structure of rutile, anatase, brookite and X-ray amorphous structure.

РФА СИ В БОТАНИЧЕСКИХ ИССЛЕДОВАНИЯХ: ЭЛЕМЕНТНЫЙ СОСТАВ РАСТЕНИЙ ИЗ ГОРНОГО АЛТАЯ (СЕМ. FABACEAE) #105

Submitted by **Elena Khramova**

For track: SR for medicine and biology application

Authors:

- Elena Khramova (CSBG SB RAS)
- Серафима Сыева (ФАНЦ Агробиотехнологий)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Дмитрий Сороколетов (Budker Institute of Nuclear Physics)

Впервые изучены особенности элементного состава растений разных жизненных форм (травы и кустарники) из сем. Fabaceae, обитающих в Чуйской котловине Горного Алтая, методом рентгенофлуоресцентного анализа с использованием синхротронного излучения (РФА СИ) на оборудовании ЦКП "СЦСТИ" на базе ВЭПП-3 Института ядерной физики СО РАН. Цель работы заключалась в выявлении особенностей элементного состава растений разных таксонов и установлении видов с высоким содержанием макро- и микроэлементов.

Материалом исследования служили образцы трав – Oxytropis argentata (Pallas) Pers (остролодочник серебристый), Astragalus tibetanus Benth. Ex Bunge (астрагал тибетский) и кустарников – Caragana Bungei Ledeb. (карагана Бунге). Растения собраны в Чуйской степи в Кош-Агачском районе Республики Алтай в июле 2020 г. в генеративный период. O. argentata и A. tibetanus произрастали в злаково-остролодочниковой ассоциации в комплексной степи с засолением на высоте 1804 м над ур.м. (N 49.92669 E 88.84287), C. Bungei – в окрестности с. Кош-Агач на высоте 1760 м над ур.м. (N 50.01888 E 88.64833). Проанализированы листья, стебли, репродуктивные органы (бобы) и почвы из точек отбора образцов.

Сравнительный анализ почв выявил превышение по содержанию Ca (62284 ppm) и Br (18 ppm) в точке отбора травянистых растений и As (50 ppm) – в точке отбора C. Bungei, содержание остальных элементов варьировало незначительно.

Показано, что концентрация K у травянистых возрастала в ряду листья – стебли – бобы, а Ca, напротив, снижалась. У кустарников наблюдалась обратная тенденция: содержание Ca выше в стеблях, чем в листьях, содержание K при этом оставалось без изменений. В целом, более высокое содержание макроэлементов установлено в листьях O. argentata (38769 ppm), низкое – в стеблях A. tibetanus (16478 ppm).

Суммарное содержание микроэлементов максимально в стеблях C. Bungei и бобах A. tibetanus (590-588 ppm), минимально – в листьях C. Bungei (376 ppm). По повышенному содержанию Mn (77 ppm) выделяются листья, а Fe (371 ppm), Br и Cr (6.2 ppm) – стебли C. Bungei. В листьях O. argentata преимущественно накапливается Sr (205 ppm), в стеблях A. tibetanus – Zn (46 ppm), Ni (11 ppm) и Cu (8 ppm). Отмечено повышенное содержание Mo в надземных органах травянистых, что может быть связано с щелочной реакцией почвы из-за высокого содержания солей кальция.

Отмечен сдвиг в соотношении некоторых элементов. Значение Fe/Mn изменяется от 2.3 в листьях кустарников до 6-7 – в травах. Значение Ca/Sr во всех образцах выше 100, что считается нормой, но у кустарника C. Bungei оно максимально и достигает 255. Величина K/Rb варьирует от 340-660 в надземных органах травянистых до 3344 у кустарников, что, возможно, связано с видовой принадлежностью и условиями произрастания.

В результате, впервые получены достоверные данные по содержанию 20 элементов в адземных органах O. argentata, A. tibetanus и C. Bungei и почвах из точек отбора растений в Чуйской котловине. Отмечена связь накопления элементов с видовой принадлежностью растений, жизненной формой, условиями произрастания. Полученные данные по элементному составу растительных образцов и почв могут быть включены в базы данных.

Авторы выражают благодарность Ольге Васильевне Чанкиной за выполнение анализов. Работа выполнена при частичной поддержке гранта РФФИ и Республики Алтай в рамках проекта № 20-44-040002 р_а.

РФА СИ ДЛЯ ИССЛЕДОВАНИЯ СИБИРСКИХ КУСТАРНИКОВ В УСЛОВИЯХ АНТРОПОГЕННОГО ЗАГРЯЗНЕНИЯ #106

Submitted by **Elena Lyakh**
For track: SR for medicine and biology application
Authors:

- Elena Lyakh (CSBG SB RAS)
- Elena Khramova (CSBG SB RAS)
- Anna Lugovskaya (bSiberian State University of Geosystems and Technologies)

- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Dmitrii Sorokoletov (Budker Institute of Nuclear Physics)

Впервые изучены особенности элементного состава кустарников в урбоэкосистеме г. Новосибирска методом рентгенофлуоресцентного анализа с использованием синхротронного излучения (РФА СИ) на оборудовании ЦКП "СЦСТИ" на базе ВЭПП-3 Института ядерной физики СО РАН. Цель работы заключалась в определении изменений элементного состава сибирских видов кустарников в условиях антропогенного воздействия для оценки качества окружающей среды и выявления толерантных к загрязнению видов.

Материалом исследования служили образцы двух видов спиреи - Spiraea chamaedryfolia (спирея дубравколистная) и S. media (спирея средняя) из сем. Rosaceae и Myricaria bracteata (мирикария прицветниковая) из сем. Tamaricaceae. Изучаемые кустарники привлекают внимание своей декоративностью, экологически пластичны, газоустойчивы, широко используются в зеленом строительстве. Растения высажены в одном из наиболее неблагоприятных с экологической точки зрения районе - Ленинском. В качестве фона выбраны растения, произрастающие на территории ЦСБС СО РАН.

Сравнительный анализ почвы из точек отбора растительных образцов показал превышение по содержанию Ca, Co, Cu, Zn, As, Br, Sr, Zr и снижение Mn в городских почвах по сравнению с контролем.

Исследование содержания макро- и микроэлементов в надземных органах растений показало, что концентрация макроэлементов K и Ca выше в листьях, чем в стеблях вне зависимости от таксона и места произрастания. В условиях антропогенного воздействия содержание K в растениях ниже, чем в фоновых условиях, а содержание Ca в листьях, напротив, возрастает. Наибольшее содержание макро- и микроэлементов обнаружено в листьях M. bracteata и стеблях Spiraea. Обнаружено, что в растениях под антропогенным воздействием повышалось содержание Ca, Ti, V, Fe, Co, Br, Sr, Y, Zr, Nb, Pb и снижалось K, Zn и Mo по сравнению с фоном. Наиболее сильное загрязнение тяжелыми металлами в городских условиях отмечено у растений M. bracteata.

Рассчитан коэффициент биогеохимической трансформации (Zv), отражающий нарушение нормальных соотношений элементов в органах растений в результате усиления антропогенной нагрузки. Наиболее существенные изменения элементного состава растений под антропогенным воздействием отмечены у растений вида M. bracteata, Zv листьев которого равно 63.7, что в 1.7-4.8 раз выше, чем у растений Spiraea. Наиболее устойчивы к загрязнению растения S. chamaedryfolia (Zv = 13.3).

В результате, впервые получены достоверные данные по содержанию 20 элементов в образцах сибирских кустарников - S. chamaedryfolia, S. media и M. bracteata в урбоэкосистеме г. Новосибирска. Выделены наиболее толерантные к загрязнению в городских условиях виды, которые могут быть рекомендованы для широкого использования в зеленом строительстве. Полученные данные по элементному составу растительных образцов и почв могут быть включены в базы данных.

Авторы благодарны Ольге Васильевне Чанкиной за выполнение анализов.

SPECTROSCOPIC (XAFS AND XPS) INVESTIGATIONS OF NANOCOATINGS DEPOSITED ON THE SURFACE OF POROUS ALUMINA #107

Submitted by **Rishat Valeev**

For track: X-ray spectroscopy

Author: Rishat Valeev (Udmurt Federal Research Center of UB RAS)
Co-author: Vladimir Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)

Novel materials science developing the methods of obtaining and studying of new materials for different applications based on nanostructured coatings. For instance, controlled deposition onto the surface of porous media can allow obtaining a new class of 2D materials possessing unique optical, magnetic, catalytic, sensory, gas and liquids filtration properties. It should be noted that a large contribution in these properties has a developed surface due to the formation of films with different surface morphology. It is also strongly affected by the structural-phase state, local atomic and electronic structure [1].

Synchrotron facilities give more precise and reliable information about structure and electronic properties of materials. For instance X-Ray Absorption Fine Structure (XAFS) technique is a powerful method of obtaining of structural information, X-Ray Absorption Near Edge Structure (XANES) as well as X-Ray Photoelectron Spectroscopy (XPS) allows to investigate the charge states of chemical elements and chemical composition. For the visualization of surface morphology the methods of Scanning Electron Microscopy (SEM) and different methods of Atomic Force Microscopy (AFM) are widely used.

In this work we propose templating approaches based on the formation of semiconductors (Ge, ZnS, ZnSe, GaAs) and 3d metals (Fe, Co, Ni) nanocoatings on the surface the porous alumina films with highly ordered and controlled diameter of holes. Porous alumina templates were obtained by anodization process of aluminum foil. The aim was to identify the influence surface morphology on chemical and local atomic structure of coatings by the methods of XAFS, XPS and SEM investigations of semiconductors and 3d metals nanocoatings to form the basis of their functional properties.

This work is supported by Russian Federation Assignment (project № 121030100002-0). XAFS investigations were done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS. XPS and SEM investigations were carried out using facilities of shared research center “Surface and novel materials” UdmFRC UB RAS.

The study was also supported by the Ministry of Science and Higher Education of Russia under Agreement № 075-15-2021-1351 in part of developing of XPS methodology.

1. R. Valeev, A. Beltiukov, et al. Mater. Res. Express 3, 015902 (2016). doi:10.1088/2053-1591/3/1/015902.

SPECTROSCOPIC INVESTIGATIONS OF IRON OXIDE NANOCOATINGS ON THE SURFACE OF POROUS ALUMINA OBTAINED BY THE AIR OXIDATION OF MAGNETRON DEPOSITED IRON FILMS #108

Submitted by **Rishat Valeev**
For track: X-ray spectroscopy
Author: Rishat Valeev (Udmurt Federal Research Center of UB RAS)
Co-author: Vladimir Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)

Due to different magnetic effects in Iron Oxide films such as spin-polarization of electrons in magnetite (Fe3O4), magnetoelectric properties in hematite (Fe2O3) and antiferromanetic properties of wustite (FeO) they have potential application in spintronics, magnetoelectricity and high density memory devices [1,2]. Moreover, we suppose Iron Oxide coatings obtained on hexagonal oriented porous media can show chirality of magnetic structure. It should be noted that the manifestation of properties mentioned above strongly connected to the thickness of coatings, their electronic and local atomic structure.

To establish the relationship between functional and structure properties synchrotron facilities can be used. For example X-Ray Absorption Fine Structure (XAFS) technique is a powerful method of obtaining of structural information, X-Ray Absorption Near Edge Structure (XANES) as well as X-Ray Photoelectron Spectroscopy (XPS) allows to investigate the charge states of chemical elements and chemical composition.

In this work for obtaining of Iron Oxide coatings on the surface of porous alumina we propose magnetron deposition technique of Fe followed by thermal annealing in oxygen atmosphere. Porous alumina templates were obtained by anodization process of aluminum foil. The aim of this work was to identify the influence of Iron Oxide films thickness and their surface morphology on chemical and local atomic structure of coatings by the methods of XAFS, XPS and SEM investigations to form the basis of their functional properties.

This work is supported by the Ministry of Science and Higher Education of Russia under Agreement N 075-15-2021-1351.

XAFS investigations were done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS.

XPS and SEM investigations were carried out using facilities of shared research center “Surface and novel materials” UdmFRC UB RAS.

1. Spintronics for Next Generation Innovative Devices / Ed. by K. Sato, E. Saitoh. Chichester: Wiley, 2015. 280 p.
2. Kang Y.S., Risbud S., Rabolt J.F., Stroeve P. // Chem. Mater. 1996. V. 8. P. 2209.

MOLECULAR STRUCTURAL DYNAMICS STUDY USING TIME-RESOLVED DIFFRACTION #110

Submitted by **Key Young Oang**

For track: X-ray structural analysis

Author: Key Young Oang (Korea Atomic Energy Research Institute (KAERI))
Co-authors:

- In Hyung Baek (KAERI)
- Hyeon Sang Bark (KAERI)
- Kyu-Ha Jang (KAERI)
- Young Uk Jeong (KAERI)
- Hyun Woo Kim (KAERI)
- Kitae Lee (KAERI)

During chemical, physical and biologically relevant reactions of various molecules in various phases, several short-lived species so-called reaction intermediates exist and change their three-dimensional molecular structures as time evolves. To assemble a puzzle of structure, dynamics and function of molecule, determining molecular structures of reaction intermediates is crucial and thus it is required to know in detail how a reaction proceeds. There are two major methodologies for studying molecular structural dynamics. One is time-resolved optical spectroscopy and another is time-resolved diffraction that replaces the optical probe pulse to structural probes, such as electrons or X-rays. Here we briefly introduce time-resolved electron diffraction and time-resolved X-ray diffraction and compare their application fields.

RESISTANCE TO HIGH-TEMPERATURE OXIDATION OF CRN/ALN COATINGS BY X-RAY PHASE ANALYSIS USING SYNCHROTRON RADIATION #111

Submitted by **Andrey Leonov**

For track: SR technological application and X-ray apparatus

Authors:

- Andrey Leonov (Institute of High Current Electronics, Siberian Branch, Russian Academy of Sciences)
- Yulia Denisova (Institute of High Current Electronics SB RAS)
- Vladimir Denisov (HCEI SB RAS)
- Mikhail Savchuk (Institute of High Current Electronics SB RAS)
- Vasiliy Tishchenko (Institute of High Current Electronics SB RAS)

- Alexander Shmakov (Budker INP)

X-ray analysis using synchrotron radiation was used to study the resistance to high-temperature oxidation and the stability of the structural-phase state of CrN/AlN coatings in the temperature range of 30÷1300 °C. The deposition of CrN/AlN coatings was carried out by the vacuum-arc plasma-assisted method on an NNV 6.6-I1 setup equipped with two electric arc evaporators with a cathode diameter of 80 mm and an additional "PINK" gas plasma source. The source of synchrotron radiation was the VEPP-3 electron storage ring. The study was carried out using a high-temperature X-ray camera NTK-2000, a position-sensitive single-coordinate detector OD-3M-350, software - a program for processing measurement results Fityk v.1.3.1. The studies were carried out for the following experimental conditions: operating wavelength λ=0.172 nm, range of diffraction angles 2Θ: 28-59 degrees, sample heating rate 10°C/min. Chromium and aluminum nitrides retain thermal stability up to a temperature of ~1110-1115°C (~1075-1080°C - with layer-by-layer deposition, when using a metal screen), after which oxidation of the coating begins, reflections of chromium and aluminum nitrides disappear at a temperature of ~1235- 1240 °C (~1255-1260 °C with layer-by-layer spraying).

PRODUCTION OF HIGH-STRENGTH WEAKLY CONDUCTIVE CERAMICS BASED ON BARIUM ALUMINATE FOR REMOVING STATIC CHARGE FROM THE INNER SURFACES OF VACUUM CHAMBERS OF ACCELERATORS #112

Submitted by **Alexandr Zhdanok**

For track: SR and FEL sources and centers

Authors:

- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
- Alexandr Zhdanok (Institute of Solid State Chemistry and Mechanochemistry Siberian Branch of the Russian Academy of Sciences)
- Zoya Korotaeva (Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk)
- Liliya Berdnikova (Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk)
- Joseph Samuel (Novosibirsk State Technical University, Novosibirsk)
- Victor Bulgakov (Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk)

A method has been developed for producing structural samples of weakly conductive ceramics for removing static charge from the inner surfaces of vacuum chambers of accelerators based on barium aluminate of the composition $BaO \cdot Fe_2O_3 \cdot 5Al_2O_3$ with conductive additives: multi-walled carbon nanotubes, silicon carbide, lithium hydroxide. The properties of such ceramics are largely determined by the concentration of components, the temperature treatment regime. The production of raw ceramic samples was carried out by semi-dry pressing of the molding mass from a powder composition with a moisture content of 13%. The pressing pressure was 200 MPa. The samples were dried in air for 24 hours and then in an oven at 200 °C. After drying, the samples were placed in a corundum crucible and covered with a heat-resistant material (fused electrocorundum). Then firing was carried out in an argon medium at a temperature of 1600 ° C.

Ceramic samples with a maximum compressive strength of 695.9 MPa, a density of 3.73 g/cm3, and a maximum electrical conductivity (at 300 °C) of 10-4 Cm/cm was obtained.

The work was carried out with support within the Federal Targeted Programme according to Agreement No. 075-15-2021-1359 of 13.10.2021 (internal No. 15. SIN.21.0015).

SUPERCONDUCTING UNDULATOR CRYOGENIC SYSTEM BASED ON INDIRECT COOLING #113

Submitted by **Sergey Khrushchev**

For track: SR and FEL sources and centers

Authors:

- Sergey Khrushchev (Budker INP SB RAS, SRF “SKIF”)
- Valeriy Tsukanov (Budker INP SB RAS, SRF “SKIF”)
- Vitaliy Shkaruba (Budker INP SB RAS, SRF “SKIF”)
- Nikolay Mezentsev (Budker INP SB RAS, SRF “SKIF”)
- Alexander Safronov (BINP SB RAS)

The indirect cooling cryogenic system of the superconducting undulator with 15.6 mm period, 1.2 T magnetic field and 7 mm magnetic gap is described in this article. Nitrogen heat pipes are used in this system as heat conductors from the first stage of cryocoolers to accelerate initial cooling down process. The cooling down without liquid helium was tested (only helium gas was used). The cryogenic system design is described and process of cooling down and operation on different modes is presented.

HALL PROBE MAGNETIC MEASUREMENTS OF THE SUPERCONDUCTING UNDULATOR #114

Submitted by **Valeriy Tsukanov**

For track: SR and FEL sources and centers

Authors:

- Valeriy Tsukanov (Budker INP SB RAS, SRF “SKIF”)
- Vitaliy Shkaruba (Budker INP SB RAS, SRF “SKIF”)
- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Sergey Khrushchev (Budker INP SB RAS, SRF “SKIF”)
- Nikolay Mezentsev (Budker INP SB RAS, SRF “SKIF”)
- Askold Volkov (Budker INP SB RAS, SRF “SKIF”)
- Artem Zorin (Budker INP SB RAS, SRF “SKIF”)

The superconducting undulator with 15.6 mm period and 1.2 T magnetic field described in this article has 7 mm magnetic gap. The magnetic measurements system in such conditions required using of special tube (ante-chamber) inside of undulator magnetic gap. The thermal insulation between cold magnet and this measurement tube does not allow to have stable temperature along this tube length. The temperature range into this tube is 70-300 K. Hall probe measurements in this case are a rather complicated problem. The features of the method of measurement and processing of results are described in this article.

ИСПОЛЬЗОВАНИЕ ПОЛУЧЕННОГО В ЛИУ КИЛОАМПЕРНОГО РЭП ДЛЯ ГЕНЕРАЦИИ ТГЦ ИЗЛУЧЕНИЯ ПРИ РАЗВИТИИ ДВУХПОТОКОВОЙ НЕУСТОЙЧИВОСТИ В ПУЧКОВО-ПЛАЗМЕННОЙ СИСТЕМЕ #115

Submitted by **Denis Samtsov**

For track: SR and FEL sources and centers

Authors:

- Denis Samtsov (Budker Institute of Nuclear Physics of Siberian Branch Russian Academy of Sciences (BINP SB RAS))
- Andrey Arzhannikov (Novosibirsk State University)
- Stanislav Sinitsky (Budker Institute of Nuclear Physics)

- Sergey Popov (Institute of Nuclear Physics 11, akademika Lavrentieva prospect, Novosibirsk, 630090 Russia)
- Danila Nikiforov (BINP)
- Magomedrizy Atlukhanov (Budker INP SB RAS)
- Dmitry Starostenko (BINP SB RAS)
- Vasilii Stepanov (BINP SB RAS)
- Semyon Vorobyov (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)
- A. Grigoriev (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin»)

Проведенные на установке ГОЛ-ПЭТ исследования механизмов генерации субмиллиметрового излучения (0.1 –0.5 ТГц) при коллективной релаксации релятивистского электронного пучка (РЭП с параметрами 0,6 МэВ/ 15 кА/ 5 мкс) в плазме с плотностью ~5 1014 см-3 продемонстрировали достижимость в потоке излучения уровня мощности ~10 МВт при микросекундной длительности [1]. Эксперименты проводятся в пробочном магнитном поле 4.5/3.2 Тл при плотности тока пучка (1-2) кА/см2. Для продвижения в генерации излучения в область частот ~1 ТГц и выше с использованием механизмов генерации в пучково-плазменной системе необходим подъём плотности тока пучка в несколько раз при поддержании его угловой расходимости на низком уровне. Пучок с такими параметрами может быть получен путём магнитного сжатия сечения пучка, генерируемого в ЛИУ [2]. Возможным затруднением к реализации процесса генерации терагерцового излучения в плазме с использованием такого пучка может оказаться его небольшая (~ 100 нс) длительность [2], которая может привести к недостаточному уровню накачиваемых пучком плазменных колебаний. Возможность преодоления этого затруднения подтверждается результатами исследований высокоэффективного коллективного торможения в плазме пучков с длительностью масштаба 100 нс, которые были проведены на установке ИНАР [3, 4].

В представляемом докладе будет проанализирована перспектива использования пучка электронов, получаемого на выходе из ЛИУ с энергией 1 МэВ, током 2 кА и длительностью ~ 100 нс, для генерации терагерцового излучения в замагниченной плазме. Этот анализ будет базироваться на отмеченных выше результатах экспериментальных исследований и теоретических представлениях о механизмах трансформации плазменных колебаний в электромагнитные волны.

Литература

[1]. Arzhannikov A.V., Ivanov I.A., Kasatov A.A., et al. “Well-directed flux of megawatt sub-mm radiation generated by a relativistic electron beam in a magnetized plasma with strong density gradients.” Plasma Physics and Controlled Fusion 62.4 (2020): 045002.

[2]. D.A. Nikiforov, A.V. Petrenko, S.L. Sinitsky et al., “Investigation of high current electron beam dynamics in linear induction accelerator for creation of a high-power THz radiation source”, Journal of Instrumentation (JINST), vol.16, P11024, 2021, https://doi.org/10.1088/1748-0221/16/11/P11024

[3]. Аржанников А.В., Бурдаков А.В., Койдан В.С. и др. Увеличение эффективности взаимодействия с плазмой//Письма в ЖЭТФ, 1978, Т. 227, вып.3. С. 173 – 177.

[4]. Arzhannikov A.V., Burdakov A.V., Burmasov V.S. et al. Plasma heating in a solenoid by relativistic electron beam. Proc. of the 3-rd Inter. Conf. on High Power Electron and Ion Beam Res. and Tech. Novosibirsk, 1979, P. 29 – 42.

DISPERSION STRENGTHENING OF COPPER USED FOR THE MANU-FACTURE OF LINERS FOR SUPERCONDUCTING INSERTION DEVICES FOR GENERATING SYNCHROTRON RADIATION #116

Submitted by **Alexandr Zhdanok**

For track: SR and FEL sources and centers

Authors:

- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)
- Alexandr Zhdanok (Institute of Solid State Chemistry and Mechanochemistry Siberian Branch of the Russian Academy of Sciences)
- Victor Kuznetsov (Institute of Solid State Chemistry and Mechanochemistry of the Siberian Branch of the Russian Academy of Sciences, Novosibirsk)
- Zoya Korotaeva (Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk)
- Liliya Berdnikova (Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk)
- Mikhail Mikhailenko (Institute of Solid State Chemistry and Mechanochemistry SB RAS)
- Natalia Stepanova (Novosibirsk State Technical University, Novosibirsk)

Cast samples (unmodified and modified with multi-walled carbon nanotubes (MWCNTs)) based on M1 grade copper were obtained. For this, MWCNTs were treated with copper powder (PMS-1) in a ratio of 5 : 95 in a centrifugal planetary shoal of AGO-3. Then a ligature was obtained: the powder mixture was diluted 5 times with copper and fused to a homogeneous state. The concentration of MWCNTs in the ligature (copper matrix) is 1 wt.%. Copper modification was carried out in a ladle and furnace, for comparison, a control sample was cast without a modifier. The metal was poured into a sand mold, which is a system of a riser in the middle and several cylinders with a length of 150 mm and a diameter of 30 mm. The metal is poured (1200 °C) into the central part (riser), from where the metal is poured by siphon (bottom-up) into other cylindrical sections; the mass of the metal in the form of 1500 g.

On the basis of electronic microphotographs, it was found that the MWCNTs are distributed fairly evenly in the ligature and are located along the grain boundaries.

Brinell hardness studies of cast samples have shown that the hardness of all samples after heat treatment decreases by 12.2-13.4%. The hardness of the modified samples (45.82-49.72 HBW) is less than the hardness of the control sample (59.47 HBW), but the standard deviations of hardness from the average values for the modified samples are 2.4-5 times less than that of the control sample, which can serve as proof that nanotubes contribute to a more uniform crystallization of the melt.

The work was carried out with support within the Federal Targeted Programme according to Agreement No. 075-15-2021-1359 of 13.10.2021 (internal No. 15. SIN.21.0015).

SOFT X-RAY SR STATION «KOSMOS» AT THE VEPP-4 STORAGE RING: STATUS AND XAFS APPLICATIONS. #117

Submitted by **Anton Nikolenko**

For track: SR technological application and X-ray apparatus

Authors:

- Anton Nikolenko (Budker INP SB RAS, SRF "SKIF")
- Anastasiya Fedorenko (NIIC SB RAS)
- Mikhail Syrokvashin (NIIC SB RAS)
- Pavel Zavertkin (Budker INP SB RAS)
- Vladimir Polkovnikov (IPM RAS)

The metrological station "Cosmos" receives radiation from the bending magnet of the storage ring VEPP-4. The station was originally intended for to various kinds of metrological work in soft X-

ray and VUV range (10-5000 eV): certification of spectrometers, optical elements, detectors, etc. At present, the station equipped by the dubble-crystal Si(111) monochromator. This upgrade has made it possible to perform spectroscopic measurements in the tendep X-ray range (2-10 keV). In the interests of station users and for the development of procedures the number of measurements of XANES spectra near the K-edges of S, P, Cl, Cu and L-edges of Nb, Mo, Zr were carried out. To expand the spectral range of available energies, a hybrid scheme with long period organic KAP and RbAP crystals paired with a multilayer mirror was developed too. The multilayer mirror has a period close to the lattice parameter of crystals (13.47 and 13 A, respectively) and servants to prevent their radiation damage. It is expected that such an optical scheme will make it possible to expand the spectral range in the soft energy region up to 500 eV, which corresponds to the K edge of oxygen. Currently, the XAFS spectroscopy procedure implemented at the station is used by our users for the development of new functional materials. However, the most important thing is the station is considered as prototype for the soft X-ray XAFS station for the new synchrotron source SKIF.

CREATION OF THE SCIENTIFIC RESEARCH CENTER «TOMSK COMPETENCE CENTER IN THE FIELD OF BEAM-PLASMA ENGINEERING AND SYNCHROTRON RESEARCH» #118

Submitted by **Anton Teresov**
For track: SR technological application and X-ray apparatus
Author: Anton Teresov (Institute of high current electronics SB RAS)
Co-authors:

- Vladimir Denisov (HCEI SB RAS)
- Nikolay Ratakhin (HCEI SB RAS)
- Nikolay Koval (HCEI SB RAS)

As part of the implementation of Agreement No. 075-15-2021-1348 dated October 5, 2021, concluded between the Institute of High Current Electronics SB RAS and the Ministry of Science and Higher Education of the Russian Federation, the Scientific Research Center «Tomsk Center of Competence in the Field of Beam-Plasma Engineering and Synchrotron Research» (SRC TCC) was created as part of the network synchrotron and neutron research infrastructure in the Russian Federation. SRC TCC was established as a structural subdivision of the HCEI SB RAS to carry out scientific-methodological, scientific and educational activities in the field of synchrotron and neutron research and to provide organizational and methodological support for work in the field of beam-plasma surface engineering, carried out by research departments of the HCEI SB RAS and third-party organizations. The main functions of the SRC TCC are:

- accumulation of data and knowledge in the field of synchrotron research, obtained by scientific groups participating in the activities of the SRC TCC, and their distribution among the participants;
- implementation of own scientific research in the field of methods of using synchrotron radiation for surface engineering;
- in the field of educational activities of the SRC TCC - assistance in the implementation of educational programs for the training and retraining of personnel by higher professional education organizations that have licenses to carry out educational activities, including programs for the training of scientific personnel in graduate school;
- development of the procedure and conditions for the use of methods and equipment of SRC TCC;
- repair and maintenance of high-tech equipment of SRC TCC;
- coordination of teams of scientific and educational institutions to carry out activities aimed at the development and creation of the station «Surface» of the resource sharing center «SKIF» (Koltsovo).

At the moment, a new unique vacuum electron-ion-plasma installation (VEIPS-1) is being created for the SRC TCC, equipped with sources of gas and metal plasma, electron beams, which

allows to carry out the processes of forming layers and coatings in a wide range of operating parameters, to diagnose generated plasma, and, most importantly, to prepare specimens and test the methodology for in situ studies of the processes of formation of layers on the surface of materials by X-ray diffraction using synchrotron radiation before its implementation at the VEPP-3 station (Siberian Center for Synchrotron and Terahertz Radiation, Novosibirsk).

DEVELOPMENT OF SPA (SINGLE PARTICLE ANALYSIS) TECHNIQUES USING SCANNING μXRF-SR AND CONFOCAL X-RAY MICROSCOPY IN THE STUDY OF NATURAL SAMPLES #119

Submitted by **Andrey Darin**
For track: X-ray fluorescent analysis
Author: Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)
Co-authors:

- Denis Rogozin (FRC «KSC SB RA»)
- Artur Meidus (FRC «KSC SB RA»)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Andrey Gogin (NRC «KI»)
- Roman Senin (NRC «KI»)

Single particle analysis is the modern section of analytic studies using electron microscopy or ICP-MS LA. This report presents the expirements results on the searh and study of single aerosol microparticles in various depozit materials. The experiment was carrying out with scanning μ-XRF using confocal x-ray microscopy (CXM) module at beamline “RT-MT” on Kurchatov synchrotron light source. The CXM and analysis techniques was developed in INP SB RAS. Experiments to study the elemental composition of individual microparticles were carried out on aerosol filters (AFA-VP) and snow cores of the Altai region. The possibility of searching and identifying natural and technogenic microparticles by elemental composition was demonstrating

Several particles (20-50 mkm size) of a round shape and composition different from the main matrix were found in the bottom sediments of Zapovednoye Lake (Tunguska Nature Reserve) in a layer dated 1908-1910 yy (Date of Tunguska event). The morphology and composition of the found particles testify to their cosmic origin.

The created equipment and methods allow searching and studying particles with micrometer spatial resolution in matrices of various compositions based on data on the content of rock-forming and trace elements.

This work was supported by RFBR grant No. 19-05-50046 (Micromir).

COMPLEX STUDY OF LOCAL ATOMIC STRUCTURE OF PROMISING TI-POWDERS #120

Submitted by **Igor Averkiev**
For track: X-ray spectroscopy
Authors:

- Igor Averkiev
- Olga Bakieva (UdmFIC of Ural Branch RAS)
- Vladimir Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)

The synthesis of two-dimensional systems became especially actual with the appearance of the first works about graphene and two-dimensional carbides and nitrides of transition metals MXenes (Mn+1XnTx, where M is a transition metal, X is C and / or N, Tx are functional groups of the -O

type, -OH, -F, etc.). For the first time, MXenes began to be discussed in 2011 [1], these materials attracted attention due to their unique properties, namely, the combination of metallic conductivity of transition metal carbides and nitrides and the possibility of attaching various functional groups to their surface [2]. The unique properties of MXenes is possible due to the method of their synthesis, namely the removal of the A element from the MAX phases (M is a transition metal, A is an element of IIIA and IVA groups, X is C and / or N). Thus, the method of synthesis of the MAX phase will effect on the characteristics of two-dimensional carbides/nitrides.

One of the ways to obtain MAX-phases is the mechanical activation of powders. In article [3], the synthesis of the Ti2AlC compound was carried out by mechanical activation of titanium, aluminum and carbon powders in petroleum ether, followed by annealing at a temperature of 1000 oC. Studies of the elemental composition, the type of chemical bond and the local atomic structure made it possible to make an assumption about the presence of the Ti-H bond in the samples after mechanical activation. Additional studies are needed to confirm this assumption. Thus, the aim of this work is to study the local atomic environment of mechanically activated powders by X-rays and electron beam. In order to determine the presence of the Ti-H bond in them, it is necessary to analyze the local atomic structure of certified titanium hydride TiH2. It is known that EXAFS (Extended X-ray absorption fine structure) and EXAFS-like methods are used to study the local atomic structure. In the present work, the spectra of the Extended Electron Energy Loss Fine Structure (EXELFS) were obtained in the mode of reflection from the surface at an excitation energy of the incident electron beam of 900 eV (analysis depth less than 5 nm). Fine structure analysis of the M2,3 excitation edge of titanium and the K excitation edge of carbon was carried out.

All EXAFS spectra of studied Ti-nanocomposites and reference samples (Ti foil and commercial TiH2) were recorded at SSTRC, Novosibirsk.

The genesis of local structures of the prepared Ti-nanocomposites and reference samples were studied by EXELFS and EXAFS. The interatomic distances and corresponded coordination numbers were determined. All possible structural models were discussed in detail. The obtained EXELFS and EXAFS results are in good agreement with XPS, XRD, SEM (EDX) data.

Acknowledgements. This work is supported by Russian Federation Assignment (project № 121030100002-0). EXELFS investigations were carried out using facilities of shared research center “Surface and novel materials” UdmFRC UB RAS.

EXAFS investigations were done at the shared research center SSTRC on the basis of the Novosibirsk VEPP-4-VEPP-2000 complex at BINP SB RAS.

References

1. Naguib, M., Kurtoglu, M., Presser, V. et.al. Two-Dimensional Nanocrystals Produced by Exfoliation of Ti3AlC2. // Advanced Materials. 2011. V. 23 № 37. P. 4248–4253.

2. Sokol, M., Natu, V., Kota, S., Barsoum, M. W. On the Chemical Diversity of the MAX Phases. Trends in Chemistry. 2019. V. 1. Is. 2. P. 210-223

3. Eryomina M. A., Lomayeva S. F., Demakov S. L. Synthesis of composite based on Ti2AlC with added nanographite via wet ball milling followed by spark plasma sintering //Materials Chemistry and Physics. 2021. V. 273. P. 125114.

TABLETOP LASER-DRIVEN PLASMA MICROFOCUS X-RAY SOURCE FOR IMAGING APPLICATIONS #121

Submitted by **Victor Asadchikov**

For track: SR technological application and X-ray apparatus

Author: Victor Asadchikov (FSRC "Crystallography and photonics" RAS)

Co-authors:

- Alena A. Garmatina
- Alexey Buzmakov (FSRC "Crystallography and photonics" RAS)
- Irina Dyachkova (FSRC "Crystallography and Photonics" RAS)
- Nikita Vladimirovich Minaev

- Vyacheslav Mikhailovich Gordienko

We developed the laboratory tabletop laser-driven plasma microfocus X-ray source for imaging applications. The femtosecond laser-plasma X-ray source driven by low energy 0.1MHz rate ytterbium fiber laser interacted with copper target in ambient atmosphere environment. The results of the generation line X-ray with energy about 8 keV and a flux more than 10^7 photons/s in 2π for X-ray imaging applications are discussed.

X-ray optical scheme include elliptical glass concentrator as condenser and Fresnel zone plate as imaging optical element. The modeling with ray tracing technique shows that system should allow to obtain spatial resolution up to 1 um.

The work was supported by the Federal Scientific and Technical Program for the Development of Synchrotron and Neutron Research and Research Infrastructure dated September 29, 2021 No. 2021-951-FP5-3.

COHERENT X-RAY BEAM-EXPANDER FOR ADVANCED LIGHT SOURCES #122

Submitted by **Zverev Dmitrii**

For track: SR technological application and X-ray apparatus

Authors:
- Zverev Dmitrii (Immanuel Kant Baltic Federal University)
- Mikhail Sorokovikov (Immanuel Kant Baltic Federal University)
- Vyacheslav Yunkin (Institute of Microelectronics Technology RAS)
- Sergey Kuznetsov (Institute of Microelectronics Technology RAS)
- Anatoly Snigirev (Immanuel Kant Baltic Federal University)

The recent trend toward fourth-generation synchrotron radiation sources has led to dramatic increases in the brightness and spatial coherence of the generated X-ray beams, compared with older designs. This has triggered the development of X-ray optics capable of fully utilizing the laser-like properties of novel sources; the most promising among these is refractive optics, the youngest of the existing X-ray optics [1]. X-ray compound refractive lenses (CRLs) have become a major tool in modern X-ray beamlines, owing to their low sensitivity to shape errors, overall ease of use, and high versatility. By modifying the shape, composition, and number of individual lenses, CRLs can be adapted to photon energies in the 2–200 keV range, enabling flexible adjustment of focal lengths for a wide range of applications. CRLs can provide beam-conditioning functions such as condensers, collimators, beam-shapers, or higher harmonics suppressors [2–5]. Moreover, CRLs are extensively used in X-ray imaging and microscopy, interferometry, Fourier optics, and spectroscopy [6–11].

Intelligent preparation and special formation of X-ray beams in advance allows to fully realize the capabilities of modern X-ray techniques, and even more, permits the creation of the necessary conditions for their effective use. At the same time, ensuring the possibility of varying the beam's transverse size, as well as controlling the photon flux density, is a desirable challenge in beam shaping and beam conditioning goals. It should be emphasized that there are well-developed and highly demanded X-ray techniques that require a high degree of spatial coherence and a large illumination area at the sample position. For example, phase-contrast imaging and spectroscopy methods require the vertical scanning of samples for imaging their full extent. The ability to control the photon flux density enables to study objects that are sensitive to radiation loads, for example, various polymers or biological samples.

We propose a beam expander based on a multilens system representing a silicon structure of 100 parallel identical planar CRLs. Under coherent illumination, a multilens system generates many diverging beams that interfere in the area where they overlap, with periodic patterns of interference fringes formed at certain distances, called Talbot distances. The optical properties of such a 100-lens interferometer, as well as the ability to control the angular size and photon flux density of the expanding beam, were experimentally demonstrated at the European Synchrotron Radiation Facility

(ESRF) in Grenoble. A theoretical analysis of the expanded beam propagation and formation of the Talbot interference patterns and the corresponding computer simulation are presented. The experimental results agree quite well with the calculated results.

1. A. Snigirev, et al, Nature, 384(6604), 49-51 (1996).
2. M. Polikarpov, et al, J. Synchrotron Radiat. 21(3), 484–487 (2014)
3. A. Snigirev, et al, Opt. Express 22(21), 25842–25852 (2014)
4. D. Zverev, et al, Opt. Express 25(23), 28469 (2017)
5. A. Narikovich, et al, J. Synchrotron Radiat. 26(4), 1208–1212 (2019)
6. D. V. Byelov, et al, RSC Adv. 3(36), 15670–15677 (2013)
7. N. Dubrovinskaia, et al, Sci. Adv. 2(7), e1600341 (2016)
8. K. V. Falch, et al, Ultramicroscopy 184(A), 267–273 (2018)
9. M. Polikarpov, et al, Acta Crystallogr. D Struct. Biol. 75(11), 947–958 (2019)
10. S. Lyatun, et al, J. Synchrotron Radiat. 26(5), 1572–1581 (2019)
11. D. Zverev, et al, Opt. Express 28(15), 21856–21868 (2020)

CORRECTION OF THE PHASE ERROR OF A SUPERCONDUCTING UNDULATOR #123

Submitted by **Pavel Kanonik**
For track: SR and FEL sources and centers
Authors:

- Pavel Kanonik (Budker Institute of Nuclear Physics)
- Nikolay Mezentsev (Budker INP SB RAS, SRF “SKIF”)
- Vitaliy Shkaruba (Budker INP SB RAS, SRF “SKIF”)
- Valeriy Tsukanov (Budker INP SB RAS, SRF “SKIF”)
- Askold Volkov (Budker INP SB RAS, SRF “SKIF”)
- Olga Tarasenko (BINP)
- Fedor Kazantsev (Novosibirsk State University)
- Sergey Khrushchev (Budker INP SB RAS, SRF “SKIF”)
- Alexandr Erokhin (BINP)
- Artem Zorin (Budker INP SB RAS, SRF “SKIF”)

The spectral brightness of the radiation from the undulator is the main characteristic of the quality of the magnetic field of the undulator. Errors in the magnetic field of the undulator can significantly reduce the spectral brightness of the radiation, especially at high harmonics. Compensation for errors in the magnetic field of the undulator is a priority task for obtaining a high spectral brightness of the radiation. The article describes a method for correcting the magnetic field for a superconducting undulator with neutral poles, manufactured at the INP, as well as a mathematical apparatus that predicts the currents of the additional power supply for correcting the magnetic field. When correcting the field and orbit inside the undulator, the main windings of the undulator are used, grouped into separate groups and powered by additional currents. This correction scheme was tested, as well as a comparison of theoretical and experimental data of the measured magnetic field and calculated phase errors. In the SPECTRA program, the SR spectra were calculated before and after the correction.

ANALYTICAL CHARACTERISTICS OF PANORAMIC (SIMULTANEOUS) DETERMINATION OF ESSENTIAL ELEMENTS IN BIOLOGICAL MATRICES BY µXRF-SR #124

Submitted by **Andrey Darin**
For track: X-ray fluorescent analysis
Author: Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)
Co-authors:

- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)

Essential macronutrients include sodium, magnesium, phosphorus, sulfur, chlorine, potassium and calcium, which are present as cations in the barrier, homeostatic system of the cell. It is customary to refer to essential micronutrients those whose imbalance in the body reliably leads to any pathological condition: chromium, manganese, iron, cobalt, copper, zinc, selenium, molybdenum, iodine. Their biological significance in the organism of higher mammals, including humans, has now been firmly established, and the main biochemical processes in which they participate have been determined. Also, essential micronutrients should be added: vanadium, nickel, arsenic, bromine, the biological activity of which has been proven in studies on experimental animals. When using μXRF-SR in the study of biological samples, it is logical to choose the experimental conditions for the simultaneous determination of the maximum number of elements with optimal detection limits. Ten elements from vanadium (23) to bromine (35) have K-series excitation energies from 5.47 to 13.47 keV. The using excitation energies of 15-16 keV makes it possible to determine more than 10 micro and 5 macro essential elements in one dimension.

Based on the study of standard samples of the composition of the graphite collector of microimpurities (SOG-30 and SOG-37), the limits of detection of a number of essential elements in the biological matrix were determined.

This work was supported by RFBR grant No. 19-05-50046 (Micromir).

FORMATION AND ANALYSIS OF MULTILAYER CERMET FILMS OF HIGH-ENTROPY ALLOYS #125

Submitted by **Yuriy Akhmadeev**

For track: SR technological application and X-ray apparatus

Author: Yuriy H. Akhmadeev (HCEI SB RAS)

Co-authors:

- Yuriy F. Ivanov (HCEI SB RAS)
- Nikita A. Prokopenko (HCEI SB RAS)
- Vladimir V. Shugurov (HCEI SB RAS)
- Oleg S. Tolkachev (HCEI SB RAS)
- Elizaveta A. Petrikova (HCEI SB RAS)
- Maria S. Petyukevich (HCEI SB RAS)
- Olga V. Krysina (HCEI SB RAS)
- Alexander N. Shmakov (Budker INP)

In the last couple of decades, research in the field of methods for the formation and study of structures based on high-entropy alloys (HEA), both purely metallic and metal-ceramic, with improved physical and mechanical properties, has become widespread. One of the approaches to the formation of such structures is the use of plasma-assisted vacuum-arc deposition of thin films, which combines the simplicity of the formation process and makes it possible to obtain multi-element structures of equiatomic composition.

The aim of this work is to analyze the results obtained in the study of the elemental and phase composition, defect substructure, multilayer multielement ceramic-metal HEA films of AlTiCrNbMoN composition by X-ray diffraction analysis, transmission diffraction electron microscopy, and also by X-ray phase analysis using synchrotron radiation.

The studied HEAs were synthesized in the form of thin films formed as a result of the deposition of a multi-element metal plasma created by electric arc plasma-assisted sputtering of several cathodes of selected elements in a working nitrogen gas atmosphere on the KVINTA ion-plasma facility developed at the Laboratory of Plasma Emission Electronics of the HCEI SB RAS and which is part

of the UNU "UNIKUUM" complex, which is on the list of unique electrophysical installations in Russia (https://ckp-rf.ru/usu/434216/). The elemental and phase composition, defective substructure were studied using the following scientific diagnostic equipment: transmission diffractive electron microscope (JEOL JEM-2100 F); scanning electron microscope (Philips SEM-515 with EDAX ECON IV microanalyzer); X-ray diffractometer Shimadzu XRD 6000; synchrotron radiation source - electron storage VEPP-3, BINP SB RAS, high-temperature X-ray camera Anton Paar HTK-2000, position-sensitive single-coordinate detector OD-3M-350.

The possibility of controlling the elemental composition of the film by changing the discharge currents of arc evaporators is demonstrated. A regime has been revealed that makes it possible to deposit thin (several micrometers) metal-ceramic HEA films with an AlTiCrNbMoN elemental composition close to equiatomic. It is shown that the formed HEA films have a nanocrystalline structure with a crystallite size of (12-20) nm.

As a result of studies of multilayer ceramic-metal HEA coatings for heat resistance and heat resistance by X-ray phase analysis using synchrotron radiation, it was found that the coatings have a structure close to that of molybdenum. When heated in air, the decomposition of the system begins at a temperature of (630-640) °C. At temperatures (1070-1080) °C, new reflections appear, presumably related to oxide compounds of the alloy components. HEA reflections completely disappear at temperatures (1260-1270) °C.

The work was carried out with the financial support of the Russian Federation represented by the Ministry of Science and Higher Education (project no. 075-15-2021-1348) within the framework of activities no. 2.1.5, 2.1.17 and 2.1.20.

DEVELOPMENT OF A 540-DEGREE MAGNETIC BUNCHER BASED ON PERMANENT MAGNETS #126

Submitted by **Shamil Lachynov**
For track: THz radiation aplication
Author: Shamil Lachynov (Novosibirsk State University, Budker Institute of Nuclear Physics)
Co-author: Nikolay Vinokurov (Budker INP, Novosibirsk State University)

Obtaining high peak current short electron bunches is necessary for many technological and research purposes. At the same time, normalized emittance must be small enough. Such bunches can be obtained by the longitudinal compression of electron bunches of a less peak current. To overcome the Coulomb repulsion, the bunching should be done at relativistic energies in a special magnetic system with a strong dependence of the flight time on the energy of a particle, the so-called magnetic buncher. A few years ago an original scheme of such a device was proposed at BINP, but no further work has been done since then. The goal of the research is to develop and create a magnetic buncher for obtaining short and large-charge electron bunches. Magnetic system elements, two magnetic mirrors, have been designed and optimised during the work. The final tuning of the magnetic mirrors parameters during its tests is planned.

PROPERTIES OF COATINGS OF THE TIB/TIBN SYSTEM DEPOSITED BY THE VACUUM-ARC PLASMA-ASSISTED METHOD #127

Submitted by **Mikhail Savchuk**
For track: SR technological application and X-ray apparatus
Author: Mikhail Savchuk (Institute of High Current Electronics)
Co-authors:

- Vladimir Denisov (HCEI SB RAS)
- Yulia Denisova (Institute of High Current Electronics SB RAS)
- Andrey Leonov (Institute of High Current Electronics SB RAS)
- Alexander Shmakov (Budker INP)

In this paper, the physicomechanical and tribotechnical properties of multicomponent TiB/TiBN and TiCrB/TiCrBN coating systems are investigated to reduce the wear of the material surface. X-ray patterns were also obtained using a synchrotron scanning source.

Coating deposition is carried out by combining of method of ion-plasma nitriding and vacuum-arc plasma-assisted deposition of functional coatings. As a result of the experiments, the values of microhardness and nanohardness of the deposited coatings were obtained. Tribotechnical tests were also carried out.

ON THE FEATURES OF AN IMMISCIBLE AU-CO ALLOY OBTAINED BY MECHANICAL ALLOYING UNDER VARIOUS CONDITIONS USING SYNCHROTRON RADIATION #128

Submitted by **Timofey Tolmachev**
For track: X-ray structural analysis
Author: Timofey Tolmachev (Institute of Engineering Science, Ural Branch of the Russian Academy of Sciences (IES UB RAS))
Co-authors:

- Vitaliy Pilyugin (M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences)
- Alexey Ancharov (Institute of Solid State Chemistry and Mechanochemistry SB RAS)
- Alexander Patselov (M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences)
- Yulia Solov'eva (Tomsk State University of Architecture and Building)

Ultrafine grained Au-Co alloys immiscible at equilibrium were prepared by mechanical alloying via high-pressure torsion technique. A consolidated alloy is formed from the initial powder mixture of components of the system in an equiatom ratio after deformation at room and cryogenic temperatures and at 8 and 11 GPa. After alloying procedure, the synchrotron radiation diffractometry of the obtained samples was carried out. It was found that after deformation an fcc substitutional supersaturated solid solution formed. Changing the deformation temperature to cryogenic results to greater dissolution of Co. The pressure changing to more elevated value leads to more Co dissolution content of supersaturated solid solution at the same temperature regime. This result corresponds to the increased mechanical and physical properties of the Au-Co alloys after cryodeformation and increased pressure than after room one.

Diffraction experiments were performed at the SR beamline №4 of the VEPP-3 storage ring. The obtaining and processing of materials were carried out at the IMP UB RAS. The research was supported by RFBR (project No. 19-32-60039) and carried out in part within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme “Pressure” No. 122021000032-5).

MAGNETIZATION MEASUREMENT AND SORTING OF PERMANENT MAGNETS FOR THE NOVOFEL VARIABLE PERIOD UNDULATOR #129

Submitted by **Oleg Shevchenko**
For track: SR and FEL sources and centers
Authors:

- Yaroslav Gorbachev (Budker Institute of Nuclear Physics)
- Oleg Shevchenko (BINP)
- Nikolay Vinokurov (Budker INP, Novosibirsk State University)

The use of variable period undulators (VPU) makes it possible to significantly increase the FEL tuning range. For example, the VPU recently installed on the second track of the NovoFEL facility

increased the lasing wavelength range to 15–120 μm. A new undulator with variable period for the first FEL of our facility is currently being developed at BINP. One of the features of the new undulator is a large aperture required to reduce radiation losses at long wavelengths. The permanent magnets used in this undulator have a special C-shape and large dimensions. The shape was optimized to obtain maximum magnetic field amplitude on the undulator axis. To carry out the magnetization measurements and sorting of these magnets, a measuring stand was developed based on four series-connected coaxial coils. In this article, we specify the tolerance requirements for sorting of the magnets and present the first measurement results.

DESIGN AND SIMULATION RESULTS OF HELICAL UNDULATOR WITH VARIABLE PERIOD #130

Submitted by **Oleg Shevchenko**
For track: SR and FEL sources and centers
Authors:

- Oleg Shevchenko (BINP)
- Nikolay Vinokurov (Budker INP, Novosibirsk State University)

A new planar undulator with variable period and large aperture is currently being developed for the NovoFEL facility. A simple modification of its design makes it possible to obtain helical undulator field. The new undulator design, like the original one, can be easily scaled to smaller undulator periods, so it can be used in in X-ray undulators. In this article we present the results of magnetic field simulations for a novel design helical undulator with variable period. These results include the dependences of both the first and higher harmonics of the magnetic field on the undulator period.

MEASUREMENTS AND ESTIMATES OF THE BREMSSTRAHLUNG DOSE RATE AT CONTROL POINTS OF THE FEL ACCELERATOR HALL #131

Submitted **Tatiana Salikova**
For track: SR technological application and X-ray apparatus
Author: Tatiana Salikova (BINP)

The bremsstrahlung power during FEL operation in the generation mode reaches several kSv/h (kilosieverts per hour), which leads to the degradation of materials and the activation of a number of installation details. The paper presents calculations of bremsstrahlung levels at control points where beam losses are probable. These data are necessary to create protection for technological units, and to install dosimetric detectors to control beam losses on the walls of the vacuum chamber when correcting the trajectory of the electron beam orbit. At “accessible points” (if the accelerator designs allow the installation of a detector), relative dose rates were measured. The distributions of the bremsstrahlung dose rate were measured along the central axis of the accelerator hall in the operating modes of the first stage of the FEL (electron energy is 12 MeV) and the third stage of the FEL (E=40 MeV).

OBTAINING AND RESEARCHING MATERIALS FOR SUPPRESSING EXTERNAL VIBRATIONS IN THE RESPONSIBLE NODES OF SYNCHROTRON RADIATION ACCELERATORS #132

Submitted by **Fedor Gorbunov**
For track: SR and FEL sources and centers
Authors:

- Fedor Gorbunov

- Aleksandra Fadina (Institute of solid state chemistry and mechanochemistry of the Siberian branch of the Russian Academy of Sciences (ISSCM SB RAS))
- Boris Tolochko (Institute of solid state chemistry and mechanochemistry)

In this study, a method for modifying polyurethane with additives during synthesis is proposed and their structure, strength and elastic deformation are compared. Inorganic additives (modifiers) were introduced into the prepolymer in the form of aluminum oxide and silicon powders of a certain dispersion in an amount of up to 1 wt.%. The properties of the obtained composites (elongation, density, tensile strength, hardness, etc.) were studied:

- the tensile strength of the unmodified polymer is – 17.6 MPa;
- tensile strength of composites - from 19.8 to 24.2 MPa;
- elongation – from 650 to 798%.

Microstructural studies have determined the sizes of polymer grains:

- unmodified – 15 microns;
- modified – 3-5 microns.

Cyclic tests of composites according to GOST P ISO 10328 with a loading force of 50-1600N at a frequency of 2 Hz were carried out.

The work was carried out with the support of the Federal Target Program in accordance with Agreement No. 075-15-2021-1359 dated 13.10.2021 (Internal number 15.SIN.21.0015).

OPERANDO XRD STUDY OF MNOX-CEO2 CATALYST OF CO OXIDATION #133

Submitted by **Zakhar Vinokurov**

For track: X-ray structural analysis

Author: Zakhar Vinokurov (BIC SB RAS)

Co-authors:

- Olga Bulavchenko (Boreskov institute of catalysis SB RAS)
- Denis Mishchenko (Boreskov Institute of Catalysis SB RAS)
- Tatyana Afonasenko (CNCT BIC SB RAS)

In this study, the catalyst reduction in CO and hydrogen were performed to improve MnOx-CeO2 catalyst activity in the CO oxidation reaction. Catalyst activation by reduction/oxidation with gas is a widely used approach [1]. We used XRD and MS for the gas phase monitoring to get detailed information about phase composition and structure of catalyst after different treatments and how it affects catalytic activity in the reaction of CO oxidation.

Mn03Ce07_600 oxide catalyst (molar ratio Mn:Ce = 3:7) was synthesized by coprecipitation of nitrates and further calcination at 600 °C for 4 h, similarly as described elsewhere [2]. Catalyst treatment steps included sequentially: 1, 3, 5 - study of the sample during stepwise heating/cooling in a mixture of 1%CO + 2%O2 to 200 °C (temperatures 150-175-200-175-150 with exposure for 2 hours at each temperature); 2 - reduction of the sample in a mixture of 10% CO at 400 °C for 2 hours; 4 - reduction of the sample in a mixture of 10% H2 at 400 °C for 2 hours.

According to X-ray diffraction, the initial Mn03Ce07_600 sample included only the Ce0.7Mn0.3O1.73 fluorite phase (based on CeO2 lattice PDF #34-394, sp. gr. Fm(-)3m , a = 5.41134). The study of the sample without pretreatment in the CO oxidation reaction (step #1) showed that the catalytic activity increases with time, and this increase accelerates with temperature. No features were observed during stepwise cooling in, however, the CO conversion rates at each of the temperatures exceeded the values obtained during initial heating. Phase separation of the solid solution after the reaction was not observed, however, the simulation showed a slight decrease in the lattice parameter and a change in the oxygen composition of fluorite, which may indicate a change in the oxidation state of manganese. The reduction of the sample in a mixture of 10% CO (step #2) resulted in the manganese segregation from the solid solution and the formation of the MnO phase (PDF #65-638, sp. gr. Fm(-)3m, a = 4.538) . Simultaneously with the appearance of the manganese

(II) oxide phase, a jump in the lattice parameter of the fluorite phase by more than 0.2% and a decrease in the value of microstrains by a factor of 1.5 were observed. Re-examination of the system during CO oxidation (step #3) showed a gradual decrease of MnO reflections with temperature. The most probable reason is the transition of MnO to other phases of manganese oxides in a more dispersed state, for example, Mn2O3 or Mn3O4, since the parameters of the fluorite phase do not show the reverse introduction of manganese into solid solution. The CO conversion values differ insignificantly, the largest difference is observed for a temperature of 150°C, which is most likely due to manganese in the composition of the MnO phase. Reduction in 10% H2 (step #4) showed similar results, with slightly less catalytic activity in the CO oxidation reaction (step #5). Summarizing the data obtained, it can be noted that the reduction treatment of the Mn03Ce07_600 catalyst leads to segregation of the solid solution with the fluorite structure and the appearance of dispersed manganese oxides, which in turn slightly increases the catalytic activity.

[1] Craciun, R., et al., Structure and redox properties of MnOx/Yttrium-stabilized zirconia (YSZ) catalyst and its used in CO and CH4 oxidation. Applied Catalysis A: General, 2003. 243(1): p. 67-79.

[2] Bulavchenko, O.A., et al., Reduction of mixed Mn-Zr oxides: In situ XPS and XRD studies. Dalton Transactions, 2015. 44(35): p. 15499-15507.

ELECTRONIC STRUCTURE WITH SB SUBSTITUTION IN TOPOLOGICAL INSULATORS MNBI2-XSBXTE4 USING SYNCHROTRON RADIATION #134

Submitted by **Igor Arkhandeev**

For track: X-ray spectroscopy

Authors:

- I. A. Arkhandeev (M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences)
- V.A. Golyashov (A.V. Rzhanov Institute of Semiconductor Physics, Novosibirsk)
- K. A. Kokh (V.S. Sobolev Institute of Geology and Mineralogy, Novosibirsk)
- O.E. Tereshchenko (A.V. Rzhanov Institute of Semiconductor Physics, Novosibirsk)
- E.I. Patrakov (M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences)
- T.V. Kuznetsova (M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences)

Topological insulators (TI) are of particular interest in recent solid state studies because of their exotic properties due to conductive, topologically protected surface states. In this paper, we report on the topological nature of the MnBi2-xSbxTe4 layered compound. The characterization of the samples will be shown using scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), as well as Raman spectroscopy. The study of the electronic structure was carried out by angle-resolved photoemission spectroscopy (ARPES). The ARPES experiments were performed at the Bloch beamline at the MAX IV laboratory (Sweden). ARPES data shows the presence of a Dirac cone. In this work we will show experimental studies of left and right circularly polarized light to topological surface states. The presence of a magnetic impurity shifted the position of the Dirac point relative to related compounds MB2T4: M = transition metal or rare earth element, B = Bi or Sb, T = Te, Se, or S. It should be noted that manganese doping has changed the atomic structure, moving from a five-layer system (quintuple layer) to a seven-layer one (septuple layer).

POTENTIAL TRACE OF THE PAEKTUSAN VOLCANO ERUPTION IN THE DATED LAYER OF THE BOTTOM SEDIMENTS OF LAKE BELE ACCORDING TO THE SCANNING μXRF-SR DATA #135

Submitted by **Andrey Darin**
For track: X-ray fluorescent analysis
Author: Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)
Co-authors:

- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Denis Rogozin (FRC «KSC SB RA»)

On the border of China and North Korea is the only active stratovolcano in the eastern part of Asia - Paektusan (other names - Baitoushan, Changbaishan). The volcano is widely known for one of the largest eruptions in the historical era, which occurred in the 10th century AD. On the volcanic activity scale (VEI), the event is rated at seven points - the largest eruption in the last millennium. Modern research shows that the eruption of the Paektusan volcano occurred in the late autumn - winter of 946 AD. This dating is supported by data obtained from the study of an ice core from North Greenland, in which traces of volcanic ash were found dating back to 947 AD.

We have studied a core sample of varves (annual layering) bottom sediments of Lake Bele (Khakassia). At a depth of 860 mm (the age according to the calculation of annual layers is 945 AD ± 30 years), a layer 2-3 mm thick was found, which differs sharply in color and texture from the rest of the core material. A thin section containing an anomalous layer was studied using a confocal X-ray microscopy. 2D scanning with 20 μm focused SR beam was carried out. A large amount of microparticles with a high content of zirconium, yttrium, and niobium was found inside the layer. The possibility of finding traces of the eruption of the Paektusan volcano is discussed.

This work was supported by RFBR grant No. 19-05-50046 (Micromir).

CURRENT STATUS OF EXAFS STATION OF SSTRC. USING XAFS SPECTROSCOPY FOR THE STUDY OF NANOMATERIALS OF COMPLEX COMPOSITION #136

Submitted by **Vladimir Kriventsov**
For track: X-ray spectroscopy
Author: Vladimir Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)

In the presented report, using the example of the work performed at the EXAFS spectroscopy station of the Siberian Synchrotron and Terahertz Radiation Center (Novosibirsk), the possibilities of the XAFS method are shown, the hardware and methodological features, methods of processing experimental data and analyzing the obtained structural information are considered. It is well known that the development of synchrotron radiation sources in the last third of the 20th century led to significant progress in the application of methods implemented in SR, such as XAFS (XANES/EXAFS) spectroscopy for research in various fields of science: materials science, solid state physics and chemistry, chemical technology, geochemistry, catalysis, inorganic and organoelement chemistry. The XAFS (XANES/EXAFS) spectroscopy method is a powerful tool for studying the state of elements and the local structure of various systems in any aggregate states: alloys, dispersed systems, solutions, ultra-diluted systems, glasses, etc. Nowadays, various methodological variants of the XAFS method have been implemented and are being successfully developed in Synchrotron Radiation Centers both abroad and in Russia - KISI-Kurchatov (Moscow) and SSTRC (Novosibirsk). It should be noted that the XAFS spectroscopy method is most effective in the study of nanoscale systems of “complex” composition, with a characteristic size of less than 10 nm and a low content of the element under study, when the use of other structural methods is not informative and obviously

problematic. The report demonstrates the capabilities of XAFS spectroscopy for a wide range of different types of nanoscale and nanostructured systems, both as an independent method and in combination with other physical research methods – XRF SR, XRD, HRTEM, XPS, SEM, etc. The prospects of the integrated approach used for the study of various functional nanomaterials of complex composition are demonstrated: nanostructured systems for storing actinoids; nanoalloys with improved characteristics, including modified with nanoscale oxide additives; model encapsulated ordered/disordered nanostructures; biological nanomaterials; low-percentage nanocomposite catalysts; test geological samples of complex composition; thin metal and semiconductor films, etc. As a result of the performed studies, new reliable information was obtained on the averaged atomic structure, elemental and phase compositions, charge states, and local structure for the studied systems. The data obtained by various methods are in good agreement with each other. This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Agreement No. 075-15-2022-263). The experiments were performed using large-scale research facilities "EXAFS spectroscopy beamline". SR investigations were done at the shared research center SSTRC on the basis of the Novosibirsk VEPP-4-VEPP-2000 complex at BINP SB RAS.

PROJECT OF DIFFRACTION-BASED METHODS FOR MEASURING MECHANICAL STRAINS AND STRESSES IN POLYCRYSTALLINE TUNGSTEN AFFECTED BY PULSED HEAT LOAD AT THE SCATTERING STATION “PLASMA” #137

Submitted by **Sergey Kazantsev**
For track: X-ray structural analysis
Authors:

- Sergey Kazantsev (Budker Institute of Nuclear Physics)
- Konstantin Kuper (Budker INP SB RAS, SRF "SKIF")
- Aleksey Arakcheev (Budker INP)

The problem of mechanical destruction of tungsten divertor plates in tokamaks affected by thermal and plasma flows is well known. One of the methods proposed for studying this problem is the X-ray diffractometry method. The essence of the method is to measure the dynamics of the diffraction pattern from a tungsten sample affected by thermal irradiation, and to restore the dynamics of strains and stresses in the sample from the obtained data.

At the shared research center SSTRC on the basis of the VEPP-4 – VEPP-2000 complex at BINP SB RAS, the SR scattering station "Plasma" is operated, This station was designed to study the deformation of materials under the action of pulsed heat load. First results were obtained by measuring the dynamics of diffraction from single-crystal samples. and deconvolution of the distribution of stresses was done. The next stage of work is the observation and measurement of diffraction from polycrystalline tungsten. The results of the first experiments on the measurement of diffraction from polycrystalline samples showed that for these experiments it is necessary to use a monochromator on the initial SR beam, which, coupled with a small number of crystallites that satisfy the constructive interference condition (Bragg condition), resulted in a strong drop in the intensity of the diffraction peak. A limitation on the variation of the experimental parameters which is in need to increase the diffraction intensity is the dependence of the change in the scattering angle, due to the presence of deformation due to thermal irradiation, on the same parameters. As part of solving this problem, it was proposed to use W/Si multilayer X-ray mirrors as a source of monochromatization.

The proposed project of a new experiment allows to obtain a temporal resolution in measuring the stress dynamics on a polycrystalline sample during pulsed heating and cooling better than 1 ms, which is sufficient to study pulsed processes during heating with parameters expected in modern fusion facilities.

AN ATTEMPT OF DETERMINATION OF CYCLICAL CONSTITUENTS IN THE SPATIAL DISTRIBUTIONS OF AU BY THE SCANNING MICRO-XRF TECHNIQUE WITHIN THE SUB-SURFACE INNER LAYER OF THE PREPARED MOUSE MIND'S SAMPLE #138

Submitted by **Dmitry Sorokoletov**

For tracks: SR for medicine and biology application, X-ray fluorescent analysis

Authors:

- Iakov Rakshun (Budker Institute of Nuclear Physics)
- Dmitry Sorokoletov (Budker Institute of Nuclear Physics SB RAS)
- Fedor Darin (Budker Institute of Nuclear Physics SB RAS)

Many biochemical processes in organisms enact cyclically (daily, hourly, and by others periods). In addition to different methods for tracking and exploring their footprints the Micro-XRF technique is to be used in some cases. An effective approaches based on the Micro-XRF technique are still being developed [1]. We have attempted to analyze the distribution of the local mass concentration of Au along two neighboring scanning lines within the sub-surface inner layer of the prepared mouse mind's sample. We used scanning micro-XRF technique [2] in two experimental schemes: with one and two x-ray polycapillary lenses (in confocal combination) for comparison.Initially it was well known that mass concentration of Au (from 0 to 2 ppm) is several times less than its limit of determination [2] for each single spatial position along scanning lines. However by applying the DFT and EMT (HHT) analysis [1] to the whole resulting one-dimensional signals of Au distribution a series of their cyclical constituents (from 1 to 3) may be restored steady. The least square method and the two-sided Kolmogorov-Smirnov statistical criteria were used in order to confirm this assumption and to determinate the tolerance intervals of all parameters of the proposed model.

The work have been carried out in the framework of RFBR project no. 19-05-50046. The work was done at the shared research center SSTRC (on the basis of the VEPP-3M/VEPP-4 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022).

[1] D. Sorokoletov, M. Chernetskaja, Ia. Rakshun, and F. Darin. An Attempt of Quantitative Analysis of Cyclical Constituents in Structure of Scanning Microfluorescence Signal from Human Hair. // AIP Conference Proceedings. In issue "Synchrotron and Free Electron Laser Radiation: Generation and Application, SFR-2020", 2020. P. 070008.

[2] A. V. Darin, Ya. V. Rakshun. A method of measurement during x-ray fluorescence analysis using x-ray concentrating optics (polycapillary lenses) (in Russian). // Nauchnyj vestnik novosibirskogo gosudarstvennogo tehnicheskogo universiteta. N2 (51) 2013. P.119-129.

ИССЛЕДОВАНИЕ УСЛОВИЙ ФОРМИРОВАНИЯ A2-ФАЗЫ В МЕХАНОКОМПОЗИТАХ СИСТЕМЫ TI-AL МЕТОДАМИ СИНХРОТРОННОГО ИЗЛУЧЕНИЯ #139

Submitted by **Alexey Sobachkin**

For track: X-ray structural analysis

Authors:

- Алексей Собачкин (АлтГТУ им. И. И. Ползунова, Барнаул)
- Александр Ситников (АлтГТУ им. И. И. Ползунова, Барнаул)
- Марина Логинова (АлтГТУ им. И. И. Ползунова, Барнаул)
- Владимир Яковлев (АлтГТУ им. И. И. Ползунова, Барнаул)
- Валерий Филимонов (АлтГТУ им. И. И. Ползунова, Барнаул)
- Алексей Негодяев (АлтГТУ им. И. И. Ползунова, Барнаул)
- Андрей Мясников (АлтГТУ им. И. И. Ползунова, Барнаул; Институт химии твердого тела и механохимии СО РАН)
- Марат Шарафутдинов (Институт химии твердого тела и механохимии СО РАН; ЦКП «СКИФ», Институт катализа им. Г.К. Борескова СО РАН)

В работе проведено in situ синхротронные исследования динамики фазообразования в механически активированной порошковой смеси Ti + Al (16 мас.%) при реализации высокотемпературного синтеза в условиях объемного воспламенения методом индукционного нагрева. Индукционный нагрев производился с помощью экспериментальной установки (VUS ver.1), разработанной для работы под пучком синхротронного излучения. Установка VUS ver.1 имеет возможность производить индукционный нагрев образца под вакуумом и позволяет разогревать образец до 1500 ºС. Исследование проводилось в Институте ядерной физики СО РАН им. Будкера (Россия, г. Новосибирск) на станции 5b «Дифракционное кино» накопителя электронов ВЭПП-3.

Объектом исследования были предварительно рассеянные порошки алюминия ПА размером частиц 50±10 мкм и титана ПТМ размером 50±10 мкм.

Экспериментально исследовано влияние времени механоактивационной обработки исходной смеси (1, 3, 7 мин.) на макрокинетические параметры синтеза. Для всех режимов механоактивации установлено, что образование как устойчивых соединений (Ti3Al, TiAl3, TiAl2, TiAl), так и метастабильных фаз (Ti9Al23, Ti5Al11, Ti2Al5, Ti3Al5) происходит на этапе первичного структурообразования, до выхода системы на тепловой взрыв. При синтезе порошковой смеси, механоактивированной в течение 7 мин., уже при 40 ºС наблюдается формирования соединений (Ti2Al5 и Ti5Al11). Также для всех режимов механоактивации высокотемпературный синтез смеси исследуемого состава проходит без образования жидкой фазы, в режиме твердофазного горения, что свидетельствует о новых механизмах диффузии и массопереноса в твердофазном горении механоактивированных структур. Увеличение времени предварительной механоактивационной обработки смеси состава Ti + Al (16 мас.%) приводит к изменению термических параметров горения: снижаются время и температура начала реагирования компонентов, для 1 мин. механоактивации с энергонапряженностью 40 g температура начала нагрева смеси составляет 603 °C, для 3 мин. механоактивации – 442 °C, для 7 мин. механоактивации – 359 °C. Максимальная температура горения составляет: для 1 мин. механоактивации – 1080 °C, для 3 мин. механоактивации – 1003 °C, для 7 мин. механоактивации – 820 °C.

Для режимов механоактивации 1 и 3 минуты с энергонапряженностью 40 g к моменту окончания реакции синтезируется многофазный продукт, состоящий из TiAl3, Ti3Al и TiAl2. Основное соединение TiAl3. Для 1 мин. механоактивации по данным количественного расчета содержание TiAl3 составляет 50 %, для 3 мин. механоактивации содержание TiAl3 составляет 60 %. Предварительная механоактивация в течение 7 мин. способствует формированию продукта с доминирующим содержанием интерметаллидного соединения Ti3Al, составляющим 68 %. Также зафиксировано присутствие TiAl2 – 26 % и TiAl3 – 6 %.

Работа проводилась в рамках государственного Задания № FZMM-2020-0002.

STRUCTURE STUDY OF IRON-SUBSTITUTED HYDROXYAPATITE BY SPECTROSCOPIC METHODS #140

Submitted by **Denis Isaev**

For track: X-ray spectroscopy

Authors:

- D. Isaev (Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk State University, Institute of Mathematical Problems of Biology - FRC Keldysh IAM RAS)
- V. Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)
- N. Bulina (Institute of Solid State Chemistry and Mechanochemistry SB RAS, Institute of Mathematical Problems of Biology - FRC Keldysh IAM RAS)
- V. Bystrov (Institute of Mathematical Problems of Biology - FRC Keldysh IAM RAS)

Stoichiometric hydroxyapatite (HAp) is a calcium phosphate biomineral compound of the Ca10(PO4)6(OH)2 composition. The chemical and structural similarity with the mineral composition of bones and tooth enamel allows the use of powdered and sintered HAp-based ceramic materials for medical applications. Biocompatibility and controlled bioresorption make HAp safe for the body. And the modified stoichiometry, cationic and anionic substitutions give HAp materials useful functional properties for dentistry and orthopaedics. HAp doped with iron ions (Fe-HAp) exhibits magnetic properties used in biomedicine for heating mediators in hyperthermic cancer therapy, as an MRI contrast agent. Also, HAP with iron ions demonstrates antibacterial properties, stimulates metabolism, and shows adsorption properties [1].

In this study, HAp samples with calcium ion substitutions for iron ions were synthesised in the planetary ball mill AGO-2. Iron (II) orthophosphate octahydrate and iron (III) orthophosphate dihydrate were used as sources of iron ions. The mechanochemical treatment of the reaction mixtures was carried out for 40 min at a drum speed of 1800 rpm. The obtained powder materials have been attestation by powder X-ray diffractometry (PXRD), Fourier vibrational infrared spectroscopy (FTIR), synchrotron thermal analysis (STA). The local structure of Fe-HAp has been studied by X-ray Absorption Fine Structure spectroscopy (XAFS) on synchrotron radiation (Fe-K edge, 7112 eV) and Mössbauer Spectroscopy (57Fe isotope).

The results of the attestation show that the synthesis reactions were successful and that the iron ions were localised in the HAp structure. Partial substitutions of the phosphate tetrahedron by the carbonate group are formed in the samples with superstoichiometric cation ratios. Results of XAFS-spectroscopy and Mössbauer spectroscopy presented data on the change in the charge state of iron ions from 2+ to 3+ from precursor compounds during synthesis. From the data obtained, the structure of the synthesised samples was clarified. Thus, iron ions in predominantly 3+ charge state occupy calcium positions and do not intrude into the hydroxyl sites. The obtained samples are characterized by the formation of non-stoichiometric defects localized as oxygen vacancies in the hydroxyl sites. The formation of these defects has been discussed in calculations using density functional theory methods [2]. The vacancy structure induces a lattice relaxation transition from hydroxyapatite to oxyhydroxyapatite.

The authors special thanks to Dr. Igor Yu. Prosanov, Dr. Konstantin B. Gerasimov, Mrs. Olga B. Vinokurova. The authors declare no competing interests.

The work was carried out with the financial support from the Russian Science Foundation (Project No. 21-12-00251) and within the framework of the “2030 Priority” of the Ministry of Science and Higher Education of the Russian Federation Program.

XAFS investigations were done at the shared research center SSTRC on the basis of the Novosibirsk VEPP-4-VEPP-2000 complex at BINP SB RAS.

[1] Tite T. et al. Cationic substitutions in hydroxyapatite: Current status of the derived biofunctional effects and their in vitro interrogation methods // Materials. – 2018. – Vol. 11. – No. 11. – P. 2081.
[2] Avakyan L. et al. Iron in Hydroxyapatite: Interstitial or Substitution Sites? // Nanomaterials. – 2021. – Vol. 11. – No. 11. – P. 2978.

FEATURES OF XANES Cl K- AND X-RAY EMISSION Cl Kβ SPECTRA OF {OsCl6}2- COMPOUNDS WITH A STRONG SPIN-ORBIT INTERACTION DEPENDING ON THE STRUCTURE OF CATIONS #141

Submitted by **Anastasiya Fedorenko**
For track: X-ray spectroscopy
Author: Anastasiya Fedorenko (NIIC SB RAS)
Co-authors:

- Igor Asanov (Nikolaev Institute of Inorganic Chemistry)
- Tatyana Asanova (Institute of Inorganic Chemistry)
- Anton Nikolenko (Budker INP SB RAS, SRF "SKIF")

Complexes with a strong spin-orbit interaction have attracted much attention in recent years due to their electrical and magnetic properties, such as superconductivity, magnetic ordering at high temperatures, anomalous and spin Hall effects, and the Rashba effect. The complexes (NH4)2[OsCl6], [M(NH3)4][OsCl6] (M = Pd, Pt) and [Co(NH3)5Cl][OsCl6] were studied to estimate the effect of spin-orbit interactions on the electronic structure and magnetic properties. The octahedral anions {OsCl6}2- are isolated centers and therefore do not participate in the superexchange interaction, which made it possible to study the correlations between the structure and spin-orbit interaction. OsCl3 and OsCl4 compounds were also studied, in which Os-Cl-Os bridging bonds are formed, which leads to the appearance of exchange interactions.

X-ray emission spectroscopy and X-ray absorption spectroscopy are sensitive methods to study changes in the electronic structure. The XANES Cl K- and X-ray emission Cl Kβ spectra of the complexes (NH4)2[OsCl6], [M(NH3)4][OsCl6] (M = Pd, Pt) and [Co(NH3)5Cl][OsCl6] and chain compounds OsCl3 and OsCl4 were obtained. Quantum-chemical calculations were carried out using the multiconfigurational CASSCF method to interpret the obtained spectra. The combined use of experimental X-ray and theoretical methods made it possible to determine the magnitude of the spin-orbit interaction depending on the cation substitution and to estimate the influence of the parameters of the electronic structure (crystal field and interelectron repulsion, spin-orbit interaction constants) on the magnetic properties and the structure of X-ray spectra.

The work was supported by the Russian Science Foundation (project 22-22-00683).

SPECTROSCOPIC AND CORROSION STUDIES OF THE TITANIUM LAYERS OBTAINED BY NON-VACUUM ELECTRON-BEAM ALLOYING FOR CHEMICAL REACTOR MATERIALS APPLICATION #142

Submitted by **Denis Isaev**
For track: X-ray spectroscopy
Authors:

- Denis Isaev (Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk State University)
- Vladimir Kriventsov (Boreskov Institute of Catalysis of SB RAS, Budker Institute of Nuclear Physics of SB RAS)
- Dmitry Volkov (Novosibirsk State Technical University)
- Eugeny Domarov (Budker Institute of Nuclear Physics SB RAS)

Structural perfection and corrosion resistance are important parameters for structural alloys for the nuclear and chemical industries. Steels such as corrosion-resistant alloys are in some cases inferior to titanium-based alloys, e.g., under conditions of boiling oxidising acid solutions. These aggressive conditions are necessary for the extraction processes in PUREX reprocessing of spent nuclear fuel from nuclear power plants. Research on the structure of resistant alloys and corrosion processes will make it possible to develop recommendations to produce special purpose alloys. This study is investigating tantalum-, zirconium- and molybdenum- electron-beam alloying titanium layers with treatment in a boiling solution of concentrated nitric acid.

Surface alloying of titanium (based on VT1-0 alloy) was carried out by electron-beam surfacing technology in the air atmosphere, in one and two passes of the beam over the layers of powder mounds. The focused electron beam was generated by an industrial electron accelerator ELV-6M (Stand UNU ELV-6, Budker INP SB RAS). Powders of titanium (99.7 %), tantalum (99.9 %), zirconium (99.8 %), molybdenum (99.9 %). Fluxes from a mixture of CaF2 and LiF were added to the bulk compositions to reduce the influence of air oxygen in the surfacing process. The modes and concentrations in the fluxes for alloying were based on the results of the Dr. Vitaly V. Samoilenko PhD Thesis.

The resulting alloyed titanium layers were examined using a variety of methods. The samples were cut and mechanically prepared for metallographic and corrosion testing. The samples were

attestation by X-ray powder diffraction, optical microscopy, scanning electron microscopy and EDX spectroscopy, durometric studies. The state and local structure of the alloys were investigated by X-ray Absorption Fine Structure spectroscopy (XAFS) on EXAFS station (SSTRC, Novosibirsk) and X-ray Photoelectron Spectroscopy (XPS) on SPECS (FRC BIC SB RAS). The obtained samples of alloyed layers were subjected to aging by boiling concentrated nitric acid for 10 h and 48 h.

The attestation of the samples confirmed the fact of non-equilibrium processes in the conditions of alloy formation under the action of the electron beam. Studies have provided data on chemical composition, microstructure and morphology of the layers, microhardness, disordered local structure, composition of passive films formed during corrosion tests, data on corrosion resistance. The assumption of the influence of disorder and defectiveness of beta-stabilized structures on reduction of corrosion resistance of the received materials is put forward.

The authors special thanks to Dr. Michael G. Golkovsky, Dr. Natalia V. Bulina, Dr. Igor P. Prosvirin, Dr. Vitaly V. Samoilenko. The authors declare no competing interests.

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (Agreement No. 075-15-2022-263).

The experiments were performed using large-scale research facilities "EXAFS spectroscopy beamline". SR investigations were done at the shared research center SSTRC on the basis of the Novosibirsk VEPP-4-VEPP-2000 complex at BINP SB RAS.

25 YEARS OF X-RAY REFRACTIVE OPTICS DEVELOPMENT - NEW OPPORTUNITIES FOR COHERENCE RELATED APPLICATIONS #143

Submitted by **Anatolu Snigirev**
For track: SR technological application and X-ray apparatus
Author: Anatoly Snigirev (Immanuel Kant Baltic Federal University)

The global trend towards the transition of modern accelerator X-ray sources to diffraction-limited synchrotrons (MAX IV, ESRF-EBS, PETRA-IV) and extremely brilliant Free Electron Lasers, provides great opportunities for coherent applications. It also poses significant challenges to the development of optical elements adapted to these sources. Knowing that highly coherent X-ray radiation easily interacts on its way with various imperfections of optical elements and spoils transmitted wavefront with aberrations, X-ray optics have to preserve unique radiation properties and also be capable of performing such functions as beam transport, nano-focusing, phase-contrast imaging, and microscopy.

Compound refractive lenses (CRLs, [1]) have become one of the main tools at modern X-ray beamlines because of their reduced sensitivity to shape errors, overall ease of use, and versatility. Being in-line optics, in addition to traditional micro-focusing applications, the refractive optics can provide the various beam conditioning functions in the energy range from 3 to 200 keV such as condensers, micro-radian collimators, low-band pass filters [2], high harmonics rejecters [3], and beam-shaping elements [4-5]. The implementation of CRL's for the beam transport concept will significantly simplify the layout of most existing and newly constructed beamlines, easily expanding their imaging and microscopy capabilities in different fields including biomedical science [6-7] and material research under extreme conditions [8-10].

The unique properties of refractive optics for beam conditioning allow the development and implementation of novel X-ray coherence-related techniques including Fourier optics [11-12] and interferometry [13-18]. The development of X-ray bright [19-21] and darkfield microscopy [22] will benefit by proposed polymer microlenses made by 3D printing, which can be used as light and ultracompact objectives [23-24].

All mentioned achievements and applications based on refractive optics are becoming especially relevant for so-called green-field synchrotrons, which are being built in Russia - SKIF in Novosibirsk and ISSI-4 in Protvino (Moscow region). Taking advantage of reduced horizontal source size, the refractive optics can be integrated into the front-end to transfer the photon beam without

losses from the source directly to the end stations. In this regard, the development of diamond refractive optics is crucial [25-30]. Recently it was demonstrated that ion-beam lithography can be applied to the fabrication of refractive diamond X-ray micro-lenses that are of interest to the field of high-resolution X-ray focusing and microscopy [31].

References

[1] A. Snigirev, et al, Nature, 384 (1996) 49.
[2] G.B.M. Vaughan, et al, J. Synchrotron Rad., 18 (2011) 125.
[3] M. Polikarpov, et al, J. Synchrotron Rad., 21 (2014) 484.
[4] D. Zverev, et al, Opt. Express, 25 (2017) 28469.
[5] D. Zverev et al., Optics Express, 29 (2021) 35038- 35053.
[6] M. W. Bowler, et al, J. Synchrotron Rad., 22 (2015) 1540.
[7] M. Polikarpov, et al, Acta Cryst. , D75 (2019) 947-958.
[8] N. Dubrovinskaia, et al, Sci. Adv., 2 (2016) e1600341.
[9] F. Wilhelm, et al, High Pressure Research, 36 (2016) 445.
[10] A. Snigirev et al., Microsc. Microanal. 24 (Suppl. 2) (2018) 236.
[11] P. Ershov, et al, Appl. Cryst., 46 (2013) 1475.
[12] D. V. Byelov, et al, RSC Advances, 3 (2013) 15670
[13] A. Snigirev, et al, Phys. Rev. Lett., 103 (2009) 064801.
[14] A. Snigirev, et al, Opt. express, 22 (2014) 25842.
[15] M. Lyubomirskiy, et ai, Optics express, 24 (2016) 13679.
[16] M. Lyubomirskiy, et al, J. Synchrotron Rad., 23 (2016) 1104.
[17] D. Zverev et al., Optics Express, 28 (2020) 21856-21868.
[18] S. Medvedeva et al, J. Synchrotron Rad., 26 (2019) 1572-1581.
[19] K. V. Falch, et al, Appl. Phys. Lett., 109 (2016) 054103.
[20] K. V. Falch, et al, J. .Mater. Sci., 52 (2017) 3437.
[21] K. V. Falch, et al, Ultramicroscopy, 184 (2018) 267.
[22] H. Simons, et al, Nature Communications, 6 (2015) 6098.
[23] A. K. Petrov, et al, Opt. Express, 25 (2017) 14173.
[24] A. Barannikov, et al., J. Synchrotron Rad., Rad., 26, 714-719, 2019.
[25] M. Polikarpov, et al, J. Synchrotron Rad., 22 (2015) 23.
[26] S. Terentyev, et al, Appl. Phys. Let., 107 (2015) 111108.
[27] M. Polikarpov, et al, AIP Conf. Proceed., 1741 (2016) 040024.
[28] T. V. Kononenko et al., Appl. Phys. A, 122, 152- (2016)
[29] S. Terentyev, et al, J. Synchrotron Rad., 24 (2017) 103.
[30] I. Snigireva et al, SPIE, 11837 (2021) 1183703.
[31] P. Medvedskaya et al, Opt. Express, 28 (2020), 4773-4785.

COMPARISON OF DEEP UV AND X-RAY LITHOGRAPHY FOR X-RAY REFRACTIVE LENS MANUFACTURING #144

Submitted by **Elena Reznikova**
For track: SR technological application and X-ray apparatus
Author: Elena Reznikova (Budker INP SB RAS)
Co-authors:

- Vladimir Nazmov (BUdker Institute of Nuclear Physics)
- N. Govorov (NSU)

X-ray refractive lenses were developed for a hard X ray transmission microscope and a confocal X-ray microscopy module with a synchrotron beam use at photon energies 15-35 keV. The lenses are rows with large number of separate bi-concave parabolic elements with periodic spaces in order to cross perpendicularly 2 linear rows forming point focusing. The maximal raw length is 10 cm. The dens polymer material of the X-ray refractive lenses is created during deep UV or X-ray lithography

processes with SU-8 negative photoresist or its analogue mr-X. It is a multi-element composition based on the monomer of diglycidyl ether of bisphenol-A novolack with small amounts of elements of a photo-acid generator, for example: C : O : H : Sb : F : S = 72.3 : 18.2 : 6.9 : 0.9 : 1.2 : 0.6. At 25 keV photon energy, the real and imaginary parts of the refractive index decrement of the SU-8 polymer are equal to 4.32E-7 and 2.61E-10, respectively. We control the current element compositions of the material by means of X-ray fluorescence analysis using INCA X-act system with the HITACHI S 3400N tip II E-beam microscope.

It was found that threshold doses of UV and X-ray absorbed radiation, which were determined from the measured characteristic curves of the photoresists with variation of the exposures, are identical both deep UV and X-ray lithography when conditions of other lithographic processes (pre-bake, post-exposure-bake) are reproduced exactly the same. To calculate the parameters of UV exposures, the spectra of the hard photoresist layers with different thicknesses from 0.2 micrometers to 2 mm were recorded by means of UV-VIS 180-3400 Shimadzu spectrometer, and the spectral specific absorbance of the layers was determined. In this work, light-emitting diode (LED) irradiated on 385 nm or 405 nm was used as a point light source for the deep UV lithography. The photoresist layers are photoactive for the LED wavelengths showing the specific absorbance values in the range of 1/mm – 1/cm. The material transparency is necessary to provide the ratio for doses of the absorbed UV radiation at the top and at the bottom of the resist layers of 0.1 - 1 mm thicknesses closed to unity. Such the UV lithographic dose ratios are comparable with X-ray lithography dose conditions and result to small diffraction distortions with high aspect ratios in the resist layer depth.

In the paper, we describe the fabrication process and properties of the X-ray refractive linear lenses with vertical sidewalls of their elements made by and the deep UV lithography and X-ray lithography as well as the X-ray refractive lens microstructures, which satisfy the X-ray microscopy applications.

DESIGN OF UNDULATOR-BASED BEAMLINE FOR APPLICATIONS IN MATERIALS SCIENCE #145

Submitted by **Ivan Bataev**
For track: SR technological application and X-ray apparatus
Authors: Ivan Bataev (Novosibirsk State Technical University), M.V. Gorbachev, I.P. Dolbnya, A.M. Korskunsky, I.V. Malyshev, N.A. Mezentsev, A.V. Murzina, V.S. Naumkin, I.V. Rakshun, A.N. Skyarov, A. Trebushinin, Y.V. Khomyakov, V.A. Chernov, N.I. Chkhalo

In this study, we present a conceptual project of an undulator-based beamline designed for material science research. The beamline allows one to quickly switch between imaging and diffraction modes, as well as implement a number of additional techniques that are of interest to materials scientists, such as USAXS, XAFS, XRF, etc. The beamline allows to hold the position of the beam spot on the sample when switching between different methods, as well as in the process of energy scanning. The size of the spot on the sample can change from about 1 mm to 100 nm. We also present the positioning of the main optical elements of the beamline, the results of thermal calculations, the ray traicing simulation, and potential applications of the beamline.

МОДЕЛИРОВАНИЕ ПУЧКОВ КОГЕРЕНТНОГО И ЧАСТИЧНО КОГЕРЕНТНОГО СИНХРОТРОННОГО ИЗЛУЧЕНИЯ ПРИ ПРОХОЖДЕНИИ ЧЕРЕЗ ОПТИЧЕСКИЕ ЭЛЕМЕНТЫ #146

Submitted by **Yuri Khomyakov**
For track: SR technological application and X-ray apparatus
Author*:* Ю.В. Хомяков (Новосибирский государственный университет, Институт ядерной физики им. Г.И. Будкера СО РАН)
Co-authors:

- Т.П. Дзюбина (Новосибирский государственный технологический университет),
- Я.В. Ракшун (Сибирский государственный университет телекоммуникаций и информатики, Институт ядерной физики им. Г.И. Будкера СО РАН)

Низкий эмиттанс новых источников синхротронного излучения (СИ) способствует росту доли когерентных фотонов в генерируемых пучках. Это приводит к ужесточению требований на оптику экспериментальных станций. В частности, существенными становятся эффекты, обусловленные искажениями волнового фронта пучков излучения на оптических элементах. Это естественным образом приводит к необходимости использования волновых подходов при моделировании распространения когерентных и частично когерентных пучков. Соответственно, подходы, основанные на трассировке лучей (геометрическая оптика) перестают корректно описывать оптические явления.

С целью развития волновых подходов к расчётам пучков СИ нами был разработан программный код, использующий проекционный метод для моделирования прохождения пучков через составные преломляющие линзы, а также split-step метод для моделирования отражения пучков от рентгеновских зеркал. Кроме того, код позволяет описывать формирование пучков френелевскими зонными пластинками. Он учитывает поглощение в материалах линз и зеркал, шероховатости поверхностей и ошибки позиционирования и наклона, что делает его перспективным инструментом как для моделирования экспериментов, так и для разработки новых станций.

ACTIVITY IN XRD DIAGNOSTICS OF FUNCTIONAL MATERIALS AT SSTRC #147

Submitted by **Alexander Shmakov**

For track: X-ray structural analysis

Author: Alexander Shmakov (Boreskov Institute of Catalysis SD RAS)

The X-ray diffraction experiments on the studies of the structure, phase composition and phase transformation of functional materials such as catalysts, sorbents, ion conductors, coatings, etc. are performing at Beamlines No.2 and No.6 of VEPP-3 and No.8 of VEPP-4M electron storage rings at Siberian Synchrotron and Terahertz Radiation Centre. The Beamline No.2 is dedicated to high resolution X-ray powder diffraction and anomalous scattering experiments; the Beamline No.6 operates as X-ray diffractometer for In Situ and Operando studies, while the facility at Beamline No.8 provides high energy X-ray diffraction within the energy range 60-120 keV. The report comprises description of the experiments on the phase transformation of mixed oxides under supercritical reaction media, oxygen mobility in Ruddlesden-Popper phases, local structure of heterogeneous catalysts by means of Total Scattering and Pair Distribution Functions technique, and so on. The attention is paid to development of XRD infrastructure for SKIF synchrotron facility.

The work is supported by budget project of SRF “SKIF”.

SYNCHROTRON RADIATION STATION ON THE VEPP-4M FOR PRACTICAL TRAINING #148

Submitted by **Boris Goldenberg**

For track: SR technological application and X-ray apparatus

Author: Boris Goldenberg (Budker INP SB RAS, SRF “SKIF”)
Co-authors:
- Ivan Gusev (BINP SB RAS)
- Yan Zubavichus (SRF «SKIF»)

The special synchrotron radiation technological station was built at the beamline #1 of VEPP-4M storage ring. Its purpose is practical training university students in synchrotron research

techniques and equipment testing. Novosibirsk universities students participate in the establishment and development of this station and it's methodic. The modular concept of the station allows its gradual introduction and implementation of various methods. This article describes the design of station, realized research methods and plan for upgrading of this facility.

The work was done at the shared research center SSTRC on the basis of the "VEPP-4 - VEPP-2000"complex at BINP SB RAS, with financial support by the Ministry of Science and Higher Education of the Russian Federation (Agreement No. 075-15-2022-263).

4TH GENERATION SYNCHROTRON RADIATION FACILITY SKIF: SCIENTIFIC PROGRAM AND FUNCTIONALITY OF THE FIRST-PHASE BEAMLINES #149

Submitted by **Yan Zubavichus**
For track: SR and FEL sources and centers
Author: Yan Zubavichus (SRF «SKIF»)
Co-authors:

- Konstantin Zolotarev (Budker INP SB RAS, SRF "SKIF")
- Eugeny Levichev (Budker INP SB RAS, SRF "SKIF")

Synchrotron Radiation Facility SKIF is a new large-scale research infrastructure project currently underway in Novosibirsk region in Russia. The 3 GeV electron storage ring designed by specialists from the Budker Institute of Nuclear Physics SB RAS will provide the record low emittance of 75 pm·rad by the date of its scheduled commissioning in December, 2024. At the first phase of the project implementation, the research infrastructure of the synchrotron radiation facility will include six beamlines dedicated to diverse techniques and X-ray spectral ranges:

1-1 «Microfocus» (5-47 keV);
1-2 «Structural diagnostics» (5-40 keV);
1-3 «Fast processes» (15-100 keV);
1-4 «XAFS spectroscopy and magnetic dichroism» (2.5-35 keV);
1-5 «Hard X-ray diagnostics» (25-200 keV);
1-6 «Electronic structure» (0.01-2 keV).

The storage ring will serve up to thirty beamlines in total, including 14 ID-based beamlines (3 wigglers and 11 undulators) and 16 beamlines utilizing light from bending magnets (both low-field and high-field ones). Key directions of the scientific program to be deployed at the SRF «SKIF» will encompass biomedicine, green technologies in chemistry and energetics, advanced engineering materials and mechanical engineering technologies. The present contribution surveys essential details of the SRF SKIF research program emphasizing functionality of the first-phase beamlines. Preliminary plans for the second-phase beamlines will be also outlined, including research-ducational beamlines of regional universities NSU and NSTU, structural virology beamline being developed by SRC VB VECTOR, etc.

This work was partially supported by the Ministry of Science and Higher Education of the Russian Federation within the budget project of SRF SKIF, Boreskov Institute of Catalysis, SB RAS.

КИЛОАМПЕРНЫЙ ЭЛЕКТРОННЫЙ ПУЧОК ЛИНЕЙНОГО ИНДУКЦИОННОГО УСКОРИТЕЛЯ – КАК ДРАЙВЕР ДЛЯ СУБМИЛЛИМЕТРОВОГО ЛСЭ #150

Submitted by **Evgeny Sandalov**
For track: THz radiation aplication
Authors:

- Evgeny Sandalov (Budker Institute of nuclear physics of SB RAS)

- Е.С. Сандалов, С.Л. Синицкий, Д А. Никифоров, А.В. Аржанников, Д. И. Сковородин (Институт ядерной физики им. Будкера СО РАН, Новосибирский государственный университет),
- В. А. Павлюченко (Институт ядерной физики им. Будкера СО РАН),
- Н.С. Гинзбург, Н.Ю. Песков, (Институт прикладной физики РАН, Нижний Новгород),
- Р. В. Протас, Д. Ю. Карасев (Российский федеральный ядерный центр — Всероссийский научно-исследовательский институт технической физики им. Забабахина, Снежинск)

В ИЯФ СО РАН совместно с ИПФ РАН был предложен проект субмиллиметрового лазера на свободных электронах (ЛСЭ) на базе релятивистского электронного пучка, генерируемого в линейном индукционном ускорителе (ЛИУ) [1]. Согласно нашему теоретическому анализу [1], электронный пучок, создаваемый в ЛИУ [2-4] (энергия E_e= 5 МэВ, ток I_b= 1−2 кА, нормализованный эмиттанс ε_n~1100 π·мм·мрад), является подходящим драйвером для генерации субГВт импульсов когерентного ЭМ-излучения в субмм диапазоне (0.3-1 ТГц). В качестве электродинамической системы такого ЛСЭ-генератора может быть использован двухзеркальный резонатор на основе сверхразмерных ($\emptyset < 50\lambda$) высокоселективных отражателей [5], либо структур Тальбо [6]. Применение таких структур позволяет обеспечить узкополосную генерацию ЭМ-излучения с $\Delta\omega/\omega \sim 10^{-4}$ при высоком электронном КПД (~5%). Для проведения экспериментов по генерации субмм излучения необходимо осуществить предварительное сжатие поперечного сечения пучка от его начального диаметра 4 см до размера менее 20λ (20 мм для 0.3 ТГц и 6 мм для 1 ТГц) в случае применения брэгговских отражателей. Для решения поставленной задачи нами была создана модель, с помощью которой рассчитаны сжатие пучка и его распространение в магнитном поле ЛСЭ, создаваемом однородным соленоидом и винтовым ондулятором. По результатам моделирования разработана конструкция магнитной системы сжатия пучка и раскачки поперечных колебаний его электронов. Успешные эксперименты по сжатию электронного пучка 5 МэВ/1 кА в прототипе системы компрессии пучка представлены в [7-8].

РНФ № 19-12-00212.

[1] A.V. Arzhannikov et al., “Powerful Long-Pulse THz-Band Bragg FEL Based On Linear Induction Accelerator”, IRMMW-THz. DOI: 10.1109/IRMMW-THz.2019.8874573

[2] E. S. Sandalov et al., "Electrodynamic System of the Linear Induction Accelerator Module," in IEEE TPS, vol. 49, no. 2, pp. 718-728, 2021, doi: 10.1109/TPS.2020.3045345.

[3] D. A. Nikiforov et al., “High-Current Electron-Beam Transport in the LIA-5 Linear Induction Accelerator”, Phys. Part. Nuclei Lett., Vol.17, no.2, pp.197-203, 2020.

[4] E. S. Sandalov et al., "Emittance Variation of a High-Current Relativistic Electron Beam in a Bend Magnet," in IEEE TPS, vol. 49, no. 9, pp. 2737-2749, 2021, doi: 10.1109/TPS.2021.3105661.

[5] N.S. Ginzburg et al., “Selective Strongly Oversized Resonators for Powerful Free-Electron Lasers Operating from Sub-THz to THz Band”, IRMMW-THz-2021, doi: 10.1109/IRMMW-THz50926.2021.9567057

[6] Y. Oparina et al., "Free-Electron Masers Based on Excitation of Talbot-Type Supermodes," IVEC, doi: 10.1109/IVEC51707.2021.9722561.

[7] D.A. Nikiforov et al., “Investigation of high current electron beam dynamics in linear induction accelerator for creation of a high-power THz radiation source”, JINST, vol.16, P11024, 2021

[8] Сандалов Е.С. и др., “Исследование поперечной неустойчивости сильноточного релятивистского электронного пучка в линейном индукционном ускорителе”, СФЖ, 2022;17(1):5-22. https://doi.org/10.25205/2541-9447-2022-17-1-5-22

X-RAY NATURAL CIRCULAR DICHROISM IMAGING OF MULTIFERROIC CRYSTALS #151

Submitted by **Mikhail Platunov**
For track: SR technological application and X-ray apparatus
Author: M. S. Platunov, (Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Akademgorodok 50/38, Krasnoyarsk, 660036, Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis SB RAS, Nikol'skiy Prospekt 1, Kol'tsovo, 630559)

The ***RE***$Fe_3(BO_3)_4$ compounds possess a huntite-type non-centrosymmetric trigonal structure that consists of helical chains of edge-sharing FeO_6 octahedra running along the *c*-axis of the crystal, interconnected by two kinds of BO_3 triangles and ***RE***O_6 distorted prisms. In the case of ***RE*** = Sm, the structure is described by the space group *R*32. Since the space group *R*32 is not centrosymmetric, there should exist two chiral atomic arrangements, left- and right-handed. In addition, the existence of inversion twins in these crystals can strongly affect electric polarization, i.e. the electric polarization can be suppressed by the existence of inversion twins possessing opposite orientation of polarization for the same spin configuration. For the $SmFe_3(BO_3)_4$ crystals, the magnetoelectric measurements have already revealed that there is disagreement with each other in the maximum magnetoelectric polarization values [1-3]. Sometimes repeated measurements of the same crystals show different polarization temperature dependencies [1].

Here we have studied structural domain distribution in a multiferroic $SmFe_3(BO_3)_4$ crystal using x-ray natural circular dichroism (XNCD) effect. XNCD [4] is defined as a difference in absorption cross sections for right σ+ and left σ– circularly polarized X-rays beams. And it is a relatively novel powerful method, which can provide a plain procedure for enantiomorphous identification using the process of high-throughput mapping. Moreover, XNCD makes it possible to determine the absolute configuration of chiral crystals similarly to natural circular dichroism or optical rotation in visible but with an element selectivity that is inherent to X-ray spectroscopy. This experimental approach can change and improve significantly our understanding of the crystallographic orientation of the racemic single crystals [5].

This work was performed within the framework of budget project for Synchrotron radiation facility SKIF, Boreskov Institute of Catalysis.

1. A. L. Freydman, D. A. Erofeev, V. L. Temerov, I. A. Gudim, Journal of Applied Physics 2018, 124(13), 134101.
2. A. A. Mukhin, G. P. Vorob'ev, V. Y. Ivanov, A. M. Kadomtseva, A. S. Narizhnaya, A. M. Kuz'menko, I. A. Gudim, JETP Letters 2011, 93(5), 275-281.
3. A. I. Popov, D. I. Plokhov, A. K. Zvezdin, Phys. Rev. B 2013, 87, 024413.
4. A. Rogalev, J. Goulon, F. Wilhelm, A. Bosak, in Magnetism and Synchrotron Radiation: New Trends, X-Ray Detected Optical Activity, Vol. 133 (Eds: E. Beaurepaire, H. Bulou, F. Scheurer, J.-P. Kapler), Springer, Berlin, Heidelberg, Germany 2010, pp. 169-190.
5. Platunov, M.S., Gudim, I.A., Ovchinnikova, E.N., Kozlovskaya, K.A., Wilhelm, F., Rogalev, A., Hen, A., Ivanov, V.Y., Mukhin, A.A. and Dmitrienko, V.E., 2021. X-ray Natural Circular Dichroism Imaging of Multiferroic Crystals. Crystals, 11(5), p.531.

DRIFTS AS QUANTITATIVE TOOL FOR STRUCTURAL CHARACTERIZATION OF PD NANOPARTICLES #152

Submitted by **Bogdan Protsenko**
For track: X-ray structural analysis
Author: Bogdan Protsenko

Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) is widely known in catalysis as a qualitative tool, mostly sensitive to light molecules, e.g. H_2O, CO, hydrocarbons and functional groups on the surface which can be used for estimation of catalytic properties of Pd

nanoparticles [1]. On the other hand, quantitative structural characterization of these catalysts is usually done with use of X-ray absorption and photoelectron spectroscopies, nuclear magnetic resonance and other methods. Such techniques require more resources and more complicated to implement than DRIFTS. Since that, utilization of DRIFTS as a tool for study both structural parameters of catalysts and parameters of absorbed gases can drastically facilitate laboratory study of palladium nanoparticles as catalysts and provide an operando approach for characterization of them in industrial applications. Using machine learning algorithms, supported by DFT calculations and experimental X-ray absorption spectroscopy data, we develop an in situ DRIFTS method for quantitative characterization of Pd nanoparticles under exposure of H_2 and carbon monoxide.
Acknowledgement: The authors acknowledge the Ministry of Science and Higher Education of the Russian Federation for financial support (Agreement № 075-15-2021-1363)
References:
[1] J. Ryczkowski, IR spectroscopy in catalysis, Catalysis Today 68 (2001) 263-381.

FINE STRUCTURE OF DIFFRACTION LOSSES IN THE SINGLE-CRYSTAL LENSES #153

Submitted by **Nataliya Klimova**
For track: SR technological application and X-ray
Author: Nataliya Klimova (Immanuel Kant Baltic Federal University(IKBFU))
Co-authors: Klimova N.B., Barannikov A.A., Sorokovikov M.N., Zverev D.A., Snigirev A.A. (Immanuel Kant Baltic Federal University, 236041 Kaliningrad, Russia), Yunkin V.A., (Institute of Microelectronics Technology RAS, 142432 Chernogolovka, Russia), Prosekov P. A., (Crystallography Institute, Russian Academy of Sciences, 119333, Moscow, Russia), Seregin A. Yu., Blagov A. E., (National Research Centre “Kurchatov Institute”, 123182, Moscow, Russia)

The best X-ray optics can be made of the single-crystal materials. Such optics are robust, well reproducible, and, the most importantly, has very low parasitic background. Unfortunately, it also has one drawback–at some conditions, undesired Bragg diffraction may occur. This leads to the situation when some part of the incident at the optics radiation is diffracted in some direction with respect to the incident and transmitted beams. And as a result, the transmitted through the optics beam loses some part of its intensity–this effect is called diffraction losses or “glitch effect”.

For studying micro- and nano-science, the x-ray beam should to match the size of the studied object. In order to do so, different x-ray optical elements are used: mirrors, zone plates and compound refractive lenses (CRLs). The CRLs have great potential due to the simple usage and great tunability. And, as already mentioned, the CRLs made of the single-crystal materials, like silicon, germanium or diamond, are one of the best options for focusing the beam of very high quality generated by 3rd and 4th generation synchrotrons as well as Free Electron Lasers. That’s why the detailed study of the glitches formation in the CRLs made of single-crystal materials is so important.

In our previous works [1-5] we have investigated the total loss of x-ray beam intensity due to the glitches in the CRLs made of single-crystal diamond. We have developed the theory describing the appearance of glitches [2,3], proposed a way how to avoid glitches during the measurements [4] and even found some constructive applications of glitches [4,5]. But the detailed picture of the glitches formation in the lenses was still missing.

In order to investigate the glitches formation in the CRLs made of the single crystal material, we have conducted an experiment at the experimental station RKFM of the Kurchatov Source of Synchrotron Radiation in Moscow, Russia [6]. For measuring the influence of glitches at the shape of the focused beam, we have used a high resolution camera with the pixel size of 0.55um and the highest achievable resolution of 1.3um. During the experiment, the Planar Compaund Refractive Lenses (PCRLs) made os single-crystal silicon [7] were used. Different number of

the PCRLs were illuminated simultaneously to form the focus at the different distance from the lenses. This allowed to measure the beam before the focus, in the focus and after the focus in each recorded image.

During the measurements two strong glitches (at 19.8keV and 20keV) were observed and recorded. The detailed analysis of the measured intensity distributions demonstrated that the glitch is formed at the different parts of the PCRLs at different energies. This can be easily explained by the refraction effect: the medium boundary changes the propagation direction of x-rays. Therefore, the Bragg's law for the refracted beam inside the medium is satisfied at different energies for the different parts of the lens. As the result, the profile of the focused beam is changing at the x-ray energies close to the energy of the glitch.

The changing shape of the focused by a PCRL beam at the energies of the glitches was observed for the first time and it is very interesting from both a fundamental and an applied point of view. This studies became possible due to the use of the high resolution x-ray camera and very small step of the energy change (0.1eV). This effect can be used in practice for the fine tuning of the focused beam shape. Such an improvement is relevant and important for the new Megascience facilities that are being built in Russia according to the Federal Scientific and Technical Program for the Development of Synchrotron and Neutron Research and Research Infrastructure during 2019-2027.

Acknowledgment.
This study was supported by the Ministry of Science and Higher Education of the Russian Federation within a State assignment for the Federal Scientific Research Centre "Crystallography and Photonics" of the Russian Academy of Sciences (project no. 075-15-2021-1362) and by the Russian Foundation for Basic Research (project No. 19-29-12043mk). The work of N.B. Klimova was supported by the Russian Federal Academic Leadership Program Priority 2030 at the Immanuel Kant Baltic Federal University. The work of V.A. Yunkin was partially supported by State assignment No. 075-00706-22-00. The work of P.A. Prosekov was partially supported as part of the work under the Ministry of Science and Higher Education within the State assignment FSRC "Crystallography and Photonics" of the Russian Academy of Sciences. The author acknowledges great support from Oleksandr Yefanov (CFEL@DESY, Hamburg, Germany).

References:

[1] M. Polikarpov, H. Emerich, N. Klimova. I. Snigireva and A. Snigirev Diffraction losses in monocrystalline X-ray refractive lenses // Proceedings of SPIE – 2017. – Vol.10235, – P. 102350H-2.

[2] N. Klimova, O. Yefanov, A. Snigirev, Predicting glitches of Intensity in single-crystal diamond CRLs // AIP Conference Proceedings – 2020. – Vol. 2299(060016).

[3] N. Klimova, O. Yefanov, I. Snigireva, A. Snigirev, Determination of the exact orientation of single-crystal X-ray optics from its glitch spectrum and modeling of glitches for an arbitrary configuration // Crystals. –2021. - Vol. 11(5):504.

[4] N. Klimova, I. Snigireva, A. Snigirev, O. Yefanov, Suppressing diffraction-related intensity losses in transmissive single-crystal X-ray optics // Crystals. – 2021; - Vol. 11(12), 1561.

[5] N. Klimova, I. Snigireva, A. Snigirev, O. Yefanov, Using diffraction losses in the single-crystal X-ray optics for precise determination of its cell parameters and tuning the monochromator // Journal of Synchrotron Radiation. – 2022. – Vol. 29. – P. 369-376.

[6] V. G. Kohn, A. G. Kulikov, P. A. Prosekov, A. Y. Seregin, A. V. Targonsky, Y. A. Eliovich, Y. V. Pisarevsky, A. E. Blagov and M. V. Kovalchuk, Synchrotron radiation diffraction in a single crystal of paratellurite investigated with a new experimental scheme// Journal of Synchrotron Radiation. – 2020. – Vol. 27. – P. 378-385.

[7] A. Snigirev, I.Snigireva, M. Grigoriev, V. Yunkin, M. Di Michiel, S. Kuznetsov, G. Vaughan Silicon Planar Lenses for High Energy X-ray Nanofocusing // Proc. SPIE. – 2007. – P. 670506 .

INVESTIGATION OF THE FACTORS DETERMINING THE EFFICIENCY OF THE INTERACTION OF ALUMINUM ALLOYS ACTIVATED BY GA-IN-EUTECTIC WITH WATER IN HYDROGEN CARTRIDGES #154

Submitted by **Alexander Nizovskii**
For track: X-ray structural analysis
Author: Alexandr Nizovskii (Boreskov Institute of Catalysis SB RAS)

A.I. Nizovskii, A.N. Shmakov, A.V. Kulikov, E.A. Suprun, V.I. Bukhtiyarov, (Boreskov Institute of Catalysis Siberian Division of RAS, Novosibirsk)

A separate direction in the use of hydrogen is the creation of energy supply systems based on low-power hydrogen fuel cells for autonomous devices such as communication equipment, video surveillance devices and remote facilities protection, etc. The use of cartridges as a source of hydrogen, in which hydrogen is obtained in the reaction of metals with water in the required amount, has a number of advantages compared to its balloon method of storage and transportation [1]. The majority of researchers who use this reaction to produce hydrogen carry it out either in a strongly alkaline medium or using specially prepared aluminum-based alloys. Often, an additional mechanochemical action is also used [2].

The fundamental difference of this work is the choice of massive structural aluminum alloys as a material for cartridges, subjected to special treatment with Ga-In eutectic. An important feature of the work is also carrying out the reaction with water at the starting room temperature and neutral pH [3]. The choice of structural aluminum alloys as starting materials for the subsequent activating treatment is due to the fact that they have an exact chemical composition and a known grain structure. The basis of the process of activating treatment by Ga-In eutectic is the Rebinder effect, which determines the features of the interaction of liquid Ga-In eutectic with a massive sample.

Using X-ray diffraction (XRD), scanning electron microscopy with local analysis (EDX) methods, grain-boundary diffusion processes were studied. The study of Al-based materials before and after the activation with the Ga-In eutectics was performed by projective X-ray microscopy and micro-tomography.

It is shown that it is the grain-boundary structure of the initial alloy that determines its efficiency of interaction with Ga-In eutectics. In the activated product, which intensively interacts with water, Ga-In eutectics is evenly distributed along the grain boundaries of the original aluminum alloy and is in a liquid state.

References

[1] Deng Z-Y, Ferreira J. M. F., Sakka Y. Hydrogen generation materials for portable applications // J. Am. Ceram. Soc. – 2008. – V. 91. – No. 12. – P. 3825–3834. https://doi.org/10.1111/j.1551-2916.2008.02800

[2] Wang H.Z., Leung D.Y.C., Leung M.K.H., Ni M. A review on hydrogen production using aluminum and aluminum alloys // Renewable and Sustainable Energy Reviews. – 2009. – V. 13. – No. 4. – P. 845–853. https://doi.org/10.1016/j.rser.2008.02.009

[3] Nizovskii A.I., Belkova S.V., Novikov A.A., Trenikhin M.V. Hydrogen production for fuel cells in reaction of activated aluminum with water // Procedia Engineering. – 2015. – No. 113. – P. 8-12. DOI:10.1016/j.proeng.2015.07.278

Научное издание

Synchrotron and Free electron laser Radiation:
generation and application (SFR-2022)

June 27 – 30, 2022

Budker INP

Book of Abstracts

Ответственный за выпуск М.В. Кузин
Сдано в набор 20.06.2022 г.
Подписано в печать 21.06.2022.
Формат 60x90 1/16 Объем 6.5 печ.л., 5.2 уч.-изд.л.
Бесплатно.