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КОМБИНИРОВАННЫЙ ПОДХОД К МОДЕЛИРОВАНИЮ ЭЛЕКТРОННОЙ СТРУКТУРЫ МАТЕРИАЛОВ, СОДЕРЖАЩИХ ТЯЖЕЛЫЕ ПЕРЕХОДНЫЕ МЕТАЛЛЫ, ЛАНТАНОИДЫ И АКТИНОИДЫ. ПРИМЕНЕНИЕ К ГАЛОГЕНИДАМ ИТТЕРБИЯ, ФЕРСМИТУ И КСЕНОТИМУ С ПРИМЕСНЫМИ АТОМАМИ УРАНА И ТОРИЯ

Dr Anatoly V. Titov (NRC "Kurchatov institute" - PNPI)

Description

Лабораторией квантовой химии НИЦ «Курчатовский институт» - ПИЯФ (http://qchem.pnpi.spb.ru) разработан комбинированный подход на основе потенциала встраивания кластера в кристалл (который мы назвали «настраиваемым под соединение» потенциалом внедрения, НСПВ, или compound-tunable embedding potential, CTEP) [1-3] для исследования различных свойств материалов (периодических структур, структур с примесными центрами, адсорбции атомов и молекул на поверхностях и других) в рамках кластерного моделирования материалов с высокой точностью. В первую очередь это касается расчётов свойств «атомов в соединении» [4], таких как химические сдвиги (ХС) рентгеновских эмиссионных (флуоресцентных) спектров (РЭС) тяжелых атомов в эффективном кристаллическом окружении, тонкого и сверхтонкого расщепления. В случае ионно-ковалентных кристаллов НСПВ может быть представлен в виде линейной комбинации нелокальных (полулокальных) псевдопотенциалов для атомов ближнего окружения и совокупности эффективных зарядов на атомах дальнего окружения без явного включения электронов атомов окружения в расчет. «Основной кластер» рассматривается в рамках обычных приближений (DFT и точные методы типа связанных кластеров), используемых в расчетах молекул. Использование кластерных расчетов с НСПВ особенно актуально для изучения электронной структуры и физико-химических свойств материалов, содержащих тяжёлые переходные металлы (d-элементы), лантаноиды и актиноиды (f-элементы), для которых требуется учет релятивистских эффектов (включая брейтовские и квантовоэлектро-динамические) и для которых не существует надежных альтернативных методов расчета. К числу таких кристаллов относятся тантало-ниобаты и другие минералы, которые рассматриваются в литературе как перспективные природные «матрицы» для долговременной иммобилизации (захоронения) высокоактивных ядерных отходов, в первую очередь актиноидов. Возможности нового комбинированного подхода продемонстрированы в пилотных расчетах галогенидов иттербия (YbF2,3 и YbCl2,3), ферсмита (CaNb2O6) и ксенотима (YPO4) с примесными атомами урана и тория. Наибольшая эффективность применения комбинированного подхода ожидается в сочетании с современными экспериментальными методами исследования соединений d- и f-элементов, в частности, с использованием источников синхротронного излучения и лазеров на быстрых электронах. Перспективы других применений нового подхода обсуждаются.

[1] DA Maltsev, YV Lomachuk, VM Shakhova, NS Mosyagin, LV Skripnikov, AV Titov, Compound-tunable embedding potential method and its application to fersmite crystal, arXiv:1907.06947 (2019)

[2] YV Lomachuk, DA Maltsev, NS Mosyagin, LV Skripnikov, RV Bogdanov, AV Titov, Which oxidation state of uranium and thorium as point defects in xenotime is favorable? arXiv:1911.00365 (2019)

[3] V.M. Shakhova, D.A. Maltsev, Yu.V. Lomachuk, N.S. Mosyagin, L.V. Skripnikov, A.V. Titov, Compound-tunable embedding potential method and its application to ytterbium fluoride crystals YbF2 and YbF3, arXiv:1911.04332 (2019)

[4] Titov A.V., Lomachuk Y.V., Skripnikov L.V., Concept of effective states of atoms in compounds to describe properties determined by the densities of valence electrons in atomic cores, Physical Review A 90, 052522 (2014).

2

THE RESEARCH OF STRUCTURE AND MORPHOLOGY OF POWDER TYPE D-16 AND MATERIAL ON IT'S BASIS OBTAINED BY METHOD OF 3D PRINTING

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Description

Aluminum alloys with copper as a structural material are widely used in various fields of industry. Currently, there is growing significant interest in the method of 3D printing of products based on ferrous and non-ferrous metal alloys using selective laser fusion (SLS) technology. In addition to choosing the type of laser and the parameters of the manufacturing process, the quality of the materials obtained is influenced by the physicochemical properties of the initial powder (the stability of oxide films on the surface of particles, the tendency to form low melting phases, etc.). The structure of the surface and volume of a 3D product obtained by the method of selective laser alloying from a powder of alloy D-16 was studied. It was found by the XPS method that on the surface of the sample there is an Al2O3 layer about 3 nm thick, and below it an Al-Cu metal alloy with a copper content of ~ 5 mass. %, which coincides with the EDX analysis performed on the initial powder by scanning electron microscopy. Local areas with a high copper content (up to 13 at. %) were found at the grain boundaries of the crystals. A high porosity of the fused sample was established (5-6%), which is almost two times higher than permissible for materials obtained by the SLS method. This is due to the crystallization features of Al-Cu system alloys associated with the transfer of matter along the interfaces, as well as to non-optimal 3D printing conditions. It is of interest to study the physicochemical properties of D-16 powder at a synchrotron radiation source.

The research was carried out within the state assignment of FASO of Russia (theme № AAAA-A19-119031890028-0)

3

AN EXAMPLE OF USING THE OPTICAL CHARACTERISTICS OF METALS OBTAINED BY THE METHODS OF SYNCHRO-TRON RADIATION AND ELLIPSOMETRY TO DETERMINE THE ELECTRONIC PROPERTIES OF ALUMINUM IN A SOLID STATE

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Description

The technique for establishing the optical characteristics of metal-lic systems from synchrotron reflection spectra allows one to establish characteristics for the required range of low energy values. It is pro-posed to use the procedure for evaluating the electronic properties of aluminum by experimentally investigating the spectrum of optical conductivity with subsequent calculation of the Kramers-Kronig inte-gral relations and the analytical between optical functions. For com-parison, the results of processing the spectrum of the optical conduc-tivity of an ellipsometric experiment are presented for a range of en-ergy values from 0.5 to 3 eV. A feature of the approach for determin-ing the electronic characteristics of metal systems by minimizing the deviation of the model optical conductivity curve from the experi-mental one is the variation in the effective mass of the electrons. When using ellipsometry data, the determined electronic characteris-tics change quite sequentially with a change in the effective mass val-ue. The use of data obtained from synchrotron spectra shows the presence of significant local jumps in the measured values at certain effective masses. Perhaps this is determined by the imperfection in the numerical approaches of interpreting the data of the synchrotron ex-periment. When

modeling optical conductivity, we can summarize the contributions from interband conductivity under the influence of pho-ton energy. In the case of permittivity, cross-contributions should also be considered. The research was carried out within the state assignment of FASO of Russia (theme № AAAA-A19-119031890028-0)

5

MODELING OF TERAHERTZ SURFACE PLASMON FOURIER SPECTROMETER

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Description

The report presents the results of research to assess the possibility of creating a terahertz (THz) Fourier spectrometer, the information carrier in which is surface plasmon-polaritons (SPPs) generated by a broadband radiation source. The key node of the spectrometer is the Michelson surface plasmon interferometer, which uses flat mirrors and plates for reflection and splitting SPP beams. The main distinctive feature of the spectrometer is the formation of interferograms by surface plasmons themselves, and not by bulk waves, one of which is generated by the SPP beam. The transition from bulk-wave optics to planar optics will not only reduce the size of the device in comparison with analogues, but will also improve the measurement accuracy due to elimination of the necessity to account for changes in the amplitudes and phases of the harmonic component of the THz radiation with its conversion into the surface waves and Vice versa; furthermore, a manifold increase in the number of recorded interferograms at different distances run by the SPPs inherent to the interferometer will contribute to the increase of accuracy of measurements as well.

This work is partially supported by RFBR grant №19-02-00353.

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EFFECT OF TiOy STOICHIOMETRY ON THE STRUCTURE OF TiOy/HAP NANOCOMPOSITE

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Description

Composite materials based on hydroxyapatite (HAP) are of much interest for biology and medicine owing to their bioactivity. The advanced strength properties of HAP can be achieved by its reinforcement with dispersed titanium and titanium oxide particles. This makes it possible to combine biocompatibility with high mechanical strength and fracture toughness. The structure of initial TiOy nanopowders and nanocomposite materials HAP/TiOy with different stoichiometry (TiO0.92 and TiO1.23) has been studied. The XRD, IR and Raman spectroscopy methods were used to establish the dependence of the shift and relative intensity of bands in the region of 144–151 cm–1 in Raman spectra on the relative content of vacancies and Ti-O bond length. Depending on the stoichiometry of additive during heat treatment, surface groups [Ti(OH)2]2+ and [TiHPO4]2+ are formed on interfaces of matrix and reinforcing additive nanoparticles, partial cationic heterovalent substitution of Ti3+ and Ti4+ for Ca2+ takes place, and new phases, in particular Ti4.5O5 and TiO2, are formed. The stoichiometry of additives affects the initial process of formation of new phase, the phase composition of nanocomposites at different annealing stages, as well as the physical properties of final product. Of interest are the in situ studies of the physicochemical properties of HAP/TiOy nanocomposites on a synchrotron radiation source, which can provide an insight into the peculiarities of interaction of additives with the matrix and the sequence of phase formation when nanoparticles come in contact.

The reported study was funded by RFBR, project number 20-03-00675.

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THE APPLICATION OF ADVANCED X-RAY DIFFRACTION IMAGE PROCESSING METHODS FOR STUDY LINEAR DEFECTS IN SILICON SINGLE CRYSTALS

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Description

The visualization and analysis of 3D fields of elastic displacements of micro-dimensional defects and dislocation structures in the volume of single crystals are important in the development of new functional materials. For this purpose, the X-ray diffraction tomography (XRDT) method is increasingly being used. We use XRDT to study the real structure of different single crystals, in particular, to visualize the spatial location of dislocation half-loops in Si (111) single crystal obtained by a four-point bending method [1]. The currently used mathematical algorithms of XRDT data processing are the evolution of absorption tomography methods. Thus, there is a motivation to modify already existing algorithms for processing experimental results in order to develop new mathematical software based on them for modeling images of micro-dimensional defects in crystals. The tools of X-ray diffraction theory, as well as modern methods of digital image processing can be used for interpretation of the obtained data. The specific feature of XRDT measurements is the impossibility to register a direct beam or its analogue (flatfield correction), which could be used to correct the background of the resulting projections. In this work, we propose a statistical method of analyzing diffraction projections to separate the noise component of the background (scattered radiation, dark current of detector, etc.) from the useful signal. In particular, an approach using antialiasing the background signal with the Hamming's kernel in a 2D implementation has been proposed. It is proposed to use an algorithm for statistical recognition using Kendall’s rank correlation criterion to recognize the boundaries and peaks in the images. Kendall’s statistic and the concordation coefficient are calculated inside the scan window of the specified width. In this case, only image trends, i.e. relative intensity values, are compared. The results of filtration depend to a large extent on the accuracy of noise dispersion estimation in the raw data. The main quality criterion of the solution is the value of the residual autocorrelation, which should correspond to a sample from a random sequence. The Durbin-Watson autocorrelation criterion [2] and several semi-empirical criteria based on the analysis of the curvature of the smoothed curve and the relative value of the systematic component in the residues were chosen as the estimation. The application of developed algorithms and software for effective automatic noise filtering and smoothing of 2D diffraction projections using the criteria of difference autocorrelation significantly improves 3D reconstruction result of the dislocation half-loops in Si (111) single crystal.

This work was supported by Russian Foundation for Basic Research (project 19-02-00556 A) in the part of image processing and the Ministry of Science and Higher Education within the State assignment FSRC “Crystallography and Photonics” RAS in part of applying tomography algorithms.

[1] V. Asadchikov, A. Buzmakov, F. Chukhovskii et al, J. Appl. Cryst. 51, 1616 (2018).
[2] J. Durbin, Biometrika 58, 1 (1971).

8

“ELECTRONIC STRUCTURE” BEAMLINE 1-6 at SKIF SYNCHROTRON FACILITY

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Description

"Electronic Structure" is a state-of-the-art beamline for methods using the Soft X-Rays range (10-2000 eV) at the 3 GeV ring of SKIF synchrotron facility. At present, three branch lines is funded, which will host an end station for Near Ambient pressure X-Ray Photoelectron Spectroscopy (NAP XPS), Spin-Angle Resolved Photo-Emission Spectroscopy (Spin-ARPES) and Reflectometry and Metrology. The NAP XPS end station will allow carrying out in situ and operando studies of the composition and electronic structure of the active component for a wide range of catalytic systems at elevated pressure; in situ studies of regularities of deactivation/ poisoning processes for catalytic systems depending on different conditions (composition of the reaction mixture, temperature, the presence of toxic agents, etc.); also in situ study of innovative functional materials. Another important technique which will be realized on a beam line (the other branch line) is Spin-Angle Resolved Photo-Emission Spectroscopy (Spin-ARPES) end station will allows to study the electronic and spin structure of solids for applications in nanoelectronics and spintronics. The third end station is Reflectometry and Metrology (the third branch line) end station will be used for certification of spectral optical elements, focusing elements and X-ray detectors; a reference detector method for absolute calibration of the spectral sensitivity of various kinds of X-ray radiation receivers in the VUV and Soft X-Rays ranges; a set of metrological techniques for calibrating the main characteristics of various kinds of X-ray detectors.

9

THE DESIGN OF «STRUCTURAL DIAGNOSTICS» BEAMLINE FOR SRF «SKIF»

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Description

The design of the user station for a fourth-generation synchrotron radiation (SR) source SRF "SKIF" has been proposed. The station is designed to solve a wide range of research and technological tasks using X-ray diffraction techniques. The concept of the station is based on the implementation of a complex approach to the structural studies of synthetic and natural objects. The most complete set of experimental diffraction techniques will allow one to benefit from the unique advantages of a modern SR source, including advanced X-ray optic solutions, high SR brightness and efficient X-ray detectors. Superconducting undulator with a magnetic period of 15.6 mm, an interpolar gap of 8 mm and a total length of 2 m will be used as insertion device (ID). In the main mode the magnetic field in the undulator will be 1.06 T (K = 1.54) giving SR harmonics generation with a step of 2.5 keV. The station includes four sections: High-resolution powder diffraction (section 1-2-1); In situ diffraction (section 1-2-2); Single-crystal X-ray diffraction (section 1-2-3); Small angle X-ray scattering (section 1-2-4). In the main operating mode of the ID all the sections are supposed to work simultaneously. This is achieved by splitting the components of the SR spectrum between different sections by three beam multiplexing monochromators (beam splitters). Flat diamond plates with an (111) orientation and a thickness of about 100 μm will be used to split the beam. The components of ID spectrum with energies of 12.50 keV / 0, 99 Å, 22.50 keV / 0.55 Å and 32.50 keV / 0.38 Å will be directed to

side sections of the station at angles of 28, 15 and 11° with respect to primary beam. For the experiments requiring energy scanning an alternative mode will be used provided by the possibility of the change of the magnetic field in the undulator. In this mode the undulator radiation transmitted to only 1-2-1 section due to the restrictions of the multibranch optical design. To obtain the necessary beam parameters we plan to use the refractive X-ray optics beryllium, diamond or aluminum lenses depending on beam energy. To detect diffraction pattern, we propose to use modern hybrid-type detectors based on sensors made of silicon or cadmium telluride for high energy applications. The work was supported by Ministry of Science and Higher Education of the Russian Federation (grant No. AAAA-A19-119020890025-3).

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OPTICAL DESIGN OF THE «STRUCTURAL DIAGNOSTICS» BEAMLINE FOR SRF «SKIF»

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Description

Herewith, we present the optical design of the «Structural Diagnostics» beamline developed for a fourth generation synchrotron radiation (SR) source SRF “SKIF”. The multi section beamline is based on a superconducting undulator (see table below) and will have a total of 4 experimental instruments, three will use fixed energy side branches and the fourth one located on the straight section will have the option of wide energy spectrum. A variety of diffraction experiments can be accomplished simultaneously at this beamline thanks to such a design. The four aforementioned sections are: High-resolution powder diffraction (straight section 1-2-1); In situ diffraction (side section 1-2-2); Single-crystal X-ray diffraction (side section 1-2-3); Small angle X-ray scattering (side section 1-2-4). [Scheme. Optical train of the High-resolution powder diffraction (straight section 1-2-1). Calculated spot size at each one of the experimental sections as well as expected fluxes will be presented. Heat management for optical components will be also discussed.][1] Table. Main machine parameters Energy [GeV] - 3 Circumference [m] -476 HF [MHz] - 178.47 Horizontal emittance [pm.rad] - 75 Coupling constant [%] - 10 Beam current [mA] - 400 No. of bunches - 510 βx, βy [m] - 13, 1.9 Table. Main undulator parameters Peak field B0 [T] 1.25 Period length λU [mm] 15.6 Minimum magnetic gap [mm] 8 Magnetic Length L [mm] ~1997 Total power Ptot (B=1.25 T, I=0.4 A, E=3 GeV) [kW] 7.18 On-axis power density (B=1.25 T, I=0.4 A, E=3 GeV) [kW/mrad2] 50

The work was supported by Ministry of Science and Higher Education of the Russian Federation (grant No. AAAA-A19-119020890025-3).

[1]: https://drive.google.com/open?id=1BoL_jAur8e0l4pLDLUpZP_yfpqwrtML-

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COMPLEX DYNAMIC STUDY OF EJECTION OF THE OF PARTICLES FROM SHOCK-LOADED TIN BY SR METHODS, A PDV LASER COMPLEX, AND OPTICAL AND PIEZOELECTRIC SENSORS

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Description

At fast acceleration of metals, a cloud of microparticles (dust cloud) appears in front of the surface. Work on the study of these processes using Synchrotron Radiation (SR) was carried out at the Budker Institute of Nuclear Physics (Novosibirsk) [1,2]. In this work, the particle flux from shock-loaded tin was recorded using X-ray radiography, but also synchronously with another 4-channel Photon Doppler Velocimetry (PDV) laser complex and piezoelectric sensors. The use of piezosensors and laser complexes PDV is widely used due to the availability and simplicity of obtaining information on the dynamic flows of microparticles. It is advisable to use these techniques in conjunction with other techniques that can evaluate mass and flow rates. The use of SR radiography is an ideal complement to them. Comparison of data on the flow of microparticles (speed and mass distributions) with the magnitude of the signal from the piezoelectric sensor makes it possible to independently calibrate the sensor readings. The simultaneous use of modern techniques has allowed not only to measure the mass distribution along the cloud, but also significantly increase the reliability of the measured values. The flows of microparticles from grooves (roughnesses) with sizes from Rz4 to Rz80 made on the surface of tin were investigated. The shock wave was created by pressed octogen. The data obtained are necessary for the numerical simulation of particle ejection processes.

[1] K.A. Ten, E.R. Pruuel, A.O. Kashkarov, I.A. Rubtsov, M.V. Antipov, A.B. Georgievskaya, A.L. Mikhailov, I.A. Spirin, V.M. Aulchenko, L.I. Shekhtman, V.V. Zhulanov, B.P. Tolochko . Detection of Particle Ejection from Shock-Loaded Metals by Synchrotron Radiation Methods. // Combustion, Explosion, and Shock Waves. Vol. 54. No. 5. pp. 606-613, 2018.

[2] K A Ten, E R Pruuel, A O Kashkarov, I A Rubtsov, M V Antipov, A B Georgievskaya, A L Mikhailov, I A Spirin, L I Shekhtman, V V Zhulanov and B P Tolochko. Dynamic registration of ejection from shock-loaded metals // Journal of Physics: Conference Series, Volume 1147, (2019) 012020 doi:10.1088/1742-6596/1147/1/012020

12

SHORT-PERIOD UNDULATORS WITH ELECTROSTATIC FIELD

Prof. Nikolay Vinokurov (Budker Institute of Nuclear Physics) **Co-author** Dr Oleg Shevchenko (BINP)

Description

Due to strong sextupole corrections, the vertical dynamic aperture of low-emittance storage ring is rather small. Therefore, in-vacuum small-period undulators may provide high enough field. In particular, significant electrostatic field value can be obtained near electrodes. To eliminate the field emission, the high-field surfaces has to be at positive electric potential. In this paper we consider the feasibility of undulator using the comb of such electrodes. It worth noting that variable-period design may be rather simple for electrostatic undulators.

Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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SIMULATION AND EXPERIMENTAL STUDY OF BEAM DYNAMICS IN NOVOFEL RF GUN AND ITS BEAMLINE

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Description

A new normal-conducting, CW, thermocathode RF gun was developed and tested at Budker Institute of Nuclear Physics recently. Providing average current up to 100 mA, this device will be used to upgrade the injector of Novosibirsk FEL facility. A beam dynamics simulation in RF

gun and its beamline was made with space-charge forces being taken into account. Comparison of the simulation results and experimental measurements is presented in this paper.
Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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PROJECT OF THE OPTICAL SCHEME FOR THE SOFT X-RAY & VUV BEAMLINE AT SKIF SYNCHROTRON FACILITY

Dr Anton Nikolenko (Budker INP SB RAS)

Description

The "electronic structure" is modern beamline for methods using the VUV and soft X-rays (10–2000 eV) on the 3 GeV ring at the SKIF synchrotron facility. The collimated PGM scheme based on a modified SX-700 monochromator is used. During monochromatization and transportation from the frontend to the sample, the SR beam passes through five reflective elements, including a plane deflecting mirror and a plane diffraction grating. The remaining three mirrors have a curved shape, and two of them are interchangeable in order to change the beam path for transportation to one of the end-stations. To reduce the contribution of high diffraction orders, it is planned to additionally use a four-mirror high orders suppression system. The calculated parameters of optical elements, estimates of the thermal load on them, and calculations of the spectral resolution of the optical system in different modes are presented.

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MONITORING SYSTEM OF NOVOSIBIRSK FEL OPTICAL CHANNEL STATE USING 1-WIRE DEVICES

Dr Sergey Tararyshkin (Budker Institute of Nuclear Physics)

Description

Monitoring system of Novosibirsk FEL optical channel state using 1-Wire devices is described

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USAGE OF EPICS CHANNEL ACCESS PROTOCOL IN NOVOSIBIRSK FEL CONTROL SYSTEM

Stanislav Serednyakov (Budker Institute Of Nuclear Physics)

Description

Examples of Usage of Epics Channel Access protocol and High level Applications in Novosibirsk FEL control system are described

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XRD DIAGNOSTICS OF FUNCTIONAL MATERIALS AT SSTRC

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Description

The studies of the structure, phase composition and phase transformation of functional materials such as catalysts, sorbents, ion conductors, coatings, etc. are performed 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 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, up to 100-120 keV. The report comprises description of the experiments on the phase composition of Ga-activated aluminum, oxygen mobility in Ruddlesden-Popper phases, reduction process of mixed oxides, local structure of heterogeneous catalysts by means of Total Scattering and Pair Distribution Functions technique, and so on.

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THE NOVOSIBIRSK FREE ELECTRON LASER FACILITY

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Description

The Novosibirsk FEL facility includes three FELs operating in terahertz, far- and mid- infrared spectral ranges. It has rather long history but its potential is not fully revealed so far. The first FEL of this facility has been operating for users of terahertz radiation since 2004. It still remains being the world's most powerful sources of coherent narrow-band radiation in its wavelength range (90 – 340 μm). The second FEL was commissioned in 2009. Now it operates in the range of 35 - 80 μm but in near future we plan to replace its undulator with a new one and its short wavelength boundary will be shifted down to 15 μm. The third FEL was commissioned in 2015 to cover the wavelength range of 5 – 20 μm. Its undulator comprises three separate sections. Such lattice suits very well to demonstrate the new off-mirror way of radiation outcoupling in FEL oscillator (so called electron outcoupling) which we also plan to do in near future. We also intend to improve the accelerator injection system. The result of this improvement will be increasing of the average electron beam current and consequently increasing of all three FELs radiation power. In this paper we present overview of the facility and discuss our recent achievements and future plans.

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THE VARIABLE PERIOD UNDULATOR MAGNETIC FIELD MEASUREMENTS AND CORRECTION OF THE FIELD ERRORS

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Description

The new variable period undulator with unique design was developed and built recently at Budker INP. It will replace the electromagnetic undulator being used now at the second FEL of the Novosibirsk FEL facility. As the result the FEL tunability range will be substantially increased. In this paper we present the results of the undulator magnetic field measurements for different periods as well as discuss the ways to reduce field errors which include magnets sorting, weakening of undulator edge poles and using of steering coils. Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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RADIATION STABILITY AND HYPERFINE MODE STRUCTURE OF THE TERAHERTZ NovoFEL

Dr Vitaly Kubarev (BINP)

Description

Radiation stability and hyperfine mode structure of the terahertz NovoFEL.

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A TERAHERTZ LOCALIZED LASER DISCHARGE AS A SOURCE OF BRIGHT VUV LIGHT

Dr Alexander Vodopyanov (Institute of Applied Physics RAS)

Description

This work describes the prospects of the point-like discharge supported by focused terahertz NovoFEL radiation as a source of UV and VUV light.
This work is partially supported by RFBR grant офи-м № 14-22-02070.

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ELECTRON OUTCOUPLING EXPERIMENTS AT THE NovoFEL FACILITY

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Description

The electron outcoupling scheme was proposed for the high power FELs with optical cavities to avoid the power limitation due to overheating of the reflecting mirrors. This can be realized if the major part of radiation power is emitted at an angle to the optical axis. For this, the electron beam should be bunched and then slightly rotated in the undulator of the FEL. At the NovoFEL facility the electron outcoupling system is installed on the third FEL based on the multiturn energy recovery linac. It consists of three undulators, dipole correctors and two quadrupole lenses assembled between them. There are two different configurations of the system since the electrons can be deflected in either the second or the third undulator. The electron beam dynamics calculations, current experimental results and the planned experiments are discussed.
Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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EPR SPECTROSCOPY STATION AT THE NOVOSIBIRSK FREE ELECTRON LASER: APPLICATION OF HIGH-POWER THZ RADIATION IN THE FIELD OF MOLECULAR MAGNETISM

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Description

In this work we present the current status of CW and TR EPR station at NovoFEL [1]. The detailed layout of the experimental user station is shown and discussed. While the CW and TR EPR X-band (9 GHz) spectrometer used is almost the same as in many EPR laboratories, it was built in the NovoFEL beamline and allows performing the unique EPR experiments with simultaneous irradiation of the sample by common UV-vis and exceptional NovoFEL light. For this purpose, multimodal THz waveguide allowing to fed NovoFEL radiation directly into the EPR resonator is used. Laser radiation of NovoFEL is passed through the collimator based on two off-axis parabolic mirrors which compress the beam diameter by a factor of 15 adjusting it to the aperture of THz waveguide used in EPR spectrometer. Electronic modulation system for NovoFEL radiation is used to decrease the average power by a factor of 100 or even higher while keeping the maximum accessible peak power[2]. Passed through the collimator and optical chopper, the NovoFEL radiation can be readily directed to the sample into EPR resonator. Different detection schemes of experiments conditioned by the initial time profile of NovoFEL radiation, its electronic modulation and the capability (CW and TR) of EPR spectrometer used are discussed. Special attention is drawn to the heat effect and its practical use for the temperature-modulated detection of very broad EPR spectra [3].
This work has been supported by the Russian Science Foundation (no. 17-13-01412).
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[2] S.L. Veber, S.V. Tumanov, et al., J Magn Reson, 2018, 288, 11.
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MEASUREMENTS AND CALCULATION OF INDUCED RADIOACTIVITY FROM TECHNOLOGICAL UNITS OF THE NOVOSIBIRSK FEL ACCELERATOR-RECUPERATOR

Dr Tatiana Salikova (Budker INP SB RAS)

Description

The article provides estimates and measurements of the levels of induced radioactivity from the technological units of the accelerator-recuperator of Novosibirsk powerful FEL. FEL operates in three modes when the kinetic energy of electrons reaches 12, 20, and 40 MeV. In the range of these energies lies a giant dipole resonance. For control, copper and stainless steel samples were irradiated. Measurements and calculations allow us to estimate the levels of induced radioactivity and the times of degradation of materials (products) under the influence of radiation.

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TECHNICAL AND SOFTWARE IMPROVEMENTS OF THE EPR SPECTROSCOPY STATION AT THE NovoFEL FACILITY: STATUS 2020

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Description

This contribution describes the current state of the X-band EPR setup at the Novosibirsk Free Electron Laser facility (NovoFEL). Recent advances in experimental hardware and software are discussed in detail. Improvements include implementations of fast detectors for recording the THz macropulses during experiment, possibility of simultaneous use of two oscilloscopes, configured at different timescale, and the development of software for on-the-fly data treatment. Modification of hardware and software of the EPR spectroscopy station at NovoFEL facility was funded by the Russian Science Foundation, grant number 17-13-01412. Synthesis of $[Co_{0.01}Zn_{0.99}(piv)_2(2\text{-}NH_2\text{-}Py)_2]$ complex was funded by IGIC RAS state assignment.

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ESTIMATES AND MEASUREMENTS OF PHOTON AND NEUTRON RADIATION DOSES OF THE NOVOSIBIRSK FEL MICRON-RECUPERATOR

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Description

The article provides estimates and measurements of the dose rate of photon and neutron radiation in the accelerator hall for three modes of operation of the Novosibirsk powerful FEL, when the maximum kinetic energy of the electrons reaches 12, 20 and 40 MeV. During the operation of the micron-recuperator, photoneutrons are generated and structural elements are activated. Measurements and calculations allow us to estimate the levels of induced radioactivity and the times of degradation of materials (products) under the influence of radiation.

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THE NovoFEL OPTICAL DIAGNOSTICS UPGRADE

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Description

Novosibirsk Free Electron Laser (NovoFEL) is based on rather complicated accelerator system. Complex uses three separate FELs installed on various Energy Recovery Linacs (ERLs). ERLs operate with high average beam current (about 5 mA). The severe restrictions on the electron bunch parameters for the lasing require the beam diagnostic system. The transverse beam profile

measurement system uses an electron beam synchrotron radiation (SR) from the bending magnet and the optical transition radiation (OTR) from the aluminum foil. This allows adjusting the beam parameters before the undulator and measuring them after lasing. This year, the diagnostic complex has been improved by the installation of additional SR monitor at the place with a large dispersion function and spectrometer for studying the undulator radiation. The recent results of the beam dynamics measurements and calculations are presented.
This work was supported by grant 18-72-00123 of Russian Science Foundation.

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SR-XRFA IN BOTANICAL RESEARCH: ELEMENTAL COMPOSITION OF SPECIES OF THE GENUS SYRINGA (OLEACEAE) UNDER TECHNOGENIC IMPACT IN NOVOSIBIRSK

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Description

A study has been first made of the element composition of both the plants of two species of the genus Syringa, growing under technogenic impact in Novosibirsk and the soil samples from their habitat by method of X-ray fluorescence analysis using synchrotron radiation (SRXRF) at the station of element analysis of SCSTR of the Institute of Nuclear Physics SB RAS (VEPP-3 store ring). The material studied was represented by the plants of two species - Syringa josikaea and S. vulgaris, represented by three cultivars: ‘Nadezhda’, ‘Olimpiada Kolesnikova’, ‘Pamjat o Kirove’, growing in conditions of technogenic impact and background, collected in August of 2017 in Novosibirsk. A comparative analysis of the soil from the points of sampling of plant samples showed an excess in the content of V, Zn, Br, Pb and a decrease in Mn in urban soils compared with the background. The study of the content of macro- and microelements in the aerial organs of representatives of the genus Syringa showed that the concentration of macroelements K and Ca is higher in the leaves than in the stems, regardless of the taxon and place of growth. The highest total content of K and Ca is revealed in the leaves of S. josikaea. It was found that in plants under technogenic impact, the content of Mn, Fe, Co, Cr, Br, Rb, Nb increased and Zn and Mo decreased compared to the control, the most severe heavy metal pollution in urban conditions was observed in plants of S. josikaea. The biogeochemical transformation coefficient (Zv) was calculated, which reflects a violation of the normal ratios of elements in the organs of plants as a result of increased anthropogenic load. The most significant changes in the elemental composition of lilac leaves under anthropogenic impact were observed in plants of the species S. josikaea, whose Zv of leaves is 37.2, which is 1.3–1.6 times higher than in plants of S. vulgaris. Plants of the ‘Memory of Kirov’ variety (Zv = 22.8) are most resistant to pollution. As a result, reliable data were first obtained on the content of 20 elements in samples of two species of the genus Syringa in the urban ecosystem of Novosibirsk. The species and cultivars that are most tolerant to pollution in urban conditions, which can be recommended for widespread use in green construction, are identified. The data obtained on the elemental composition of plant samples and soils may be included in the databases.
This work is partially supported by RFBR grant № 16-44-040204.

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W-CONTAINING PMMA-BASED NANOCOMPOSITE

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Description

The development of polymer nanocomposites has been an area of advanced scientific and industrial interests in the last ten years in connection with advances in improving the properties of materials based on a combination of a polymer matrix and, as a rule, inorganic nanomaterial. As a result, new materials are formed with improved properties such as mechanical resistance, strength and stiffness, electrical conductivity and thermal conductivity, increased flame retardant properties, lower diffusion coefficient of vapors and gases. Nanocomposites can also demonstrate unique engineering capabilities that guarantee the benefits of creating functional materials with desired properties for specific applications. Therefore, it is promising to use new materials in micromachining to obtain functional microstructures. Some micromachining technologies are based on the use of photo and electronic resists, which are just an organic polymer or prepolymer, and the introduction of inorganic particles into it increases the chemical and thermal stability and mechanical stability of microstructures. One of the promising applications of LIGA technology is the formation of an X-ray detector with high spatial resolution. The introduction of inorganic particles of the inorganic particles of the GdO2S2 scintillator with a grain size of several microns into the technological layer of the resist promotes the conversion of X-ray radiation, but significantly limits the spatial resolution. On the other hand, large particles scatter the generated radiation in the visible range of the spectrum. Therefore, we have developed a method of in-situ polymerization of dispersing PMMA particles of submolecular size into an electronic resist, which stimulate the transformation of X-ray radiation into visible-spectrum radiation. The results of the resulting X-ray detector based on a polymer nanocomposite are reported in this report.
This work is partially supported by RFBR grant № 19-42-540014.

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SELF-ALIGNED SINGLE EXPOSURE DEEP X-RAY LITHOGRAPHY

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Description

Microdevices are usually made up of several interacting components that can be assembled on the basis of 3-dimensional LIGA structures, using various techniques to fulfill the required positioning accuracy - the so-called combined LIGA technology [1]. As a part of the LIGA technology, deep X-ray lithography enables the formation of 3-D microstructures of significant size in each of the three dimensions; however, it is often possible to improve positioning accuracy by using self-alignment technique when patterning with the use of X-ray mask, as shown in [2]. In our work, we consider single-exposure with self-alignment technique for the creation of microdevices of technological material, which can demonstrate new physical capabilities.

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DIRECT WRITING ON PBWO4 MONOCRYSTALLINE USING X-RAYS

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Description

The lithographic profile on the material surface is usually based on making structural changes in the intermediate - technological layer using radiation, and the subsequent transfer of the resulting topology to the underlying layer of the functional material. However, not all materials enable the

removal process that meets the sufficient selectivity value. This report presents the results of direct writing a relief on an inorganic PbWO4 crystal using synchrotron radiation in the X-ray range.
This work is partially supported by RFBR grant № 19-42-540014.

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HIGH-P,T DIFFRACTION STUDIES OF DEHYDRATION OF MAGNESIUM SILICATES RELATED TO THE DEEP EARTH'S WATER CYCLE

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Description

In the context of the global H2O cycle, an active interest is taken in water recycling associated with subduction of oceanic plates into the mantle. Mineral serpentine, Mg3Si2O5(OH)4, is regarded as the main water reservoir in oceanic litosphere [1], and therefore its dehydration can produce a large impact onto seismic activity and magma generation in subduction zones. Since the dehydration temperature can be effectively decreased in the presence of alkali chlorides [2], we explore this effect on serpentine dehydration. Here we report the results of in-situ X-ray diffraction and Raman spectroscopy studies of two serpentine minerals, chrysotile and antigorite, in the presence of sodium chloride at high P-T conditions relevant to subduction zone (1-4 GPa, 400-800oC). The dehydration temperature of both minerals is about 200 degrees lower compared to salt-free H2O-saturated conditions, which is important for the localization of dehydration reactions in subducting slab.
This work is supported by the Russian Foundation for Basic Research (grant No 18-05-00312). Diffraction experiments were performed at SSTRC, Novosibirsk (project RFMEFI62119X0022) and the PETRA III (DESY, Hamburg), and supported by approval of PETRA III Proposal I-20190140.

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INVESTIGATION OF THE LOCAL PHASE COMPOSITION AND MORPHOLOGY OF LASER WELDED JOINTS BASED ON TITANIUM AND ALUMINUM ALLOYS BY HARD SYNCHROTRON RADIATION DIFFRACTION METHODS

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Description

Laser welding is one of the most promising methods in comparison with other methods of welding dissimilar materials. This method does not require the use of additional materials, special edge processing, and also has a high welding speed. The aim of the work was to study the phase composition and morphology of various zones of the welded joint between alloys based on aluminum and titanium. . The phase composition and morphology of the welds were studied at the experimental station of the 4th SI channel from the VEPP-3 storage ring. We used the technique of shooting in the light. A thin beam (0.1 mm across the width of the seam and 0.4 mm along the length of the seam) of monochromatic synchrotron radiation passes through the welded joint and gives a two-dimensional diffraction pattern recorded by a two-coordinate flat detector. The use of synchrotron radiation made it possible to identify the fundamental laws of the formation of the micro and nano structure of the weld, to determine the main phase composition.

Scanning with a thin SR beam for the first time investigated the structural-phase composition of laser welded joints of dissimilar materials in different zones of the weld from titanium to aluminum at different displacements of the laser beam. This allowed us to choose a welding mode in which the strength of a heterogeneous weld increased by 2.5 times. This method, due to the small diameter of the focused radiation, makes it possible to obtain a thin diffusion zone in which intermetallic compounds are formed, vary the width of this zone due to the movement of laser radiation, and thereby change the mechanical characteristics of the resulting dissimilar welded joints.

The work on optimizing welding conditions and studying the microstructure was carried out in the framework of the Program of Fundamental Scientific Research of the State Academies of Sciences for 2013-2020 (project AAAA-A17-117030610122-6). The work was carried out using the equipment of the Mechanics and Processing Center (ITAM SB RAS). Diffraction studies were carried out using the infrastructure of the Siberian Center for Synchrotron and Terahertz Radiation as part of the state task of the Institute of Chemical Technology and Technology of the SB RAS (project No. AAAA-A17-117030310280-6).

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THz SENSING BASED ON SUBWAVELENGTH GRATING IN ATTENUATED TOTAL REFLECTION CONFIGURATION

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Description

THz sensing is very important tool in biological and medical applications. In this paper, we study the possibility of creating a sensor on a subwave grating in the attenuated total reflection (Otto) configuration. Using theoretical analysis and numerical simulations, the optimal parameters of the gold grating with liquid water solutions under test were found. The sensitivity of the grating sensor has been estimated.

This work is partially supported by RFBR grant №16-32-00678 мол_а.

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TECHNIQUES FOR GENERATION OF ANNULAR SURFACE PLASMON POLARITONS WITH REFRACTIVE BINARY AND REFLECTIVE CYLINDRICAL DIFFRACTION GRATINGS

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Description

The propagation length of surface plasmon polaritons (SPPs) increases with increasing wavelength, which makes it possible to use radiation from the far-infrared and terahertz ranges to create communication devices in which SPPs will be carriers of information. In this paper, we consider methods for implementing the multiplex transmission of information along cylindrical conductors using a combination of SPPs with orbital angular momentum.

It is shown that there are two methods for generating ring surface plasmon polaritons (SPPs) using high-order Bessel beams. In the first method, free radiation is transformed into an SPP using a binary phase axial grating illuminating a cylindrical diffraction grating connected to a cylindrical waveguide. The second method uses the diffractive coupling of a Bessel beam to an axisymmetric conductor. In this case, as an option, before the capture, the beam can be first transformed by a lens, forming an annular vortex beam at its focus. After passing through the waveguide, the mode composition of the beam is decoded, for example, using diffractive optical

elements, and each communication channel is registered by an individual detector. A device that implements these methods is demonstrated.
The work was supported in parts by the RSF grant No. 19-12-00103.

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THE USE OF POLYCHROMATIC SYNCHROTRON RADIATION TO STUDY FAST PROCESSES IN SOLIDS. ADVANTAGES AND CHALLENGES

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Description

Theoretical analysis has been carried out and test experiments have been implemented on the use of polychromatic synchrotron radiation to study fast processes in solids. The obvious benefits and challenges are outlined.
This work was supported by RFBR grant 14-03-00770.

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DEVELOPMENT OF SRXFA METHOD WITH THE HARD X-RAY RANGE FOR PALEOCLIMATE RECONSTRUCTION (REGION OF LAKE BAIKAL) ON THE STORAGE RING VEPP-4M

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Description

The aim of the research was to identify trends and changes of moisture supply, global and local climate regime of the Central ecological zone of the Baikal natural territory (the Selenga River). For this, wet sediment core samples were analyzed by scanning X-ray fluorescence spectrometry (SRXFA scanning) in the context of paleoclimate studies. The new SRXFA station on the VEPP-4M storage ring (BINP RAS) was used to determine the elemental composition of wet cores, which allows us to significantly expand the set of detectable elements to 35 or more, including lanthanides (La, Ce, Pr, Nd, Sm). The use of this technique in the study of wet bottom sediments showed a high relevance of this method when displaying short-period climatic fluctuations. The obtained data can be used in an interdisciplinary aspect, and in particular, when predicting the water content of Lake Baikal and as a result when planning the activities of the Angarsk HPP cascade.
Work is partially supported by RFBR gant 17-29-05016 офи_м.

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MEASURING INSTALLATION FOR DETERMINING CURRENT-VOLTAGE CHARACTERISTICS AT LIQUID HELIUM TEMPERATURE

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Description

Measuring plant are made on the base of cryostat КГ-60/300-1 in internal cavity of which, in liquid helium medium, solenoid is located, and in its central part insert-holder with sample is located. Power supply of solenoid and tested sample, by current leads located in the upper cover of cryostat, are performed by power supplies of Danfysik - system 8800 company with the help of PC and control program developed in BINP. In order to test the plant for determination of current–voltage characteristics (CVC) in superconductors at helium temperatures, test measurements were carried out according to the method MVI 400-423/8-2018 developed by JSC VNIINM [2]. Measurements were made on composite wire samples based on the Nb-Ti alloy,

0,08 m long and 0,5 and 0,85 mm diameters cut from the wires of standard batches, with CVC being indicated by the manufacturers of these superconductors. He calculated value of the critical current specified by the manufacturer of the measured superconducting wires at the 7 T shall be 200 A and 372 A. The value we have obtained is 212 A and 382 A, which is less than 10% [4] and this corresponds to the limit of the permissible basic absolute error of the meter B7-99 which is ± (1, 5·10-3 + 4, 5·10-5 | U |) mV (U - measured voltage, mV). As can be seen, the operability of the measuring unit for determining the actual critical current values is confirmed, and obtaining a more accurate measurement result will allow modern precision digital measuring equipment, with the permissible basic absolute error of ± 0,0025%+ 0,02 nV.

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A DEVELOPMENT OF COMPACT COMBINED PUMP FOR SRF SKIF

Dr Alexey Semenov (BINP SB RAS) **Co-author** Dr Vadim Anashin (BINP)

Description

It is required an ultra-high vacuum (near 10^{-11} Torr in the beam absence mode) in the synchrotron source of 4+ generation SFR “SKIF”. Owing to the vacuum chambers have small molecular conductivity and it exists the space limitation for pumps location, compact combined pumps application is required, i.e. pump on the base of non-evaporable getter and sputter ion pump. The modern pumps NEXTorr (SAES Getters, Italy) are not implemented the all of requirements on the inert gases such as argon and methane for SFR “SKIF”. Therefore, it is necessary to create similar combined pumps by Russian manufacture. The first pumping speed calculations for one cell of triode type sputter ion pump and the whole of pump are presented here. Also experimental results of pumping speed measurements depending on the magnetic field, diameter and length of cell for sputter ion pump are given.

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DETECTORS FOR FAST TIME-RESOLVED STUDIES AT SSTRC, STATUS AND FUTURE

Lev Shekhtman (Budker INP)

Description

The detector developments for fast and super-fast time-resolved studies at SR beams will be reviewed. Two detectors based on Si micro-strip technology are developed at present at Budker INP SB RAS. The detector for imaging of super-fast processes at a nanosecond scale, DIMEX-Si allows to improve by more than a factor of ten maximum detected photon flux, with respect to the gaseous version of such detector, that is operating at VEPP-3 for more than 15 years; the frame rate is increased up to 50 MFr/s and spatial resolution is improved to about 50 microns. The new full-size detector prototype for the studies of tungsten deformations under pulse heat load in a microsecond scale is recently developed. Its has significantly better spatial resolution and sensitivity compared to the DIMEX-G detector that was used for these studies before.
Part of the work reviewed in this presentation related to the measurements with the prototype of the DIMEX-Si detector is supported by the RFBR grant No.19-42-540006.

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MICROELEMENTAL LIMITATION OF LYMPH NODES STRUCTURE ACCORDING TO THE X-RAY FLUORESCENT ANALYSIS WITH A SYNCHROTRON RADIATION

Prof. Vladimir Gorchakov (Novosibirsk State University) **Co-authors** O.V. Gorchakova[1], Yu.P. Kolmogorov[1], V.N. Gorchakov[1,2*], G.A. Demchenko[3], S.N. Abdreshov[3]
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Description

Unique properties of X-ray fluorescent analysis with synchrotron radiation and classical morphological method allowed to reveal interrelation between the trace elements content and structure of lymph nodes. Belonging of lymph nodes to different regions is defining in formation of a certain microelemental profile and features of the microanatomic organization of lymph nodes. Lymph nodes have different functional specialization with prevalence of immune or drainage function and a certain microelemental composition. The inguinal lymph node has active drainage function because of the developed sinus system at the maximum of Mn, Fe, Zn concentration; immune function prevails in a tracheobronchial lymph node at the low content of all trace elements; the mesenteric lymph node has evenly developed drainage and immune functions at the maximum of Cu, Se contents. The content of trace elements is considered as the leading mechanism limitation the structural organization of lymph nodes. Innovative approach helped to reveal formation of lymphoid-microelemental association. Features of this association modify the structural organization of lymph nodes depending on localization (region specifics).

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THE PROJECT «DIAGNOSTICS IN THE HIGH-ENERGY X-RAY RANGE» BEAMLINE AT THE SIBERIAN SYNCHROTRON SKIF

Dr Konstantin Kuper (BINP)

Description

The project of the beamline “Diagnostics in the high-energy X-ray range” will become the basis for advanced scientific experiments in the materials science, geophysics, archaeologists, paleontology, byology and medicine. A number of research techniques will be implemented at the station using high-resolution introscopy, diffraction, and X-ray scattering.

48

APPLICATION OF COMPLEX STUDIES OF TEST SAMPLES FOR THE IMPLEMENTATION OF COMBINED SR METHODS FOR THE STUDY OF MICRO-OBJECTS

Dr Vladimir Kriventsov (BIC SB RAS) **Co-authors** Fedor Darin (Budker Institute of Nuclear Physics SB RAS) Mr Dmitry Sorokoletov Dr Iakov Rakshun Andrey Darin (Sobolev Institute of Geology and Mineralogy SB RAS)

Description

This work shows the results of the study of trial test samples of technological and natural origin, and using a complex composition for the development of combined methods based on synchrotron radiation (SR), such as μ-XANES/EXAFS, μ-XRF, and others. Main goal of the study is to adapt the developed integrated approach for the study of micro-inclusions and microparticles by SR methods in the near future. All the spectra of the studied samples were recorded using standard methods, both at the experimental module of x-ray confocal microscopy located at NRC “Kurchatov Institute” (Moscow) and at XRF-, EXAFS- stations of Siberian Synchrotron Terahertz Radiation Center (SSTRC, Novosibirsk).

The studied test samples with a complex composition (such as low-percentage metal oxide nanocomposites, nanoalloys, and samples of natural origin) were synthesized and/or selected from existing collections. Test samples and benchmarks necessary for testing and developing SR techniques were studied by a set of methods (μ-XANES/EXAFS, μ-XRF, XAFS, XRF, HRTEM, XPS, SEM, EDX, etc.). New information about phase and element compositions, atomic structure, morphology, and structural parameters was obtained for the test systems under study. The data obtained by all the methods are in a good agreement. The possibilities of the proposed approach for the study of microparticles and micro-inclusions of complex composition by methods implemented using synchrotron radiation are demonstrated.

The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk

FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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RESEARCH OF NANOSCALE SYSTEMS OF COMPLEX COMPOSITION BY XAFS METHOD AT THE EXAFS SPECTROSCOPY STATION OF SSTRC

Dr Vladimir Kriventsov (BIC SB RAS)

Description

This work shows the results of the study of trial test samples of technological and natural origin, and using a complex composition for the development of combined methods based on synchrotron radiation (SR), such as μ-XANES/EXAFS, μ-XRF, and others. Main goal of the study is to adapt the developed integrated approach for the study of micro-inclusions and microparticles by SR methods in the near future. All the spectra of the studied samples were recorded using standard methods, both at the experimental module of x-ray confocal microscopy located at NRC "Kurchatov Institute" (Moscow) and at XRF-, EXAFS- stations of Siberian Synchrotron Terahertz Radiation Center (SSTRC, Novosibirsk).

The studied test samples with a complex composition (such as low-percentage metal oxide nanocomposites, nanoalloys, and samples of natural origin) were synthesized and/or selected from existing collections. Test samples and benchmarks necessary for testing and developing SR techniques were studied by a set of methods (μ-XANES/EXAFS, μ-XRF, XAFS, XRF, HRTEM, XPS, SEM, EDX, etc.). New information about phase and element compositions, atomic structure, morphology, and structural parameters was obtained for the test systems under study. The data obtained by all the methods are in a good agreement. The possibilities of the proposed approach for the study of microparticles and micro-inclusions of complex composition by methods implemented using synchrotron radiation are demonstrated.

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SUPERCONDUCTING INSERTION DEVICES CONSTRUCTED BY BUDKER INP

Dr Nikolay Nikolay Mezentsev (Budker INP SB RAS)

Description

The main generators of radiation in fourth-generation sources are insertion devices which are installed in special straight sections of light sources. Multipole magnetic systems such as wigglers and undulators are used to produce high brightness due to a large number of magnetic poles. Multipole magnetic systems are manufactured using conventional electromagnets, permanent magnets, and superconducting magnets. A multipole wiggler/undulator type magnet is a sequence of magnets with a changing sign of the transverse field along the electron orbit. The main characteristics of such magnetic systems are the field amplitude, the period of field change, and the pole gap into which a chamber with an ultra-high vacuum is inserted for the electron beam. Despite the progress in the development of permanent magnet systems, the use of superconducting magnets has a fairly large advantage in creating multipole magnetic systems with identical geometric dimensions. The most common material used for superconducting magnets is niobium-titanium alloy in a NbTi/Cu copper matrix. The report provides an overview of superconducting insertion devices already used in various synchrotron radiation centers and are planning to be used in the future on 4+ generation light sources.

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COMPRESSION AND HIGH-PRESSURE TORSION TECHNIQUES FOR DIFFRACTOMETRY IN SYNCHROTRON RADIATION AND NGR-SPECTROSCOPY

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Description

To implement a soft stress state scheme used to obtain high quasi-hydrostatic pressure and large plastic deformations, Bridgman type static anvils and anvils with mutual axial rotation - shear under pressure - are most suitable. The last technique has been given the name high pressure torsion (HPT). This method is widely used to study the features of phase transitions under pressure and also to obtain and study bulk nanocrystalline materials. Depending on the task, anvil punches are used with different bandwidths of x-rays and gamma rays. To study the kinetics, degree, and hysteresis of baric phase transformations, superhard materials with a relatively high permeability of gamma and X-rays are used: cubic boron nitride (c-NB), synthetic sapphire, and also the skeleton - artificial finely dispersed diamond with SiC binder. A vacuum pumping or an inert gas medium is used to create a chemical inert medium. To produce nanocrystalline structures of metals and alloys, the anvil punches made of tungsten carbide with a cobalt binder are mainly used: WC-6. To solve a number of spectroscopy tasks under conditions of high static compression and deformation of materials, a set of HPT methods was created on the basis of hydraulic presses with an effort of 106 and 5 * 10^6 N and also portable cameras for studying *in situ* phase transitions. Operating ranges of varied parameters: pressure 1.0 - 18 GPa, temperature 20 - 800 K, true logarithmic deformation up to ($e \leq 7$). A device for measuring the moment of the resistance force of samples to deformation by torsion was created with conversion to the resistance to torsion. The device is based on a strain gauge and an electronic dynamometer with data transfer and recording to a computer. To avoid the influence of low and high temperatures, the strain gauge is moved away from the anvil block on the lever 0.52 m from the axis of rotation of the anvils. The portable chamber for compression and HPT with anvils made of cubic boron nitride is made of stainless steel. The supporting parts for the c-NB anvils are made of WC -6, the rotating anvil is supported by a thrust bearing. The camera is used *in situ* for two methods: Mössbauer spectroscopy with E = 14.4 eV and also for X-ray diffractometry, mainly on synchrotron radiation (SI) $\lambda = 3685$ nm at the SR beamline №4 of the VEPP-3 storage ring of BINP SB RAS. In the portable chamber, the features and hysteresis of the baric phase bcc-hcp direct and reverse transition both in single-crystal and nanocrystalline samples of pure iron were studied. The exposure time of the spectra using the SI and Mössbauer spectroscopy methods was 1 hour and 60 hours, respectively. The experiments of the samples produced by mechanical alloying by HPT of non-soluble elemental powder mixtures of Fe-Cu, Ag-Cu, Au-Co were carried out. It is found that non-equilibrium nanostructured solid solutions were obtained in all concentrations of powder mixtures.

The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme Pressure No. AAAA-A18-118020190104-3), supported in part by RFBR (project No. 19-32-60039).

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CONSTRUCTION OF A BIOSENSOR SENSITIVE TO TERAHERTZ RADIATION BASED ON THE GLUTAMINE SYNTHASE GENE PROMOTER

Sergey Peltek (Institute of Cytology and Genetics SB RAS (Novosibirsk, Russia))

Description

In this study we performed a differential proteomic analysis of the total E.coli soluble protein fraction after exposure to THz radiation. Glutamine synthase was one of the proteins overexpressed in response to THz radiation. We constructed the E.coli/pGlnA-GFP biosensor

based on the promoter of the glnA gene and the GFP protein and demonstrated that it could detect THz radiation.

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FT-IR INVESTIGATION OF NETLIKE POLYMERIZATION OF SU-8 RESIST LAYERS DURING PHOTO- AND X-RAY LITHOGRAPHY PROCESSES

Dr Elena Reznikova (Budker INP SB RAS) **Co-authors** Dr Vladimir Nazmov (Budker INP SB RAS) Arina Neustroeva

Description

Layers of multi-component SU-8 resist, which includes a diglycidyl ether of bisphenol A novolac as a monomer, were investigated by the FT-IR spectroscopic method for a wave number range of 600 - 5000 cm^{-1} after each step of the photo and X-ray lithography processes (coating, pre-exposure baking, exposure, post-exposure baking, development). The doses of absorbed both photo and X-ray radiation were varied from 0.1 to 6000 J/cm^3 with uniform dose distribution in the layer depth. It was found that the monomers are bonded to each other in initial pre-polymer by means of the end disrupted epoxy groups. The band intensity at the 914 cm^{-1} wave number is decreased after heating of exposed SU-8 layer with an increase of a dose of absorbed radiation because of a disruption of the glycidyl groups. The disrupted bonds of the pre-polymer molecules connect to each other with a net polymer formation, and the intensities of FT-IR spectral bands at 1076, 1110, 1128 and 1150 cm^{-1} are enhanced. In contrast to photolithography, an X-ray exposure results to a disruption of the epoxy groups of the pre-polymer molecules as well as a formation of polymer ester bonds -C-O-C- during both the exposure process and post-exposure baking. The relative quantity of disrupted epoxy groups and the correspondent amount of a new formed polymer bonds in the resist layer are grown with an increase of the dose of the absorbed radiation up to saturation at about 1000 J/cm^3. The dose dependence of a relative number of monomers in the insoluble phase of the residual polymer area after the development process corresponds to the characteristic curve of a relative residual thickness of the resist layer. The dose of about 1 J/cm^3 is a threshold for an appearance of the insoluble phase of the layer on a substrate surface. At approximately 30-60 J/cm^3 the shrinkage and swelling of the layer with the insoluble phase becomes close to zero. The mass ratios of the insoluble and soluble phases in the resist layer in dependence on the dose of absorbed X-ray radiation were determined, the quantity of absorbed photons and the track lengths of photo- and Auger-electrons were calculated in order to model the SU-8 netlike polymerization. The physical-chemical properties of SU-8 polymer, the mechanism and optimization of X-ray lithography processes using synchrotron radiation are discussed.

This work is partially supported by grant №19-42-540014 of Russian Foundation for Basic Research and Government of Novosibirsk Region.

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RELAXATION TIMES OF DONOR BOUND ELECTRONS IN SILICON AND GERMANIUM

Roman Zhukavin (Institute for Physics of Microstructures) **Co-authors** Prof. Boris Knyazev Heinz-Wilhelm Hübers (German Aerospace Center (DLR) and Humboldt University Berlin) Dr Konstantin Kovalevsky (ipm ras) Dr Nils Dessmann (FELIX laboratory, Radboud University) Roman Zhukavin (Institute for Physics of Microstructures) Sergey Pavlov (German Aerospace Center) Valery Shastin (IPM RAS) Dr Veniamin Tsyplenkov (ipm ras) Yulia Choporova (Budker Institute of Nuclear Physics)

Description

The results of pump-probe experiments devoted to investigation of relaxation of bound electrons in elemental semiconductors will be presented. The radiation of free electron lasers was used to excite the donor and measure the relaxation times. Several donors were investigated to uunderstand the common features as well as difference originated from different chemical nature

of particular donor. The uniaxial stress was used to modify the multivalley donor states. The typical relaxation times of bound electrons while emitting acoustical phonons in silicon were measured to be in the range of hundreds or tens of picoseconds. The optical phonon assisted relaxation yields picosecond times. The applied stress allowed to suppess the relaxation rates in the case of the resonances with intervalley phonons. In the case of donors in germanium the typical relaxation times are in the subnanosecond or nanosecond range. The binding energy of group-V donors in germanium is less than optical phonons (10-14 meV) thus the intervalley phonons which could influence the relaxation are of TA type. The stress application to germanium crystal results in increase of lifetimes for some donor states. For the case of Ge:As the pump-probe experiments allow to determine lifetime for 1s split off state. The latter result helps to suppose the possible inversion in the system under optical pumping.
The results of pump-probe experiments devoted to investigation of relaxation of bound electrons in elemental semiconductors will be presented. The radiation of free electron lasers was used to excite the donor and measure the relaxation times. Several donors were investigated to uunderstand the common features as well as difference originated from different chemical nature of particular donor. The uniaxial stress was used to modify the multivalley donor states.

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TEST RESULTS OF THE 7 T SUPERCONDUCTING SOLENOID FOR THz LASER SPECTROSCOPY

Alexey Bragin (Budker Institute of Nuclear Physics) **Co-authors** Dr Vitaly Kubarev Dr Vitaly Shkaruba (BINP) Nikolay Mezentsev (Budker Institute of Nuclear Physics) Dr Sergey Khrushchev (BINP)

Description

This project is related to new spectroscopy method in less researched THz range. The method is founded on using of a free electron laser with high spectral power radiation which can be smoothly tuned in desirable range of spectrum. The objects of research of this method are fast processes in physics, chemical and biological reactions. Uniform magnetic field of 6 T value in the research area can considerably increase possibilities of this method. The magnetic field will modulate free induction decay (FID) radiation of molecules on characteristic frequencies of the Zeeman splitting that gives more possibilities of identification of molecules having even weak magnetic momentum. Moreover, the use of magnetic field allows essentially increase sensitivity of this method due to almost complete polarized separation of weak measuring FID signals from powerful radiation of the laser. The operational characteristics of the superconducting solenoid providing the field up to 7 T will be presented. The magnetic field measurements results will be discussed.

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BEAM-BEAM COMPENSATION IN A COLLIDER BASED ON ENERGY RECOVERY LINAC AND STORAGE RING

Shamil Lachynov (Novosibirsk State University, Budker Institute of Nuclear Physics) **Co-author** Prof. Nikolay Vinokurov (Budker INP)

Description

One of the aims of new circular collider projects is further increasing in their luminosity. The high space charge electromagnetic field at the meeting points limits the achievable current densities and consequently the luminosity. Non-linear focusing compensation in a storage ring done by the opposite-charge beam circulating in another storage ring was proposed and tested many years ago. Ya. S. Derbenev has shown that such a scheme suffers from tune shifts of coherent betatron oscillations, which move betatron frequencies toward the nearest integer or half-integer resonance. In this paper, the collider based on electron energy recovery linac (ERL) and “figure-8” positron storage ring with beams of equal currents is considered. Positrons are circulating in a two-loop storage ring (positron-positron collider), and electron-electron collider

uses ERL, as in original Tigner's proposal. Thus, a collision of four bunches and space-charge compensation in a multi-bunch mode can be ensured. The mathematical and numerical analysis of this configuration is presented.
Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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MAGNETIC FIELD EFFECT ON THE FREE INDUCTION DECAY OF HYDROXYL RADICAL (OH) IN THE TERAHERTZ REGION

Evgeniy Chesnokov (Istitute of Chemical Kinetics) **Co-authors** Dr Vitaly Kubarev (Budker INP) Lev Krasnoperov (New Jersey Institute of Technology)

Description

Effect of external longitudinal magnetic field on the optical Free Induction Decay from a free radical is observed for the first time. The experiments were performed on a rotational transition of hydroxyl radical, OH ($2\Pi 3/2(J=1) \Downarrow 2\Pi 3/2(J=0)$ at 83.8 cm^{-1}) using Terahertz Free Electron Laser. In contrast to the results of the experiments with a stable paramagnetic molecule, NO, the observed effect of external magnetic field on the Free Induction Decay from hydroxyl radicals is more complicated. Longitudinal magnetic field leads to the rotation of the polarization plane of the FID radiation as well as to an additional modulation of the signal intensity. The angle of the rotation of the plane of polarization is large, in agreement with the theoretical predictions. The observed FID kinetics in the time domain are in semi-quantitative agreement with the modeling. This observation opens an opportunity of selective detection of weak signals of short-lived reactive paramagnetic free radicals from overwhelming signals that originate from stable non-paramagnetic species by polarization discrimination.
This work is partially supported by RFBR grant №15-03-05352.

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MAGNETIC MEASUREMENTS IN SMALL APERTURE OF INDIRECT COOLING WIGGLER

Sergey Khrushchev (BINP) **Co-authors** Mr Aleksandr Safronov (Budker INP SB RAS) Artem Zorin (BINP) Askold Volkov (BINP) Nikolay Mezentsev (Budker Institute of Nuclear Physics) Pavel Kanonik (Budker Institute of Nuclear Physics) Valeriy Tsukanov (BINP) Vitaliy Shkaruba (BINP) Dr Vladimir Lev (Budker INP SB RAS)

Description

Several last superconducting wigglers fabricated in Budker INP are of indirect cooling. They all have small aperture with cryogenic temperature. This feature makes measurements enough complicated task. Magnetic measurement system designed especially for one of such wigglers are described in this article. The results of magnetic measurements both by Hall probe and by stretched wire method are also presented.

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EVALUATION OF CCD DETECTOR ABSOLUTE RESPONSIVITY WITH THE AID OF SYNCHROTRON RADIATION

Dr Eugene Vishnyakov (P.N.Lebedev Physical Institute of RAS) **Co-authors** Mr Andrey Shugarov (Institute of Astronomy of RAS) Mr Denis Ivlyushkin (Budker INP SB RAS) Mr Pavel Zavertkin (Budker INP SB RAS) Dr Anton Nikolenko (Budker INP SB RAS) Mr Viktor Chervinskiy (P.N.Lebedev Physical Institute of RAS) Dr Andrey Pertsov (P.N.Lebedev Physical Institute of RAS) Mrs Nataliya Erkhova (P.N.Lebedev Physical Institute of RAS) Prof. Sergey Kuzin (P.N. Lebedev Physical Institute of RAS)

Description

We have employed VEPP-4 synchrotron radiation to measure CCD detector absolute responsivity in vacuum ultraviolet (115-310 nm) spectral range. The detector is designed in the form of a stainless steel enclosure containing a backside-illuminated CCD to protect the CCD

from contamination. The entrance window of the enclosure is a round MgF2 spectral filter transparent for ultraviolet radiation with wavelengths longer than 112 nm. The measurements were carried out at Kosmos Metrological Station at the operating temperature of -100°C on the sensitive surface of the CCD. We utilized SPD calibrated silicon photodiode with 1 cm^2 sensitive area and a known spectral sensitivity profile as a reference detector. The resultant measurements show a clear CCD responsivity dip near 280 nm, and a great potential to improve the CCD responsivity values using specially designed anti-reflection coatings.

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FEATURES OF USING OF THE HARD X-RAYS (60 – 120 KEV) OF SYNCHROTRON RADIATION FOR DETERMINATION THE TRACE CONCENTRATIONS OF RARE-EARTH AND HEAVY ELEMENTS BY THE SRXFA METHOD

Mr Aleksandr Legkodymov (Budker INP)

Description

The analysis of the elemental composition of samples by their X-ray fluorescence spectra were performed at the synchrotron radiation station using radiation from the 9-pole wiggler on VEPP-4M at the Siberian Center for Synchrotron and Terahertz Radiation (SSTRC). The excitation energy for the determination of rare-earth elements (La-Lu) and heavy platinoids (Os,Ir,Pt) and also Au was 60 - 120 keV. The Compton and the multiple scattering of radiation from samples was analysed. The samples Russian and International standarts were used.

The work was done using the infrastructure of the Shared-Use Center "Siberian Synchrotron and Terahertz Radiation Center (SSTRC)" based on VEPP-4M of BINP SB RAS (Novosibirsk, Russian Federation, using equipment supported by project RFMEFI62119X0022. This work is partially supported by RFBR grant 17-45-540618.

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INVESTIGATION OF THE CHEMICAL COMPOSITION OF BOTTOM SEDIMENTS BERING SEA

Ivan Kirichenko (IGM SB RAS) **Co-author** Dr Sergey Gorbarenko (V.I. Il'ichev Pacific Oceanological Institute)

Description

The chemical composition of the bottom sediments of Bering Sea (north-west of the Pacific) was measured by method of X-ray fluorescence analysis using synchrotron radiation (SRXRF) at the collective station, VEPP 3 (Institute of Nuclear Physics, SB RAS). Column length is 560 cm. The study of the chemical composition of this column is a continuation of large-scale work aimed at studying the climate of the North Pacific. The aim of the work is to construct several climate change schemes for the Bering Sea and the subarctic of the Pacific for the characteristic time slices of the last two glacier-ice cycles: the maximum of the last glaciation, the Marine Isotope Stage 4 (MIS 4), the maximum of the last interglacial glaciation (MIS 5.5), the maximum of the penultimate glaciation (Heinrich event 11, MIS 6.2) and the warmest possible MIS 6.5. The general characteristic patterns of orbital and millennial environmental, climate and ventilation changes in the Bering Sea and the Pacific subarctic that have occurred during global climate change over the last two glaciation-ice cycles (190-0 thousand years ago) will be established. Analysis of mutual influence of environment and climate parameters between the subarctic of the Pacific Ocean and the Bering Sea over the last 190 thousand years. The experiment is aimed at studying the distribution of chemical elements, markers of paleoclimatic changes along the core of bottom sediments in order to identify orbital and rapid climate changes in the last two cycles of glaciation-icing. And also to clarify the role of the region in changes in the palaeoceanology of the world's oceans and in the interaction of water and atmosphere that had occurred during orbital and millennial climate changes. As part of the work were obtained distributions of chemical elements (from K to Mo for K-series and U, Th, Pb for L-series) along the column under study in 1 cm steps. The conducted cluster analysis showed the presence of

two large groups of elements. The first one reflects the terrigenous component of the sediment (K, Rb, Nb, Th, Y, Zr, Mo, Ti, Fe, etc.) and the second - biogenic (Ca, Sr, U, Ge, As, Br). In the Fourier and wavelet spectra of the distribution of the chemical elements were found periodically components comparable with periods of D-O events.
This work was supported of the grant RFBR № 19-05-00663

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RECENT EXPERIMENTS IN TERAHERTZ PHOTONICS, PLASMONICS, AND SPECTROSCOPY AT THE NOVOSIBIRSK FREE ELECTRON LASER FACILITY

Prof. Boris Knyazev (Budker INP)

Description

A review is given of the experiments in the field of photonics and plasmonics, recently performed on the Novosibirsk free electron laser (NovoFEL). The parameters of NovoFEL radiation and user workstations are described. Considerable attention is paid to the development and testing of quasi-optical elements designed for this range and to methods for the formation of powerful beams of terahertz radiation with a given mode composition. The use of terahertz radiation in the spectroscopy of gases and semiconductors, in the generation and study of surface plasmon polaritons, as well as the use of the latter for the study of surfaces and in the communication applications, are described.
The work was supported in parts by the RFBR grant No. 15-02-06444 and the RSF grant No. 19-12-00103.

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CALCULATION OF THERMAL LOADS OF X-RAY MIRROR OPTICS OF A SYNCHROTRON RADIATION SOURCE SKIF

Nikolay Razumov (Институт химии твердого тела и механохимии Со РАН) **Co-author** Prof. Boris Tolochko (Institute of solid state chemistry and mechanochemistry SB RAS)

Description

The work is devoted to the problem of the occurrence of large thermal loads on x-ray optics when it is irradiated with a 69 kW synchrotron radiation beam from a superconducting wiggler installed on a SKIF synchrotron radiation source. The task was to reduce the temperature gradient on the surface of the mirror, which lead to mechanical thermal stresses and, consequently, to geometric distortions of X-ray mirrors. The task of this work was: 1) calculation of the thermal load on X-ray mirror optics when it is irradiated with a synchrotron radiation beam with a power of about 80 kW, which leads to a temperature gradient and, accordingly, to mechanical thermal stresses, which lead to geometric distortions of X-ray mirrors; 2) choosing the geometry of the cooling system; 3) choosing a refrigerant for the cooling system; 4) optimization of the exposure time of x-ray mirror optics of the experimental station "Fast processes"; 5) conducting test (calibration) experiments to study the heating of elements of X-ray mirror optics on beams of synchrotron radiation from the wiggler of the VEPP-4 accelerator. In this work, we simulate the heating of an X-ray mirror for synchrotron radiation from the SKIF superconducting wiggler, as well as for the VEPP-4M wiggler. The beam characteristics, such as power, divergence, and spatial distribution, are calculated. In the calculation of the emission spectrum, the SPECTRA program was used. To calculate the passage of synchrotron radiation

through the material of filters and mirrors, as well as to calculate the reflected spectrum from the mirror at the angle of total external reflection, the XOP 2.3 program was used. Using the data obtained, the distribution of the thermal power of the beam in the near-surface layer of the mirror was simulated. Further, using the obtained distribution and the ANSYS Workbench program, the local heating of the X-ray mirror under various modeling conditions was calculated, which made it possible to construct a map of the temperature distribution over the mirror surface. A control experiment was carried out to measure the surface temperature of a mirror when irradiated with a SI beam from a VEPP-4 wiggler. This made it possible to verify the calculations performed by the ANSYS Workbench codes. In the case of VEPP-4M, the mirror was cooled convectively by air. For the SKIF wiggler, computer simulation of radiation heating of a mirror was calculated for various cases, both of the cooling geometry and of various refrigerants, including liquid nitrogen.
This work was supported by RFBR grant 16-29-01050.

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NUMERICAL SIMULATION OF THE INTERACTION OF TERAHERTZ WAVES WITH DIFFRACTION METAL GRATINGS AND CONDITIONS FOR THE GENERATION OF SURFACE PLASMONS

Mr Oleg Kameshkov (Bukder INP) **Co-authors** Prof. Boris Knyazev, Dr Vasily Gerasimov (Budker INP)

Description

In the terahertz plasmonics, it is widely used wavelength 1D grooved metal gratings for excitation of surface plasmon polaritons (SPPs). SPPs are traveling charge density waves at the surface of conducting materials. Since these modes have a non-radiative nature, it is possible to excite them only if the configuration providing the wavevector-matching condition between the incident light and SPP dispersion law. The wavelength gratings are the most suitable and cheaper solution to satisfy this requirement. The careful optimization of the most suitable experimental parameters by the numerical simulations leads to the enhancement of surface plasmon resonance response. In this paper, numerical results of grating optimization with different groove profiles are discussed. The work was supported by RFBR grant 18-32-20226.

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FIRST EXPERIMENTS ON NEW SYNCHROTRON RADIATION TECHNOLOGICAL STATION ON THE VEPP-4M

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Description

A new synchrotron radiation technological station at beamline #1 from the VEPP-4M storage ring was constructed and experimental work started. The station is intend for practical training of students to carryout experiments on synchrotron radiation. The modular concept of construction of station allows us to put station in to operation in stages, also it allows us to realize various research methods. The article presents the design of the station, SR beam characteristics and test experiments on X-ray fluorescence analysis.
This work is partially supported by RFBR grant № 19-05-50046. The work was done at the shared research center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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THE CONDUCTION BAND OF THE LANTHANIDE DOPED CHROMIUM DISULFIDES CuCr0.99Ln0.01S2 (Ln=La, Ce, Gd): XANES INVESTIGATIONS

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Description

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], the ionic conductivity [2], the helimagnetic arrangement [3-4], 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-xMxS2 exhibit promising thermoelectric properties. The key aspect to control the electrophysical properties of thermoelectric materials is the understanding of 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. 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. Thus, this study involves a purposeful synthesis of the lanthanide doped solid solutions CuCr0.99Ln0.01S2 (Ln=La, Ce, Gd) and detailed study of their electronic and band structure. A comprehensive experimental and theoretical study of the X-ray absorption edges of the matrix elements and doped-lanthanide atoms in the cation-substituted disulfides CuCr0.99Ln0.01S2 was carried out. Based on the obtained results, the cationic substitution with lanthanide atoms affect to the conduction band structure was studied.

The study was carried out with a funding from the Russian Science Foundation (project No. 19-73-10073). The software program design for the experimental XANES spectra shape correction was supported by RFBR grant №16-32-00612.

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STATUS OF THE DEVELOPMENT OF THE SILICON MICROSTRIP DETECTOR FOR ULTRA-FAST DYNAMIC STUDIES

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Description

New silicon microstrip detector for ultra-fast dynamic studies is being developed in the Institute of Nuclear Physics SB RAS. The first prototype of such detector with a silicon sensor with 50 um strip pitch, 30 mm strip length and with 96 active channels equiped with specially developed ASIC is now operating at the SR beam line 8 of the VEPP-4M storage ring. The new prototype demonstrated about 20 times higher limit of the detected photon flux that the detector can measure as compared to the current detector DIMEX-G, based on gas technology. Spatial resolution of the new prototype is ~4 times better and frame rate is about 6 times higher than in the gaseous detector. The first results of operation in multi-bunch mode with VEPP-4M storage ring will be demonstrated in the presentation.

This work is supported by RFBR grant number 19-42-540006.

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SUPERCONDUCTING 3 TESLA 54-POLE INDIRECT COOLING WIGGLERS WITH A PERIOD OF 48 MM FOR KURCHATOV SYNCHROTRON RADIATION SOURCE

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Description

Two identical 54-pole indirect cooling wigglers with a 3 Tesla magnetic field and a period of 48 mm were designed and manufactured by BINP SB RAS as the insertion devices for X-rays generation on the Kurchatov Synchrotron Radiation Source. After being delivered to the Kurchatov Institute these wigglers were tested in 2019 with a full test cycle to demonstrate operating parameters and installed on the storage ring for commissioning with electron beam. The main features of magnetic and cryogenic system design and tests results of these superconducting insertion devices capable of autonomous operation for a long time on the storage ring without maintenance and consumption of liquid helium are presented.

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ANALYSIS OF THE INDIVIDUAL ANNUAL LAYERS ELEMENTAL COMPOSITION IN THE LAKE KUCHERLINSKOE (ALTAI) VARVES SEDIMENTS WITH SUBMICRON SPATIAL RESOLUTION BY SCANNING MICRO_XRF-SR WITH X-RAY OPTICS (POLY CAPILLARY LENSES)

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Description

Samples for analysis (optical thin section) were prepared for several core intervals of Lake Kucherlinskoe bottom sediments with well visually distinguished separate annual layers (varves). The annual nature of the layers was previously confirmed by the coincidence of varvechronology (layer counting) with isotopic dating (Cs-137, Pb-210, C-14). The thickness of the annual layers ranged from <1 to 3-4 mm. To study the internal structure of annual layers, we used the scanning micro_XRF-SR with focusing x-ray optics (poly capillary lenses). The experiments were carried out at the Siberian Center for Synchrotron and Terahertz Research (INP SB RAS, Novosibirsk) and the Kurchatov Complex of Synchrotron-Neutron Research (KISI, Moscow) using a confocal X-ray microscope, as well as at the Shanghai Synchrotron Center at the micro_XRF-SR station. The excitation energy in all cases was 22 keV. The size of the scanning spot was determined by the used focusing poly capillary lenses and amounted to 15-25 microns.The scanning step coincided with the exciting radiation spot size on the sample. The measurement time was determined by the counting rate and ranged from 10 to 100 seconds per point. Scanning profiles were superimposed on the optical images of the thin section obtained with a high-resolution scanner. Given that the thickness of the thin section is less than 20 μm, a change in elemental composition reflects visual changes in the structure of the bottom sediment. Thus, while tracking visual changes in the structure and elemental composition of individual annual layers, seasonal geochemical features and boundaries between the layers can be distinguished. The obtained changes in the elemental composition made it possible to calculate the annual layers by the found lithological and geochemical indicators of the layer boundaries (Rb / Sr ratio).

The work was carried out in the framework of the RFBR projects no. 19-05-50046. The work was done at the shared research center SSTRC on the basis of the VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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COMPARISON OF THE GEOCHEMICAL PROFILES OF LAKE KHINDIKTYKOL (TUVA) BOTTOM SEDIMENTS CORES ACCORDING TO THE SCANNING μXRF-SR

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Description

Two cores (67 and 105 cm) of high mountain Lake Khindiktykol (Tuva) bottom sediments were sampling by a hummer gravity corer from depths of 64,7 m in the middle of the lake and of 31,3 m in the small bay. The upper 170 mm of each core was studied by scanning micro-XRF with synchrotron radiation (μXRF-SR). The analysis was carried out at the experimental station "Elemental analysis" in the joined Research Center SSTRC. Experimental conditions: excitation energy 23 keV, dimensions of the exciting radiation beam 1.5 mm in height and 10 mm in width of the sample. The scanning step was 2 mm in height of the sample. The distributions of more than 20 rock-forming and trace elements over the core depth were obtained. The distribution of Ti, Mn, Fe, Ni, Ga, Y in both cores coincides well. This suggests one source of terrigenous material and similar sedimentation rates. Large discrepancies are visible in the distribution of Ca, As, Br, Sr, Mo. These elements are characteristic of carbonates and biogenic material. The obtained data indicate differences in the sources of matter entering the bottom sediments in different parts of the lake. Additional lithological and geochemical studies are required when choosing bottom sediments will be used to climatic reconstructions.

This work was financially supported by the RSF project. № 20-17-00110. The work was done at the joined Research Center SSTRC on the basis of the VEPP-4 - VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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STUDY OF AU-CO ULTRAFINE GRAINED ALLOY BY SYNCHROTRON RADIATION DIFFRACTOMETRY

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Description

Ultrafine grained Au-Co alloys were prepared by high pressure torsion (HPT) technique. The severe plastic deformation was carried out at room and cryogenic temperatures. A consolidated alloy is formed from the initial powder mixture of metals in an equiatom ratio after mechanical alloying. Then, synchrotron radiation diffractometry of the obtained samples was carried out. It was found that after deformation at room temperature an fcc substitutional supersaturated solid solution formed. Changing the deformation temperature to cryogenic leads to greater dissolution of Co. This result corresponds to the increased mechanical and physical properties of the Au-Co alloys after cryo-HPT processing than after room one.

Diffraction experiments were performed at the SR beamline №4 of the VEPP-3 storage ring. The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme “Pressure” No. AAAA-A18-118020190104-3), supported in part by RFBR (project No. 19-32-60039).

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A STEP-WISE TAPERED UNDULATOR FOR THE QUICK-EXAFS BEAMLINE AT THE SIBERIAN CIRCULAR PHOTON SOURCE

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Description

Synchrotron radiation (SR) provides a powerful tool for studying materials with X-rays in a wide energy range. A combination of high photon flux and flexibility in photon energy tunability allows exploiting SR for absorption and emission spectroscopy techniques such as XAS, XANES, XES. Some sophisticated techniques like, for example, quick X-ray Absorption Fine structure (qXAFS) spectroscopy allow to quickly measure the XAS spectrum. qXAFS is based on the use of a fast monochromator that scans through a broad spectral range (1 keV) providing data acquisition in less than 100 ms. However, modern SR sources equipped with superconducting undulators require new approaches for generating radiation with such bandwidth and still retain the advantage of undulator radiation compared to other broadband sources. In this research, we propose to use a stepwise tapered magnetic field configuration for the superconducting undulator: we gradually change the magnetic field along the device. An undulator is effectively split into cells, each with a slightly different magnetic field, such that a given harmonic of the radiation emitted in each cell is shifted by half of its bandwidth. The contribution from the segments sums up to a continuous spectrum with the desired total bandwidth of 1 keV. We studied the performance of this device both analytically and numerically including propagation of the emitted radiation up to the sample location. We also studied how propagation and spatial filtering affects radiation spectral density. This research serves as a conceptual design for the quick-EXAFS beamline at the Siberian Circular Photon Source (SKIF — the Russian acronym) in Novosibirsk, Russia.

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METHOD FOR POLARIZATION SHAPING AT FREE-ELECTRON LASERS

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Description

X-ray free-electron lasers (FEL) deliver high-power, ultra-short polarized X-ray pulses, where the polarization state is determined by the electron beam trajectory in the FEL undulator. In this way, the polarization state depends on the kind of a magnetic structure used, and is fixed along the entire pulse. However, it would be beneficial to control the dependence of the polarization shape on time over the scale of one single pulse duration (about tens of femtoseconds). Such radiation may enable study of ultrafast molecular dynamics and magnetism. In this contribution, we discuss a new method to control the polarization state of a single FEL pulse longitudinally (in time) and/or transversely (spatially) on the scales of 100 femtoseconds and several micrometers respectively. We propose to use a crossed-undulators setup consisting of a pair of two co-axial Apple-X undulators. These undulators are scheduled for installation downstream the nominal SASE3 undulator line of European XFEL and they may be tuned to emit radiation pulses with two orthogonal polarization states, e.g. linear (vertical and horizontal) or circular (right and left). Both pulses upon reaching the sample are overlapped both spatially and temporally with some phase difference. Their interference yields polarization states, circular or linear respectively, with orientation that depends on that phase difference. If the frequency of one of the pulses is detuned, polarization of the resulting radiation will be shaped temporally. If the distance between the undulator cells is considerable, a difference between the wavefront curvatures allows shaping the resulting polarization spatially. We investigate possibilities to maximize or minimize both effects with a focusing system and demonstrate it with numerical simulations.

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LINEAR DICHROISM OF NEXAFS SPECTRA AND MOLECULAR ORIENTATION IN POLYPYRROLE AND POLYANILINE FILMS ELECTRODEPOSITED ON HOPG AND VITREOUS CARBON

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Description

In this work, we have studied the structural anisotropy of polyaniline and polypyrrole films depending on the type of conductive carbon substrates, including highly oriented pyrolytic graphite (HOPG) and vitreous carbon being a fullerene-like material in its structure. The NEXAFS spectra were measured at both carbon and nitrogen K absorption edges. To analyze the chemical structure of the polymers, X-ray photoelectron spectra were additionally measured. The measurements were performed at the Russian-German beamline at BESSY II (HZB, Berlin). It has been found that polyaniline films are predominantly disordered, regardless of the substrate material used. Most polypyrrole films have shown a pronounced dichroism of the NEXAFS spectra, indicating their structural anisotropy. The nature and intensity of the changes observed in the NEXAFS spectra when varying the measuring geometry turned out to be the same for the HOPG and vitreous carbon for most of thin films, which indicates a weak effect of the substrate structure on the molecular arrangement of polypyrrole films. The spectra measured at both edges have shown a significant decrease in π^* resonances observed on going from grazing incidence to normal one. Based on the data obtained, the tilt angle has been estimated to be approximately 40 degrees for the pyrrole rings of the polymer. It has been found that the substrate affects molecular arrangement only in thick long-term-deposited films. In contrast to HOPG, the films deposited on vitreous carbon have shown greater fraction of charge carriers, which are bipolarons and quaternary nitrogen derivatives, in the polymer structure. Such films have demonstrated a relatively weak linear dichroism of the spectra, which may indicate a disordering of the films due to the indicated change in the chemical structure of the polymer.

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SUPERCONDUCTING ELLIPTICAL UNDULATOR

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Description

Circularly polarized photons are widely used for conducting experiments to study the magnetic structures of matter. On the basis of superconducting coils developed at the Budker Institute of nuclear physics for a short-period superconducting planar undulator, a superconducting elliptical undulator with a period of ~2.2 cm and an elliptic coefficient of ~ 0.7 is proposed. The poles of the upper and lower halves of the undulator are located at an angle of 45 degrees to each other in the horizontal plane, which creates a periodic vertical and horizontal elliptical field of up to 1 T vertically and 0.7 T horizontally. There is a possibility to create a fast switching left and right polarizations of radiation at a zero angle from two sequentially installed undulators by quickly switching the electron orbit using correction magnets external to the cryostat (up to hundreds of Hertz). A short prototype of an elliptical superconducting undulator was made and magnetic measurements were made in the bath cryostat. The paper presents numerical calculations of the undulator fields, its spectra, and the experimentally measured field.

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SUPERCONDUCTING UNDULATOR WITH A VARIABLE CONFIGURATION OF THE MAGNETIC FIELD

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Description

Based on coils developed at the Budker Institute of nuclear physics for a superconducting undulator with a period of 15.6 mm, a model of a superconducting undulator with variable polarization (SCUVP)with a period of ~32 mm is proposed. The undulator consists of two superconducting undulators placed mutually perpendicular and powered by currents independently. Depending on the different currents values in the windings of the undulator, there is a possibility to create both an elliptical undulator with different elliptic coefficients, and planar undulators with linear radiation polarization at a zero angle both horizontally and vertically. The paper presents numerical calculations of the undulator fields and its spectra.

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SYNCHROTRON RADIATION APPLICATION IN THE BINP

Konstantin Zolotarev (Budker Institute of Nuclear Physics)

Description

The Siberian Siberian Synchrotron and Terahertz Radiation Center is the oldest Russian center for synchrotron radiation applications. The center combines the research efforts of numerous scientific groups, mostly from institutes of the Novosibirsk Scientific Center, as well as groups from institutes and universities of other Russian cities. The center provides research groups with access to most popular synchrotron radiation applications and research techniques. A big part of the activity is devoted to developing new original approaches for synchrotron radiation usage. The report covers activity on synchrotron radiation applications at the Siberian Synchrotron and Terahertz Radiation Center, as well as some bright results of recent research.

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PULSED WIRE FIELD MEASUREMENTS OF 38-PERIOD SUPERCONDUCTING UNDULATOR PROTOTYPE

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Description

In this paper, a pulsed wire method (PWM) for magnetic measurements was described. Experimental setup was developed and assembled. The results of measurements on superconductive 38-pole 0.75 T undulator are given. Two different wires were used – 200μm and 140 μm diameter. For 140μm the calibration curve was obtained, wire position sensor has high sensitivity – 0.28 V/μm. A dispersion correction algorithm was applied to the raw data from sensor and corrected signals were given. The results and further works are being discussed.

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IN SITU SYNCHROTRON X-RAY DIFFRACTION STUDY OF FACE-CENTERED CUBIC PLATINUM HYDRIDE AND PHASE DIAGRAM OF PTH

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Leonid Dubrovinsky (Bayerisches Geoinstitut, Universitaet Bayreuth) Dr Sergey Rashchenko (Sobolev Institute of Geology and Mineralogy, SB RAS)

Description

Recent extensive research on high-temperature superconductivity in compressed binary hydrogen-rich compounds generat-ed a large corpus of phase stability calculations with an evident lack of their experimental verification. Pt-H system at high pressure represent a typical example of inconsistency between computational approach, which predicted stability of eight PtH structures, and experiments revealing the existence of only two modifications: hexagonal close-packed (hcp) PtH (alt-hough at drastically lower pressures than predicted), and trigonal PtH (not foreseen by ab initio calculations). Of particular interest is face-centered cubic (fcc) platinum hydride - a product of hydrogen intercalation into the native structure of fcc Pt. This phase was predicted to be nearly isoentalpic to the hcp PtH and stable between 93 and 105 GPa, but has been never observed experimentally. Here we report the first synthesis of the fcc PtH using laser heated diamond anvil cell. The fcc plat-inum hydride was found to occupy high-temperature area of the phase diagram in a wide pressure range of 20 – 100 GPa. It can be quenched, although with partial transformation into the hcp phase, thus being metastable at room temperature. Our results look promising for uncovering weak approximations in current ab initio approaches, used for computational model-ling of high-pressure hydrides stability. Moreover, here we clarify the view on the inertness of Pt as a heat absorber in laser-heating high-pressure experiments with hydrogen-containing systems.The research was carried out at PETRA III (DESY), P02.2 Extreme conditions beamline, proposal #I-20180048.

This work was supported by RFBR grant №18-35-20047.

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THE STUDY OF THE AEROSOL IMPURITIES SEASONAL ACCUMULATION IN A SNOW COVER BY SCANNING μXRF-SR

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Description

Snow cover is an ideal deposition medium in which aerosol particles of both natural and technogenic origin are fixed and accumulated during the winter period. As a rule, environmental studies analyze the total amount of aerosol accumulated. This paper presents a study of the aerosol accumulation dynamics in the vertical section of snow cover with high spatial (temporal) resolution. Sampling over the entire height of the snow cover accumulated during November 2019 - March 2020 was carried out on the Novosibirsk region territory using polypropylene pipes with a diameter of 100 mm and a length of 1 m. The cores were selected to the entire depth of the snow cover to the base. After that, the pipe was shut up from below by a tight stopper, and from above the snow was pressed by the top stopper to a total core height of 40 cm. This was done to achieve a uniform snow density over the entire core height. Mixing of snow layers did not occur. Samples were transported to the laboratory of the IGM SB RAS in a frozen state. The pipes were opened along the sampling axis and placed horizontally in a plastic box, cooled with liquid nitrogen. Snow sublimated during the day without the formation of a liquid phase. The solid components remaining in the pipe were transferred onto a conductive adhesive tape without disturbing their vertical distribution. The analysis was carried out using the μXRF-SR according to the standard certified method at the experimental station "Elemental analysis" in the shared research center SSTRC. Experimental conditions: excitation energy 23 keV, dimensions of the exciting radiation beam 1.0 mm in height and 10 mm in width of the sample. The scanning step was 1 mm in height of the sample. The distributions of more than 20 rock-forming and trace elements over the sample depth were obtained. The data obtained make it possible to calculate the dynamics of aerosol accumulation. Analysis of individual particles is used to identify their sources.

The work was carried out in the framework of the RFBR projects no. 19-05-50046. The work

was done at the shared research center SSTRC on the basis of the VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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SEARCH FOR AND ANALYSIS OF COMPOSITION AND STRUCTURE OF SUBMICRON-SIZE PARTICLES IN GEOLOGICAL SAMPLES

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Description

A technique combining SR XRF, XRF mapping, μ-XRF, and μ-XAFS for search for microparticles in different matrices and determination of particle size, as well as analysis of their composition and structure, has been developed at Budker Institute of Nuclear Physics. The technique is based on comprehensive examination of sample with gradually increasing the spatial resolution and constricting the study area for locating the desired microparticle. The beam size for preliminary studies ranges from 1 mm to 100 um in height and 10 mm in width. The next stage is examination using X-ray optics (polycapillary lenses) with single-lens and confocal schemes. The apparatus function of each lens is measured, which enables controlled variation of the focal spot size from 10 um to 70 um. This multifacet technique was tested on search for and study of micro-inclusions of light platinum group metals (Ru and Pd) in Bushveld (South Africa) Intrusive Complex samples. An area with high concentration of Pd has been found. The particle sizes (~ 50 um) have been identified. A localized particle was studied using the μ-XAFS method. Forms of Pd stabilization in the particle have been established; their structural parameters (interatomic distances and coordination numbers) have been determined.

The work was carried out in the framework of the state assignment for IGM SB RAS and RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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MEASUREMENT OF THE RESIDUAL STRESSES DYNAMICS IN TUNGSTEN DURING HEATING

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Description

In a thermonuclear reactor plasma interacts with the divertor walls in the form of periodic heat pulses as well as constant heat load. As a result, residual plastic deformations and mechanical stresses can occur, which cause destruction of the divertor material. However, these residual deformations and stresses can be relieved under the influence of constant flux of plasma and the consequential high temperature of the material. The goal of this work was the study of residual stresses dynamics in a heated 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. To compare heat load and residual stress profiles the measurements were conducted with spatial resolution. SR scattering station “Diffraction movie” was used for measuring the dynamics of residual stresses during heating. As a result of these experiments scattering angle – temperature dependencies were obtained. Residual stresses relaxation was measured and turned out to be ~75 MPa.

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TERAHERTZ PHOTONICS OF DENCE MEDIUM: FROM GAS TO LIQUID

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Description

We present results of our research on generation of THz radiation in liquid nitrogen. We used a dual-frequency scheme when emissions of the main laser frequency and its second harmonic are mixed in the same medium. The research showed a possibility of effective conversion of optical radiation into THz radiation.

Summary

The source of electromagnetic radiation in the THz band on the basis of laser spark was firstly presented in many years ago. An experiment in which a liquid, namely, water was used for the conversion of femtosecond radiation into the THz one is also described. Water is a polar liquid which has high absorption in the THz frequency range and the authors of previously published works have to use for the experiments the very thin water films. Unlike water, considerable absorption both in THz and NIR ranges is absent in liquid nitrogen. In our experiments the laser beam ω is directed vertically from top to bottom with the help of a set of mirrors and is focused by a lens inside the LN in Dewar vessel. The Dewar vessel is mounted on a microscopic translation stage and can be moved vertically, which enables the regulation of the position of the lens focus regarding the surface level of the LN. THz radiation generated in the beam-waist is reflected from a flat aluminum mirror and is collimated by the parabolic mirror.

First of all, we obtained the THz radiation with the use of a dual frequency scheme in an experimental set-up without liquid nitrogen, from a routine optical air breakout. After that, the laser beams on the fundamental and the second harmonic was focused into LN and the THz radiation was also observed. IN the talk we show the dependences of the THz pulse energy on the lens focus position regarding the surface of liquid nitrogen (the laser beam waist is located inside the liquid if $z < 0$ and in the air if $z > 0$). The intensity of the generation changes exponentially as the beam-waist position varies and a and a leap in the level is observed when the level of the surface is passed.

Also we have studied how THz yield scales with laser pulse duration and its energy, angle of rotation of the BBO crystal and measured spectra of the THz radiation.

The present work describes broadband generation of THz radiation first obtained in liquid gas. Unlike previous attempts to generate THz radiation in water, in our experiments we used liquid nitrogen, and the results enabled us to suggest a physical mechanism of this process.

This work is partially supported by RFBR grant №18-29-20104.

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ЧЕГО ХОТЯТ ПОЛЬЗОВАТЕЛИ В ОБЛАСТИ МАКРОМОЛЕКУЛЯРНОЙ КРИСТАЛЛОГРАФИИ ОТ СОВРЕМЕННОГО СИНХРОТРОНА?

Sergey Arkhipov (Novosibirsk State University)

Description

В докладе будут рассмотрены основные потребности пользователей синхротронного излучения, задачей которых является рентгеноструктурный анализ монокристаллов биополимеров (белков, нуклеиновых кислот и их комплексов) и дальнейшая расшифровка структуры, необходимая для решения изначально поставленной биологической задачи. Для сбора информации автор консультировался с исследователями, регулярно проводящими эксперименты на станциях различных синхротронов (ESRF, DESY, SSRF, Spring-8, MAX IV), изучал тематическую литературу и информацию представленную в

базе данных кристаллических структур биополимеров (PDB, protein data bank). Будут затронуты техники сбора данных и доставки кристаллов для метода "серийной синхротронной кристаллографии" (SSX) и требуемое для этого оборудование, подходы к уменьшения радиационного разрушения образца, значение кристаллизационных комнат в непосредственной близости от синхротрона, методы транспортировки кристаллов на экспериментальную станцию, подходы к сбору данных без извлечения кристаллов из кристаллизационного резервуара.

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HIGH ENERGY IMAGING AND DIFFRACTION AT DIAMOND LIGHT SOURCE BEAMLINE I12: 11 YEARS OF EXPERIENCE AND LESSONS LEARNED

Dr Thomas Connolley (Diamond Light Source)

Description

The I12 Joint Engineering, Environmental and Processing (JEEP) beamline, was constructed during Phase II of the Diamond Light Source. The beamline started operating in November 2009. It is located on a short (5 m) straight section of the 3 GeV Diamond storage ring. The insertion device is a 4.2 T superconducting multipole wiggler. User experiments are possible with filtered white beam or monochromatic X-rays in the energy range 53-150 keV from a bent Laue monochromator. The beam energy enables good penetration through large or dense samples, combined with a large beam size from the wiggler fan (1 mrad horizontally × 0.3 mrad vertically). These beam characteristics permit the study of materials and processes inside environmental chambers and on sample sizes that are more representative of bulk materials. X-ray techniques available are radiography, tomography, energy-dispersive diffraction and monochromatic 2D diffraction/scattering. I12 has established a broad user community in materials science and processing, chemical processing, biomedical engineering, civil engineering, environmental science, palaeontology and physics. The majority of experiments are time resolved, in-situ studies, often involving processing equipment brought by users.

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ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY (I05-ARPES) BEAMLINE AT DIAMOND: GETTING INSIGHT INTO ELECTRONIC STRUCTURE OF SOLIDS

Timur Kim (Diamond Light Source)

Description

Angle-resolved photoemission spectroscopy (ARPES) has proven to be particularly successful for the investigation of the electronic structure of solids and their surfaces. A synchrotron radiation beamline in a vacuum ultraviolet (VUV) to soft x-ray photon energy range of 18-240 eV and a photon flux up to 2·10^13 ph/s have been constructed at the 3 GeV Diamond Light Source storage ring. The instrument features a variable polarisation undulator, a high resolution monochromator, a re-focussing system to form a beam spot of 50 × 50 μm2. The end station for high resolution photoemission spectroscopy includes a 6-degrees-of-freedom cryogenic sample manipulator operating in the range from 7-300K. The beamline design and its performance allow for a highly productive ARPES experiments at an energy resolution of ~10 meV for fast momentum-space mapping studies and at 3 meV for high resolution measurements.
Second branch has nano-ARPES end-station that uses a scanning microscopy piezo driven sample stage and a photons in the energy range 60-100eV. Photon beam is focused to sub-micron beam-spot using Fresnel Zone plates. Sample can be cooled down to 25K, giving total energy resolution of about 30meV.
The overall high productivity of the instrument performance is best judged by the publication output - see website of I05–ARPES beamline for more information (http://www.diamond.ac.uk/I05).

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THz GYROTRONS: NOVELTY, ACHIEVEMENTS AND APPLICATIONS

Mikhail Glyavin (IAP RAS)

Description

THz Gyrotrons: novelty, achievements and applications

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STUDY OF THIACALEXARENE CONFORMATION EFFECT ON THE ELECTRONIC STRUCTURE BY X-RAY ABSORPTION SPECTROSCOPY AND QUANTUM CHEMISTRY METHODS

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Description

Calixarenes (CA) and thiacalixarenes (TCA) are macrocyclic compounds. Calixarenes (CA) and thiacalixarenes (TCA) structure include the upper and lower rims. These molecules can be in cone conformation, partial cone, 1,2-alternate and 1,3-alternate. An important feature of CA and TCA is the ability to functionalize molecules by substitution of upper and / or lower rims by different functional groups, substitution of methylene bridges for S, SO, SO2, N, NO bridges, etc., and by changes the conformation of molecules. This makes it possible to widely change the selectivity and binding efficiency of various substrates [4], which allows them to be used in extraction processes, and opens up great opportunities for the use of CA and TCA molecules in various fields of chemistry, biology, and physics.

Accordingly, the question arises of the effect of conformation on the electronic structure and, as a consequence, on the physical and chemical properties of CA and TCA molecules. The methods of X-ray emission (XES), X-ray absorption spectroscopy (XANES, EXAFS) and X-ray photoelectron spectroscopy (XPS), as well as quantum-chemical methods are highly characteristic and effective methods for studying the electronic structure of various chemical compounds.

In this paper, we studied the electronic structure of TCA molecules by XES, XPS, XANES, and quantum chemistry. The influence of molecular conformation on RES and XANES was studied. The X-ray absorption spectra of the acyclic molecule TCA and cone conformation and 1,3-alternate were obtained. Quantum-chemical calculations of TCA molecules electronic structure in the cone 1,3-alternate conformation were carried out by DFT in the ADF software package. Carbon XANES spectra were calculated in the ground state of the molecules and the Z+1 model by ADF software package and by FMDNES program. The experimental K-edges of carbon absorption of TCA molecules cone, 1,3-alternate and acyclic molecules are compared and compared with the results of quantum chemical calculations. Based on the carried out theoretical calculations, it was shown that, the LUMO of the studied TCA molecules were constructed with the participation of 2p AO carbon atoms of CH, CS, CO fragments constituent TCA. It is also shown that, when passing from cone conformation to 1,3-alternate conformation, the LUMO structure changes and the contribution of 2p AO CH fragments becomes dominant.

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SMALL-ANGLE SCATTERING APPLICATIONS TO THE ANALYSIS OF APTAMER STRUCTURE AND CONFORMATIONAL CHANGES

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Description

At present different agents are developing for diagnostics and treatment of cancer - one of the main reasons of human deaths. Especially perspective examples are aptamers - single-stranded DNA or RNA molecules which are compact analogs of the antibodies with low immune response, have a short length (10-100 nucleotides), well-defined spatial structure and surface charge distribution providing highly specific binding with their targets - proteins in the tumor cells. It allows one to use aptamers as the agents for the visualisation the cancer cells and tissues in organism and also as the carriers for active molecules, labels, nanoparticles, toxic entities to deseased tissue cells. To define the function and parameters of the activity for the aptamers and to localize the specific binding epitopes on the surface of both aptamers and the target proteins, it is necessary to know the spatial structure of these molecules. For this purpose the Small-Angle X-ray Scattering (SAXS) method was used, which is applied in a high quality at the synchrotron radiation sources due to the high intensity of the emitted X-rays, ability to change the wavelength and beam size for the experiment. SAXS method is used to carry out the measurements on the biomolecules in solution, without crystallisation which is mostly impossible for single-stranded nucleic acids. One can create a native environment for the molecules under study, or inversely to track the conformational changes during varying temperature, pH and other parameters. Here we present the results of revealing and adjusting the 3D spatial structures of the DNA molecules using the SAXS method in solution and the molecular simulation method based on the experimental SAXS data. This combination yields an information about the molecule structure, possible conformational changes, parameters of the aptamer-protein complexation, that in a perspective will be useful to optimize the development procedure of the theranostics agents against the socially important deseases.

This work is partially supported by RFBR grant №18-32-00478.

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STUDYING THE EFFECTS OF ELECTRON BEAM IRRADIATION ON THERMAL PROPERTIES AND PARTICLE SIZE DISTRIBUTION OF MAGNESIUM HYDROXIDE

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Description

The aim of this work is to study the effects of electron beam irradiation on thermal properties and particle size distribution of magnesium hydroxide. The sample was irradiated by the high-energy electron beam at the different irradiation doses in air at room temperature. The high-energy electron beam was generated by electron accelerator model ILU-6 which is located in BINP SB RAS, Novosibirsk, Russia. The changes of thermal behaviours and particle size distribution of studied sample were analyzed by using thermogravimetric analysis/ differential scanning calorimetry, SR-XRPD and image analysis, respectively. The TGA and DSC data show that there was no changes occuring in Tmax (the temperature of maximum rate of mass loss) values of the sample before and after irradiation. However, the irradiated sample began to lose mass at the lower initial temperature as compared with this temperature of the sample without irradiation and the quantities of released water of irradiated specimen are higher than these values of non-irradiated one. In addition, DSC profiles indicate that the endothermic effects of irradiated sample are stronger than that of the sample without irradiation. The SR-XRPD results also agrees with the previous TGA and DSC results. The the median particle size value (d50) of all irradiated samples is lower than d50 of non-irradiated one. The results of studying of thermal

behaviours and particle size distribution of magnesium hydroxide before and after modifying by high-energy electron beam irradiation in this work are possitive and greatly important, especilally in studying polymer composite materials using magnesium hydroxide as a flame retardant. All results indicate that high energy electron beam irradiation significantly improve the flame-retardant properties of studied magnesium hydroxide.
This work was supported by RFBR grant 19-29-12045 and Ministry of Science and Education of Russia grant AAAA-A17-117030310280-6.

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SINGLE-COLOR PUMP-PROBE SETUP AT THE NovoFEL FACILITY FOR MEASURING THE TEMPORAL DYNAMICS OF RELAXATION IN Ge:As

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Description

The short, narrow-band THz pulses produced by the Novosibirsk free electron laser (NovoFEL) in combination with a pump-probe experimental setup are a powerful tool to reveal information on the dynamics of resonant processes. In this work, we present our experimental setup and show some recent results on the relaxation of electronic impurity states in germanium at low temperatures.

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ЦЕЛЬНОМЕТАЛЛИЧЕСКИЕ МИКРОСТРУКТУРНЫЕ ЭЛЕМЕНТЫ УПРАВЛЕНИЯ ТЕРАГЕРЦОВЫМ ИЗЛУЧЕНИЕМ

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Description

Описаны конструкция и способы изготовления самонесущих сеточных структур, используемых в качестве квазиоптических селективных элементов для управления электродинамическими характеристиками пучков излучения в диапазоне субтерагерцовых (субТГц) и терагерцовых (ТГц) частот электромагнитного спектра (0,1÷10 ТГц). Толщина изготавливаемых микроструктур может меняться в диапазоне от 10 до 1000 мкм. Тонкие структуры изготавливаются путём плазмохимического травления фольги толщиной 10-30 мкм тяжелых тугоплавких металлов (в частности вольфрама - W и тантала - Ta) через маску, сформированную посредством фотолитографии. Толстые микроструктуры толщиной 200-1000 мкм изготавливаются посредством применения глубокой рентгенолитографии и гальванопластики. Толщина самонесущих сеточных структур оказывает влияние на АЧХ квазиоптических селективных элементов, что иллюстрируется расчетными графиками спектральной зависимости энергетического коэффициента пропускания нулевой дифракционной гармоники для высокочастотных фильтров с шестиугольными отверстиями (сотовая упаковка), характеризующихся различной толщиной металла.
При выполнении работы использовалась инфраструктура Центра коллективного пользования «Сибирский центр синхротронного и терагерцового излучения (СЦСТИ) на

базе накопительного комплекса ВЭПП-3/ВЭПП-4М ИЯФ СО РАН, поддержанного Министерством образования и науки РФ (проект RFMEFI62117X0012).

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СПОСОБ ИЗГОТОВЛЕНИЯ LIGA-ШАБЛОНОВ НА ОСНОВЕ ТАНТАЛОВОЙ ФОЛЬГИ

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Description

Описаны конструкция и способ изготовления высококонтрастных самонесущих перфорированных (со сквозными отверстиями) сеточных LIGA-шаблонов, используемых в рентгеновском диапазоне длин волн $\lambda \approx 0{,}5 \div 3$Å. Способ основан на плазмохимическом сквозном травлении танталовой фольги через металлическую алюминиевую маску, сформированную на поверхности фольги посредством фотолитографии. Шаблоны предназначены для формирования толстых резистивных масок толщиной 250-1000 мкм, в частности, из негативного резиста SU-8, что позволит создавать толстые планарные металлические микроструктуры, предназначенные для управления потоками электромагнитного излучения терагерцевого диапазона. В качестве исходной заготовки LIGA-шаблона использовалась танталовая фольга толщиной 30 мкм и диаметром ~80 мм. Заготовка шаблона проводилась через следующую последовательность операций:
1. Напыление на рабочую поверхности заготовки тонкого (толщиной ~ 1,5 мкм) слоя алюминия (Al).
2. Формирование резистивной маски на рабочей поверхности заготовки посредством контактной фотолитографии из позитивного резиста SPR 220 (7.0).
3. Жидкостное травление алюминия через резистивную маску и удаление остатков резистивной маски.
4. Плазмохимическое травление тантала через алюминиевую маску на глубину 30 мкм.
Доклад содержит СЭМ-фотографии, иллюстрирующие как процесс изготовления LIGA-шаблона. По результатам работы оформлен и получен патент RU №2721172 на изобретение: «Способ изготовления самонесущего рентгеношаблона» / Генцелев А.Н., Дульцев Ф.Н. - Опубл. в Б.И., 2020, №14.

При выполнении работы использовалась инфраструктура Центра коллективного пользования «Сибирский центр синхротронного и терагерцового излучения (СЦСТИ) на базе накопительного комплекса ВЭПП-3/ВЭПП-4М ИЯФ СО РАН, поддержанного Министерством образования и науки РФ (проект RFMEFI62117X0012).

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THEORY OF MULTIBUNCH STORAGE RING WITH TRANSVERSE FEEDBACK

Prof. Nikolay Vinokurov (Budker INP)

Description

Most of contemporary storage rings operates in multibunch mode. In this case the transverse dynamics in the presence of feedback may be complicated. Indeed, in general case, the amplified signal of a beam position monitor kicks all circulating bunches. In this paper the stability of such system with many degrees of freedom is considered. Damping times are estimated for the simplest cases.

Results of researches supported by RBRF grant 15-02-07776 were used in this work.

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DEVELOPMENT OF SILICON MICROSTRIP DETECTOR WITH INTEGRATING READOUT FOR TIME-RESOLVED STUDIES IN MICROSECOND SCALE

Lev Shekhtman (Budker INP)

Description

First results from the tests of a new full-size prototype of a silicon microstrip detector with integrating readout for studies of material deformations under pulsed heat load are presented. The prototype includes the silicon microstrip sensor with 1024 30 mm long strips with 50 um pitch, half of which are connected to the inputs of analogue pipeline ASICs APC128. The readout electronics can integrate charge released in the sensor under synchrotron radiation within exposure time from 100 ns to tens microseconds. Spatial resolution measured at an energy of X-rays about 70 keV is close to 100 um (FWHM). Next steps of this development including the change of sensor material to GaAs and usage of the new ASIC DMXG64B for the readout electronics are discussed.

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“IN SITU DIFFRACTION AT EXTREME CONDITIONS” END-STATION AT SKIF

Dr Sergey Rashchenko, Mr Alexander Romanenko (Sobolev Institute of Geology and Mineralogy, SB RAS)

Description

The “Microfocus” beamline of SKIF storage ring is a multi-branch undulator beamline to be commissioned in 2024. The “in situ diffraction at extreme conditions” end-station is designed for X-ray diffraction (powder, single crystal, and multi-grain techniques) and total X-ray scattering from samples under high-pressure conditions (up to several million atmospheres) combined with high (up to 6000 K) and cryogenic temperatures. Extreme conditions will be achieved using diamond anvils cells (DACs) of various designs, as well as compact toroid (Paris-Edinburgh) presses. The end-station offers beam parameters suitable for solving the most demanding user tasks in the fields of Earth and planetary sciences, materials science, physics and chemistry of the extreme state of matter etc. The section will use radiation of the 15th harmonic of superconducting undulator (resonance energy of 30.9 keV), with source dimensions (r.m.s.) of 9×8 μm, divergence of 16×13 mrad, and integrated flux of about 2×10^13 phot/s/0.1% b.w. The “in situ diffraction at extreme conditions” end-station will consist of two experimental setups: a laser heating (LH) and general purpose (GP), where experiments can be carried out using DACs with resistive heating or cryogenic cooling, toroid press, etc. To reach the smallest beam focus, a compound refractive lens (CRL) with ~1 m focal length will be placed in front of the sample, collecting a 10^10 phot/s flux into a 0.3×0.3 μm (FWHM) spot. A moderate focus mode using a pre-focusing CRL located in an optical hutch near the diamond monochromator will be also available. Using the pre-focusing CRL , almost the entire photon flux transmitted by the monochromator can be transported to the aperture of the focusing CRL. This configuration provide focusing of larger flux (10^11 phot/s) into a 1.6×1.4 μm spot (FWHM). The flux density in both modes is about 1011 ph/s/μm2, allowing the proposed scheme to compete with capabilities of similar beamlines of main world synchrotron facilities both in the tight focusing, and in flux density.

The reported study was funded by RFBR according to the research project #18-35-20047.

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PDF ANALYSIS OF ALUMINA CONTAINING SYSTEMS

Dr Kristina Shefer (Boreskov Institute of Catalysis SB RAS) **Co-author** Prof. Ella Moroz (Boreskov Institute of Catalysis)

Description

Alumina containing systems are of great significance for catalysis due to the unique properties of this oxide. These systems usually exist in nanoscale state. Their composition and

physicochemical properties depend on the preparation conditions. The appearance of novel methods of alumina synthesis give a new stimulus to the study of their structure and properties. Therefore such substances are interesting objects for research. The most reliable structural information is extracted from direct structural diffraction methods. In the case nanoscale catalytic systems, using special methods which take into account the specific features of X-ray scattering from small objects is required. In this work, structural features of alumina-containing systems are examined using PDF method. Applying this method needs obtaining diffraction data in a wide range of angles and with high intensity. X-ray diffraction patterns for constructing the experimental curves were obtained on a high-resolution diffractometer at the Siberian Synchrotron and Terahertz Radiation Center (Institute of Nuclear Physics, SB RAS, Novosibirsk). The considered aluminum oxides were obtained by different methods with varying synthesis parameters: deposition method, aluminate method, sol-gel method, CTA method.
The work was supported by Russian Foundation for Basic Research (project #19-03-00595) and by Ministry of Science and Higher Education of the Russian Federation (project # AAAA-A17-117041710079-8).

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STATUS OF THE STUDIES OF THERMAL STRESSES AND DEFORMATIONS IN MATERIALS CAUSED BY PULSED HEAT LOADS IN BINP

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Description

The operation of fusion reactor on the base of tokamak geometry of magnetic field is expected to be accompanied by pulsed heat loads to divertor. The loads lead to formation of plastic deformations and residual mechanical stresses. The stresses may result in mechanical destruction of tungsten armor of divertor. Typically it appears as a crack formation. The cracks decreases the heat removal from the surface, spoils the geometry of plasma flow to divertor, make easier the formation and ejection of micro particles, etc. The optical and X-ray diagnostics are applied to studies of the stresses and deformations in tungsten caused by pulsed heat loads in Budker Institute. The optical diagnostics are applied at the facility BETA (Beam of Electrons for material Test Application). The measuring of thermal radiation and scattered on the surface laser radiation during pulsed heating gives information about the surface temperature, roughness and curvature of the surface, etc. Among the most significant discoveries made using these diagnostics, we can note the detection of a delay between the end of the pulse heating and the formation of cracks by several orders of magnitude compared to the expected values. Recently, a new optical diagnostic has been developed, which allows determining the radius of curvature of the surface by changing the focal length. The results of the diagnostics confirmed the previous results on the delay. In addition, measuring the dynamics of surface curvature allows calculating the distribution of deformations and stresses along the depth of the sample. Of course, the results of such calculations depend on the applied strain models. The more direct methods for measuring residual stresses are used at stations of X-ray scattering «Precision diffractometry and anomalous scattering» and «Diffraction "movie"» at the VEPP-3 source of synchrotron radiation. The residual stresses may be calculated using the dependence of the scattering angle on the inclination of the sample. The station «Precision diffractometry and anomalous scattering» was used to make measurements of residual stresses with the spatial distributions. The decreasing of residual stress during slow heating simulating the result of continual heating of divertor was measured at the station «Diffraction "movie». The station of X-ray radiation «Plasma» at the VEPP-4 source of synchrotron radiation is oriented to measurements of deformations and

mechanical stresses in during pulsed heating simulating by laser radiation. The previous experiments demonstrated the possibility of the measurements of the depth distribution of deformations in single-crystal tungsten with the time resolution about 10 μs. The first demonstrative experiments on the measurements of the diffraction on polycrystall tungsten were carried out. The acceptable magnitude of signal were measured with the whole exposure 150 ms. The time resolution is admissible for measurements of the dynamic of the stress between the pulsed heating and crack formation.

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APPLICATION OF SYNCHROTRON RADIATION TO STUDY THE SURFACE ATOMIC STRUCTURE OF 2D MATERIALS

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Description

An important task of studying the properties of modern materials is to study the surface, including determining the atomic and electronic structure of solid. A special place is occupied by 2D materials where the surface structure determines the properties of the material, such as topological insulators and other low-dimensional systems. Topological insulators, because of the special properties of the topologically protected surface, are promising materials for creating spintronic devices. In this regard, the knowledge of the atomic surface is an actual issue that requires the use of structural methods. Among the methods that allow to obtain information about the structure of the local environment, we can distinguish the method of X-Ray photoelectron diffraction (XPD). Photoelectrons are generated by x-ray photons, creating an internal source of electrons inside the sample, and therefore the technique is sensitive to the type of atom. Core-level electrons have a high probability of being located in the inner part of the potential, and they can be considered as a source of localized monochromatic electron waves propagating from the center of the potential. Combined use with the method of photoelectron holography allows to obtain high-quality results of reconstruction of the atomic position. Although it is possible to obtain diffraction patterns on laboratory electronic spectrometers, the use of synchrotron radiation has a number of advantages. First, synchrotron radiation can range from low energies (less than 100 eV) to several keV. This implements to perform photoelectron diffraction with scanning by energy (energy-scanned XPD), diffraction with scanning by angle (angle-scanned XPD), as well as angle-scanned XPD at different energies. Second, the photon flux must be high enough to accumulate a large number of points in the angular and energy spaces. This paper presents the results of using synchrotron radiation to implement the method of X-Ray photoelectron diffraction on the surfaces of topological insulators - bismuth chalcogenides. The experiments were performed at the Bessy II synchrotron center on the U49-2 PGM1 line using p-polarization. The obtained experimental diffraction patterns are applied in the photoelectron holography method to reconstruct the surface atomic structure of solid.

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SECONDARY MINERAL FORMATION MONDMILCH FROM BOTOVSKAYA CAVE (EASTERN SIBERIA)

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Description

Mondmilch, or moon milk, is a special type of speleothems (secondary mineral formations formed in a cave environment from a primary mineral as a result of physical and chemical reactions). This mineral formation is a soft clay-like substance with a high water content, which becomes fluid when touched. In caves, mondmilch is found in the form of covers, leaks, lumps on the walls and on the floor, extensive deposits and small solitary formations. The composition of moon milk dependes on the rocks in which the underground cavity is located. It can be carbonate, gypsum, aluminosilicate and phosphate [1]. The questions of the moon milk origin and the variability of its crystalline structure are con-troversial. It remains uncertain as the thixotropic characteristics (fluidity) of the sediment and water content are changing in accordance with the features of the crystals formed the formation. It is possible that there are some regularity between the composition, structure of the crystals and the physical properties of this type of sediment. There is also a hypothesis about the biogenic origin of the moon milk. It is known that microorganisms of different physiological groups were found in the secondary formation content [2], and it can be assumed that microorganism cells can act as crystallization centers during the formation of moon milk, but the hypothesis that the microbiota is secondary in the content of moon milk and the sedimentation is its habitat. This paper presents the data on chemical composition and morphology of crystals of the samples of moon milk (mondmilch) from Botovskaya cave, which is the largest in Russia. It was determined that moon milk is characterized by increased concentrations of Ca and Sr and lower contents of Ti, Mn and Fe relatively to the host rocks. The morphology of mondmilch crystals indicates that the genesis of this secondary mineral formation is based on both abiogenic and biogenic mechanisms. It should also be noted that this type of sediment has been studied using the XRF SR method for the first time. The examination of sampled specimens provides new information on chemical composition and structure of moon milk in caves of carbonate karst. This paper provides the information on chemical composition and morphology of crystals of moon milk samples (mondmilch) from Botovskaya cave, the largest in Russia. This type of sediment has been studied with the application of XRF SR method for the first time. The research of sampled specimens provides new information on chemical composition and structure of moon milk in carbonate karst caves.

This work is partially supported by RFBR grant №13-05-90780.

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DETERMINATION THE PATTERN OF SPREADING AND ACCUMULATION OF ESSENTIAL AND TRACE ELEMENTS AT THE BENTHIC SAMPLES BY USING SCANNING micro-XRF-SR

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Description

For river ecosystems, one of the site of chemical elements accumulation is benthic assemblages. In our research 20 benthic samples were collected from small rivers and streams from industrial and nature areas of Novosibirsk region. Benthic invertebrates were fixed at 75% ethanol and identified up to the family taxonomical level at the laboratory. After identification samples were dried up to stable weight, animals from each taxonomical group were placed at the conductive tape for further investigation. The analysis was carried out using the μXRF-SR according to the standard certified method at the experimental station "Elemental analysis" in the SCSTR (Budker INP SB RAS). Experimental conditions: excitation energy 21 keV, dimensions of the exciting radiation beam 0.5 mm in height and 10 mm in width of the sample. Measuring time for one

point was 100 s. The contents of more than 20 elements, including essential Cl, K, Ca, Mn, Fe, and trace elements Ti, V, Cr, Ni, Cu, Zn, As, Rb, Sr, Y, Zr, Nb, Mo, Pb were determined. The concentration range for essential elements was 150 - 10000 ppm, for trace elements 0.3 – 1500 ppm. Scanning was done in two directions – the length and width of the sample animal. The profile of scanning was compared with photos from the electronic microscope. That gave us an opportunity to find out a specific locus of accumulation of some elements. Results obtained shown patchy spreading distribution of elements in the samples, that could be interpreted by various forms of chemical compounds, which included explored elements. So, some elements concentration could be determined as a part of the exoskeleton or outside contamination on the surface of an animal. For more complete result 3d scanning with the function of focused X-ray optics could be used. All obtained data will be applied for the determination of the role of benthic communities' mechanisms of essential and trace elements accumulation in river ecosystems. Moreover, our data will be useful for the assessment of the ecological statement of rivers and streams of industrial areas of Novosibirsk region.
The work was carried out in the framework of the RFBR projects no. 19-05-50046. The work was done at the shared research center SSTRC on the basis of the VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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CHARACTERISTIC OF D-F STATES IN DyNi2Mn and ErCo2Mn COMPOUNDS WITH STRONG ELECTRONIC CORRELATIONS BY RESONANT PHOTOEMISSION

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Description

Investigation of intermetallic compounds have been increasingly attractive due to their structural and magnetic properties and the possibility of developing new functional materials based on them. The compounds RT2Mn (R = Dy, Er; T = Ni, Co) crystallize in cubic MgCu2 – type structure by alloying 3d transition metal (T) and rare-earth (R). Certain amount of manganese is introduced in compounds of this type led to a change in the characteristics of materials. The interplay of d-and f-elements and its effect on the formation of the electronic structure in such compounds as DyNi2Mn and ErCo2Mn are studied. The method used resonant x-ray photoemission spectroscopy allows to select the contributions of the various components in the valence bands (VB). We can study not only the ground state, but also the lifetime of the excited (a core-level hole – VB electron) state, determine energies of the VB single-particle states and two-hole states at selected atoms, see reactions to sudden appearance of the core-level photo-hole. Resonant photoemission in narrow-band materials is described by the sum of first- and second order transitions, their quantum-mechanical interference leads to an increase in the spectrum from the valence bands and the appearance of an asymmetric dependence on the photon energy. Recently, these effects were studied theoretically and experimentally using the example of three-component intermetallic compounds TbNi2Mnx. The competition between the elastic and inelastic photoemission channels leads to a different dependence of photoemission spectra from nickel and manganese on photon energy. The elastic channel is realized on atoms with large magnetic moments, the inelastic Auger decay occurs on atoms with small moments.
The research was supported by RFBR project № 20-02-00541.

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ENHANCING RESOLUTION OF TERAHERTZ SURFACE PLASMON RESONANCE MICROSCOPY BY GHOST IMAGING USING FEL RADIATION

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Description

Surface plasmon resonance (SPR) microscopy is one of the most sensitive label-free microscopy method, however, it has a low lateral resolution. This drawback is primarily caused by the fact that surface plasmon polaritons (SPPs) excited by terahertz (THz) radiation propagate from their excitation spot to macro distances (about ~100 λ), thereby blurring the observed region by analogy with a scattering medium. To eliminate this disadvantage, we propose to adapt method known as ghost imaging (GI), which is notable for its tolerance to environmental aberrations between object and camera. The GI established itself in the classical optical visible-range nanoscopy, allowing to obtain a high resolution. In the report we will present an optical scheme of SPR microscopy for the THz range with an additional optical arm to implement the classical GI. In the GI the image of an object $O(x,y)$ is reconstructed by calculating the second-order correlation function (mutual intensity) between the spatial distribution of the intensity $P(x,y)$ of the probing beam (patterns) and the integral intensity S (registered by a single-pixel receiver) of the reflected (or transmitted) light in two optical arms (x,y) and (x',y'):
$O(x,y) \propto \sum i=1N(Si-\langle S\rangle)(P(x,y)i-\langle P(x,y)\rangle)\rangle=\langle P(x,y)i\cdot Si\rangle-\langle P(x,y)\rangle\cdot\langle S\rangle$,
where $\langle\ldots\rangle=1N\sum Ni=1$ is the averaging operator, N is the number of independent patterns, $R(x',y')$ is the object response function, $S=\int R(x',y')P(x',y')idx'dy'$. The restored image is called a ghost image, because it uses information about the spatial structure of light that did not interact with the object. In the THz range, the classical GI in the far field has not yet been demonstrated because it requires a THz radiation source having a sufficient second-order coherence length exceeding the wavelength by at least 2-3 orders of magnitude. This requirement is met by light from a powerful coherent THz source of radiation transmitted through a transparent turbulent medium or reflected from a rough surface, as a result of which the radiation acquires the statistical properties of a thermal source. To implement the classical GI in the THz range, we propose to use the Novosibirsk free electron laser (NovoFEL) as a THz radiation source. The high beam power of the NovoFEL provides a speckle structure with a pronounced profile, which is necessary to achieve a high level of contrast in the obtained image. And large coherence length of radiation of the NovoFEL is necessary to ensure a large degree of correlation between the beams emerging from the beamsplitter, which allows reconstructing an image with a lower noise level. This report will consider the advantages of implementation the ghost imaging method to surface plasmon-polariton resonance microscopy in the THz range and presents an analysis of factors affecting the resolution of proposed method.

The work was supported by the Russian Foundation for Basic Research (project 20-52-54004).

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Ni NANOCOATINGS ON POROUS ALUMINA: STRUCTURAL PROPERTIES VS MATRICES POROSITY

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Description

During last decade materials science developing the methods of obtaining and studying of new materials for magnetic and catalytic aplications based on nanostructured thin films and

nanostructures of different metals [1,2]. Nickel due to there high magnetic and cathodic properties has technological and scientific interest. It should be noted that the magnetic and catalytic properties depend on the size of material nanoparticles, so there is an increased interest in the literature to nickel based materials having a developed surface due to the formation of metal nanoparticles with different morphology [3]. This is due to the large contribution of surface electronic states of the metal with particles size decreasing. It is also strongly affected by the structural-phase state, local atomic and electronic structure, surface morphology.
Synchrotron facilities give more precise and reliable information about structure and electronic properties of materials. For instance Extended X-Ray Absorption Fine Structure (EXAFS) technique is a powerful method of obtaining of structural information and X-Ray Absorption Near Edge Structure (XANES) allows to investigate an electronic structure of materials. For the visualization of surface morphology a method of Scanning Electron Microscopy (SEM) are widely used.
In this work we propose templating approaches based on the formation of Ni nanocoatings on the surface the porous alumina films with highly ordered and controlled diameter of holes. Porous alumina were obtained by anodization process of aluminum foils at different (40, 80 and 120 V) voltages. We trying to identify the influence of pores sizes on the surface morphology and local atomic structure of materials. All of the above defines the scope of work: EXAFS and SEM investigations of Ni nanocoatings to form the basis of their magnetic and catalytic properties.
This work is supported by Russian Federation Assignment (project № AAAA-A17-117022250040-0), RFBR project № 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022. SEM investigations were carried out using facilities of shared research center “Surface and novel materials” UdmFRC UB RAS supported by project RFMEFI62119X0035.
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THE NONGAUSSIAN BEHAVIOUR OF THE SPREAD FUNCTION OF THE X-RAY POLYCAPILLARY LENS: CHARACTERISTICAL CASES AND NEW NONSTANDARD APPROXIMATION MODELS

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Description

The spread function of a x-ray polycapillary lens may be approximated very accurately by a laterally symmetrical gaussian function [1]. However it is true statement for the spacial fields whose are near to a focus of the lens only. We carried out the research to clarify a specifics of the lateral spacial distribution of the intensity of x-ray radiation around more spacious areas (placed more farly from lens' focus along axial directions). As the result we found that in many cases a range of characteristical features of nonstandard behavior for the spread function are exist. They may be asymmetrical behavior of gaussian peak (most frequently), superposition of two peaks (whose are respectively big and small), strong nongauss behavior, etc. We consider for all these effects to be explained fully by a nonaccuracy adjustment of angles and position of the polycapillary lens because of a limited precision of applied piesomechanics. Herewith most acceptable of the quality of the adjustment of the lens refers to cases of asymmetrical behavior of gaussian peak of the spread function of the lens. In the frame of this research a range of series of scanning experiments for detecting the spread function of the x-ray lens was carried out. The numbers of these series and the experiments of each series were be about 10. (Each series corresponded to an individual case of adjustment of the polycapillary lens, whereas a single

experiments in each series referred to an individual case of spacial position of interesting field of spread function along the axial direction.). We selected the range of the cases of the detected spread functions in order to be proceed by the quantitative analysis (approximation) those refer to the cases of most good quality of lens' adjustment. After that a various of approximation models (asymmetrical gaussians, extreme, logistpk, lorentz peaks [2], some our models) were tested by us. As the result it was shown that most good results refer to the cases of the extreme peaks approximation model additionally modified by us. The scanning experiments were carried out at Synchrotron and Terahertz Research (INP SB RAS, Novosibirsk) and the Kurchatov Complex of Synchrotron-Neutron Research (KISI, Moscow) using a confocal X-ray microscope.
The work was carried out in the framework of the RFBR projects no. 19-05-50046. 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, using equipment supported by project RFMEFI62119X0022.
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ON THE EFFICIENCY OF BACKWARD COLLINEAR ACOUSTO-OPTIC INTERACTION BETWEEN TERAHERTZ RADIATION AND ACOUSTIC BEAM IN HEXANE

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Description

One of the leading areas in telecommunication technology is the development of high-speed devices. At present, the use of the acousto-optical (AO) effect to control radiation is promising. Devices based on this effect are used in the ultraviolet, visible and infrared ranges. One of the main problems of using the AO effect in the terahertz (THz) range is the low diffraction efficiency (four orders of magnitude less than in the visible range) due to an increase in the radiation wavelength. This work is devoted to modeling the operation of the AO filter of a THz radiation, in which the collinear geometry of the interaction of the radiation beam with the ultrasound beam is used. In contrast to the well-known works in which the sound beam was assumed to be homogeneous and the chalk plane wave front, we used the model structure of the sound beam. The nonpolar liquid hexane (C6H14) was chosen as the AO interaction medium, since it is characterized by acceptable values of transparency and attenuation of ultrasound.
The work was supported by RSF grant No.18-12-00430.

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LUMINESCENT SPECTROSCOPY OF Pr3+ IONS IN SOME PHOSPHATES, BORATES AND SILICATES USING X-RAY SYNCHROTRON RADIATION FROM VEPP-3 STORAGE RING

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Description

This paper reports the spectroscopic properties of praseodymium-doped phosphates, borates and silicates. Spectra of X-ray excited luminescence and its decay kinetics were measured. Studied samples demonstrate interconfigurational 5*d*-4*f*, intraconfigurational 4*f*-4*f* transitions and defect-related luminescence. Comparative analysis of spectroscopic properties and application perspectives is presented.

Inorganic scintillating materials are being actively investigated in terms of their application in fields of nuclear physics, medicine tomography and detecting systems. Ce3+ ions impurity are widely used, but praseodymium ions are able to shift the emission spectra of interconfigurational

transitions to higher energy region. The Pr3+ 5*d*-4*f* emission appears, when a sufficiently strong crystal field shifts the lowest 4*f*15*d*1 excited state below the 1S0 level 1. Polycrystalline samples KLuP2O7, Li6Y(BO3)3, LiY6O5(BO3)3, LiSrPO4, Sr9Sc(PO4)7, K3Lu(PO4)2, K3LuSi2O7 doped with Pr3+ ions were synthesized using a solid state reaction and XRD verified for phase purity at the Laboratory of Luminescent Materials, University of Verona (Italy). The measurements of emission spectra and luminescence decay kinetics upon excitation with non-monochromatic X-ray synchrotron radiation (E = 3--60 keV, pulse FWHM ~ 1 ns, frequency ~ 8 MHz) were performed at the beamline #6 of the VEPP-3 storage ring at Budker Institute of Nuclear Physics (Russia). Stroboscopic method of electron-optical chronography with sub-nanosecond time resolution was used. The detection system included a SOL Instruments MS2004 monochromator equipped with a high-speed LI-602 dissector [2].
For example, Fig. 1, (a) demonstrate spectra of X-ray excited luminescence of some studied samples, LiSrPO4:Pr3+, K3LuSi2O7:Pr3+ and Li6Y(BO3)3:Pr3+. Two principal regions can be observed there: 220-350 nm -- region of interconfigurational 5*d*-4*f* transitions in Pr3+ impurity ions, and 480-650 nm -- region of intraconfiguration 4*f*-4*f* transition. Decay kinetics of interconfigurational radiation transitions are presented in Fig. 2, (b). Each of them can be approximated with multiexponential description $I(t) = \Sigma(A_i * \exp(-t/\tau_i) + I0$. Obtained luminescence lifetime parameter τ_i is vital for understanding of luminescence dynamics.
This paper reports the spectroscopic properties of praseodymium-doped phosphates, borates and silicates. Spectra of X-ray excited luminescence and its decay kinetics were measured. Studied samples demonstrate interconfigurational 5d-4f, intraconfigurational 4f-4f transitions and defect-related luminescence. Comparative analysis of spectroscopic properties and application perspectives is presented.
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ELECTROMAGNETIC UNDULATOR WITH SWITCHABLE PERIOD FOR SOFT X-RAY APPLICATION IN THE SKIF PROJECT

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Description

The “Electronic structure” beamline is dedicated for realization different photoelectron spectroscopy application in the SKIF project, requires intense photon flux in the soft X-ray and VUV ranges (10 - 2000 eV). The generation of the undulator radiation in this range is very problematic for electron beams with 3 GeV energy. For keeping the opportunity to cover whole range, the special undulator design with possibility doubling of the period was proposed. The commutation of the coils groups provides change the undulator period from 10 to 20 cm with keeping the amplitude magnetic field (0.5 T). The undulator mode (5 cm period) gives a big flux for high energy edge of the range and the wiggler mode (with period 20 cm) provides the sufficient number of the photons for soft region (down to 10 eV). Some details of the undulator design are presented in the report.

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STRUCTURAL ANALYSIS OF CATALYSTS USING THE ATOMIC PAIR DISTRIBUTION FUNCTION

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Description

The elaboration of catalytic materials is related to abilities to effectively probe nano-scale structures. There is significant drawback to common XRD methods addressed to well-crystallized materials, since catalyst components are often highly dispersed and present at low concentrations. The Pair Distribution Function (PDF) analysis based on operating with total scattering data is one of the techniques of choice for structural characterization of catalytic materials. Structural characterization of catalysts by the PDF analysis has attracted particular interest in the last years; the method has already proven itself a powerful technique for the study on highly dispersed, defect-rich and amorphous components of catalysts. The PDF describes local atomic structure of the material and provides structural information in the form of a radial distribution function of inter-atomic distances. In the 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 supported nanoparticles in catalysts will be shown for some examples: 1) mono- and bimetallic (Pt, Rh)/γ-Al2O3 catalysts for hydrocarbon oxidation; 2) Ni/CeO2 catalyst for CO methanation 3) MoS2/Al2O3 hydrotreating catalysts. The data will illustrate that the PDF analysis is effective tool for study on structural organization of the supported catalysts and can be used to not only determine the nanoparticle structure but also assess particle shape, size of atomic ordering.

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THE CODE FOR PROCESSING OF THE SRXRF SPECTRA

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Description

The X-ray fluorescence (XRF) analysis with using synchrotron radiation (SR) is a powerful technique for resolving elemental composition of the different samples with high sensitivity and good special resolution.

For precise quantitative analysis, the procedure for robust and reliable processing of the XRF spectra is necessary. Especially, such code is very important for realization scanning mode of the XRF analysis for the operative treatment big spectral data.

As a rule, the specialized codes for conventional XRF systems are not suitable for this aim because of the SR excitation provides a big variety of the analysis modes. Thus, the proposal of the code for processing of the SRXRF spectra is very actual.

The modern program libraries provide a simple ways for organizing robust fitting XRF peaks with keeping a prior data for X-ray lines. In current work the reliable code for estimation of the XRF peaks areas was proposed. Algorithm suitable for calculation net areas of the peaks in the case of series overlapping and in case violation of the mutual intensity ratios of the line in the series due to sample absorption and due to difference in the registration efficiency.

Code was tested in the new beamline for hard XRF analysis was supported by RFBR grant 17-29-05016 офи_м.

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NITROGEN DOPED DIAMOND SINGLE CRYSTALS FOR X-RAY OPTICS APPLICATIONS

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Description

Here we present our latest achievements regards diamond single crystal growth and characterization by means of X-ray diffraction. Synthetic diamond crystals were grown by the temperature gradient method using a high-pressure apparatus of the ‘‘split sphere’’ type (BARS) at P=5.7 GPa and T=1550 °C with the use of a Ni0.7Fe0.3 alloy as a solvent-catalyst. It has been shown that dislocation-free regions in these crystals occupy about 58 mm3. Two diamond plates oriented by (111) plane with 3x3 mm2 surface area were cleaved from the outer parts of two single crystals, followed by mechanical polishing from both sides. It was found that the plates contained nitrogen impurities predominantly in the form of isolated substitutional atoms (C-centers, type Ib) with concentrations in the range of 100–150 ppm.
Diamond plates were characterized by means of high-resolution rocking curve imaging (RCI) performed at P01 beamline at DESY. The samples were studied at room temperature in the Bragg geometry using monochromatic radiation with energy of 14.41 keV. The energy resolution provided by high-resolution Si (4 0 0)(10 6 4) monochromator was $\Delta E/E = 10\text{-}7$. Rocking curves were collected from (333) reflection in a pixel-by-pixel manner by 2D-detector with 55-μm pixel size with a total surface area of 256x256 pixels. RCI showed an overall good quality of the diamond plates close to the central area. The FWHM mean value at the defect- and strain-free areas lie in scope of 0.5 μrad deviation from the theoretical value that is suitable for XFEL and 4th generation synchrotron sources optical applications like beam splitters and monochromators. Defect- and strain-free areas were found to be 1x2.2 and 1x1.6 mm2. The working area of the crystal #1 exceeds 50% of the whole crystal surface. Further improvement of the cutting in couple with polishing process will lead to the large Ib diamond crystals (more than 6 mm2) with larger working area.

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THE MODIFICATION OF OPTICAL PROPERTIES OF THE SURFACES BY THE GLANCING ANGLE DEPOSITION OF TiO2

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Description

This work considers the optical properties and structure of thin films of titanium dioxide formed by glancing angle deposition to improve light yield of scintillation materials. The experimentally obtained value of the refractive index was about 1.2, which is almost two times less than the refractive index of crystalline titanium dioxide. This allows you to use this method to modify the optical properties of the surfaces of scintillators with a large refractive index.
This work is partially supported by RFBR grant №19-42-540009 p_a.

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DEVELOPMENT OF INDIRECT COOLING CRYOGENIC SYSTEM WITH NITROGEN AND HELIUM HEAT PIPES FOR SUPERCONDUCTING INSERTION DEVICES IN BINP

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Description

The using of indirect cooling cryogenic system based on cryocoolers for superconducting insertion devices (wigglers and undulators) gives opportunity, in contrast to magnets immersed into liquid helium, to reduce the size of the magnetic gap due to the removal from it the walls of

the helium vessel and increase the magnitude of the magnetic field. To increase the cooling efficiency of such a magnet, which is in vacuum and does not have direct thermal contact with cryogenic liquids, the heat pipes of siphon type filled by nitrogen and helium is used as the heat conductors for connecting of superconducting magnet with cryocoolers stages. The article describes the principle of operation, design and application features of the heat pipes on several indirectly cooled superconducting insertion devices created in BINP.

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IN SITU XRD ANALYSIS WITH THE TIME-RESOLUTION (0.4 MS) OF STAINLESS STEEL IN DURING SELECTIVE LASER MELTING

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Description

Selective laser melting is an additive technology that is gaining popularity due to its ability to produce complex metal components that cannot be manufactured using traditional technologies.To achieve high quality components created using SLM, it is necessary to control the processes of melting and subsequent crystallization in metals. Using the high synchrotron radiation (SR) intensity from a 9-pole wiggler (VEPP-4M), we obtained data on phase transformations in AISI 304 stainless steel with a time resolution of 0.4 ms. For SLM, we used a 500 W ytterbium fiber laser with a wavelength 1070 nm. , The work was performed on the SR beamline "Phase Contrast Radiography", created with the support of the RFBR project No. 12-02-12071

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GENERATION AND USE OF COHERENT X-RAY BEAMS AT FUTURE SKIF STORAGE RING

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Description

In 1990s, the emergence of the 3rd generation synchrotron user facilities equipped with undulator sources, stimulated pioneering works on interaction of coherent X-ray beams with matter (Brauer et al. 1995), resulted in the development of X-ray photon correlation spectroscopy (XPCS) technique, capable to probe nanoscale fluctuations up to kHz frequencies using dynamics of speckle pattern given by scattering of coherent X-ray beam from the sample. More recently (and highly aided by the development of modern high-throughput data analysis algorithms), coherent X-ray diffraction imaging (CXDI), also known as lensless imaging, revolutionized the field of X-ray microscopy, finally bringing users the possibility of non-destructive 2D and 3D imaging of complex structures with unprecedented ~10 nm resolution. However, strict requirements to transverse coherence of X-ray probe put serious limits on further development of CXDI-based techniques at the 3rd generation facilities, where coherent flux after spatial filtering becomes unacceptably small at energies above ~20 keV. At the same time, the latter was used as one of the strongest arguments of the user community for push towards construction of MBA-based 4th generation of storage rings with ultra-low-emittance.
Since coherent flux can be simply expressed as $Fcoh=\lambda 24B$, where λ is X-ray wavelength, and B – source brightness, the demand for higher coherent flux is often translated as demand for higher brightness – a recognizable motto for both accelerator and user communities. From the same relationship one can also easily see that even more brightness is needed to obtain the same coherent flux at shorter wavelengths / higher energies. Another expression $Fcoh=\lambda 216\pi 2F/\varepsilon tot$, where F is total flux, and εtot – 4D phase volume of X-ray beam, illustrates that it is the phase volume of the undulator X-ray source that should be minimized in order to deliver a maximum number of coherent photons to end-user (given total flux has already reached its limit imposed

by machine current and undulator technology). Whereas at the 3rd generation facilities the phase volume of undulator source was dominated by electron beam emittance with negligible influence of other factors, the estimation and minimization of undulator source phase volume at 4th generation facilities requires more elaborate approach taking into account electron beam energy spread, undulator phase error, and matching of phase-space ellipses between electron and X-ray beams.

In our contribution we will present estimations of coherent flux at different energies available for future users of ultra-low-emittance SKIF storage ring (to be commissioned in 2023) and discuss ways of its optimization, as well as future scientific program of user experiments with diffraction-limited X-ray beams.

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EXPERIMENTAL AND THEORETICAL X-RAY SPECTROSCOPIC STUDY OF ELECTRONIC STRUCTURE OF SULFUR-CONTAINED TRANSITION METAL COMPLEXES

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Description

Tasks arising with the growing need for alternative renewable energy sources and environmentally pure catalytic technologies stimulate the search for new functional materials. At present, growing interest is in compounds containing chalcogenide and dichalcogenide groups, which may perform as active catalytic centers. In this regard, binuclear and trinuclear transition metal clusters modified with various terminal ligands have great prospects as catalysts or precursors with higher catalytic activity, and could be considered convenient structural models of active centers of industrial catalysts. The coordination of terminal ligands of various nature affects the electronic structure of clusters, which could improve functional properties such as nonlinear optical properties, reactivity, and other physicochemical properties.

An important issue in obtaining new functional materials is the characterization of their atomic and electronic structures. Thus, the electrocatalytic activity of materials based on dichalcogenide molybdenum clusters or MoS_2 nanoparticles with different morphologies is associated with a large number of disulfide groups in the catalyst structure. X-ray spectroscopy provides information about both the atomic and the electronic structure of the studied compounds.

In the present work, the electronic structure of a series of binuclear and trinuclear transition metal clusters with disulfide and sulfide ligands was studied by X-ray spectroscopy methods. The S K-edge, S $L_{2,3}$-edge XANES spectra, and S Kβ, M Lβ X-ray emission spectra of complexes with various cluster core ($\{M_2S_4\}$, $\{M_3S_7\}$, $\{M_3S_4\}$, M = Mo, Nb, V, W) were studied. Based on quantum chemical calculations, the X-ray absorption and X-ray emission spectra of sulfur atoms were interpreted, providing information on the energy position and partial atomic composition of the HOMOs and LUMOs, and the electron density distribution in the clusters under study. Based on the obtained experimental and theoretical data, the effect of external sphere ligands on the nature of the electronic interactions of cluster core, the electronic structure of bridge sulfide and disulfide ligands was studied. The electronic structures of transition metal disulfides and disulfide clusters were compared.

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The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4 - VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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FOCUSING SYSTEM OF SYNCHROTRON RADIATION WITH REFRACTIVE MOSAIC LENSES FOR THE STATION "EXTREME STATE OF MATTER" OF THE VEPP-4

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Description

The purpose of the work is to create a system for focusing synchrotron radiation for the station "Extreme state of matter" on a VEPP-4 [1]. For experiments at this station, there is a problem of insufficient radiation intensity, which worsens the statistics in fast processes experiments with an exposure time of diffraction patterns of 100 ps [2, 3, 4, 5, 6]. This problem can be solved through the use of refractive focusing optics made of a polymer (epoxy resin SU-8). An x-ray mosaic lens was chosen for focusing [7]. The system makes it possible to focus SR into a smaller spot by increasing the radiation intensity and allowing realizing a local structural analysis. The following tasks were solved:

1) the mechanical precision parts of the detector alignment and fastening system are designed and manufactured;
2) a control program for the adjustment device is designed;
3) a calculation was made of the heat absorption on the lens and its heating under monochromatic and polychromatic radiation using the ANSYS program;
4) the system is installed and debugged on the channel No. 8 VEPP-4;
5) an experiment was conducted to focus synchrotron radiation on a monochromatic beam.

In the experiment it was shown that the lens stably works on monochromatic radiation, but it heats up strongly (heating rate of 17 deg / s) on polychromatic radiation. A scheme of the pulsed operation of the lens (active interval of 100 ms) for the study of fast-flowing processes on polychromatic radiation is proposed.

This work was supported by RFBR grant 19-29-12045 and Ministry of Science and Education of Russia grant AAAA-A17-117030310280-6.

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SILICON AND DIAMOND DIFFRACTIVE LENSES WITH CONTINUOUS PROFILE FOR FOCUSING HIGH-POWER TERAHERTZ RADIATION

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Description

An increase in the radiation power of THz sources creates the need for the development of new optics operating with it. Here, we propose and realize the fabrication of silicon and diamond diffractive lenses with a continuous profile by the method of direct and indirect laser ablation, respectively. The fabricated lenses were tested with a free-electron laser at the wavelength of 141 μm and demonstrated high diffraction efficiency and a good agreement with the theoretical prediction. The work was supported by RFBR grant 18-32-20226.

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APPLICATION OF XAFS SPECTROSCOPY FOR STUDY OF MICROPARTICLES OF SIKHOTE-ALIN METEORITE

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Description

The presented work shows the new results of a study of microparticles of the Sikhote-Alin meteorite using XANES and EXAFS methods. XANES / EXAFS spectra (Ni-K, Fe-K, W-L2), using μ- and standard methods, for meteorite microparticles and reference comparison samples were obtained both on experimental module X-ray Confocal Microscopy situated on NRC “Kurchatov Institute” (Moscow) and at XRF-, EXAFS- stations of Siberian Synchrotron Terahertz Radiation Center (SSTRC, Novosibirsk). Some differences in the local structure and phase composition in different microparticles of the studied meteorite samples were determined. The interatomic distances and the corresponding coordination numbers were calculated. Various options for structural models are considered. Additionally, the chemical and phase compositions, and the morphology of the samples were studied by SEM, EDX, and XRF methods. On the example of a test meteorite, the possibilities of the proposed approach for the study of microparticles of complex composition are shown. The data obtained by all the methods are in a good agreement.
The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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STRUCTURAL STUDY OF PT-COMPLEXES IN AQUEOUS SOLUTION BY EXAFS

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Description

This work is devoted to the study of the process of hydrolysis of chloride Pt(II) complexes and Pt(IV) nitrate complexes existing in aqueous solutions of different nature by EXAFS spectroscopy. The deposited platinum catalysts are inevitable in various industrial oxidation and reduction processes due to their unique properties,. The variety of catalytic properties is determined by the possibility of varying the dispersion and lability of the active component. It is quite obvious that the development of methods for fine control of Pt dispersion is necessary to study the fundamental relationships between the size, state of the active component nanoparticles, their detailed electronic structure, and the actual properties of a catalyst in a chemical reaction. As a rule, various precursor solutions based on Pt(IV) and Pt(II) salts are used for the synthesis of platinum catalysts; after precipitation to a carrier the system undergoes various heat treatments. The main factor affecting the dispersion of Pt forms existing in salt solutions is the ongoing hydrolysis process. To implement the research goals, ~0.01-0.05 M aqueous solutions of K2 PtCl4 and nitrate solutions of Pt (IV) with different ligand environments were prepared and EXAFS spectra (Pt-L3 edge) of studied samples were recorded at SSTRC, Novosibirsk. The composition and structures of the hydrolysis products being polynuclear platinum (II) hydroxocomplexes (PHC-Pt) were studied. It was found that during the hydrolysis reaction of [PtCl4]2-complexes, oligomeric chains containing Pt-O-Pt fragments are formed, in which neighboring Pt atoms are connected by a single O–bridge atom. Aging of solutions containing PHC-Pt for a long time, by formation of 3D-oxide structures. does not take place, in contrast to solutions of PHC-Pd (II) and PHC-Pt (IV). Increase in size of PHC-Pt particles is shown to take place while the process of oligomerization of Pt(II) mononuclear complexes proceeds. It was shown that during hydrolysis of Pt(IV) nitrate solutions, Pt(IV) polynuclear hydroxocomplexes were formed. It was established that the nearest environment of Pt in these solution is always octahedral, with the distortion caused by replacing the O part with the N part. However, formation and stabilization of various agglomerated Pt-containing forms of different nuclea are possible. It was found out that the nuclearity of various forms and their resistance to hydrolysis depend on the preliminary history of the sample and the nature of O, N-ligands in the platinum coordination sphere platinum in the solutions. The Pt-O, N, and Pt-Pt distances and corresponding coordination numbers are determined. Variants of possible structural models are considered. Additionally, all prepared samples of solutions were examined by NMR, TEM methods. Data from all these methods agree with each other.

The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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XAFS STUDY OF ZIRCONIUM OXIDES MODIFIED BY YTTRIUM AND MAGNESIUM

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Description

Today the mixed oxides with a fluorite structure of the composition (Zr, Y) O2-x are widely used to harden ferritic steels used as fuel element cladding materials for the new generation of fast neutron reactors operating under irradiation and high temperatures. This work is devoted to study of the state and local structure of samples of zirconium oxides modified by yttrium and magnesium, prepared by coprecipitation and calcined at a temperature of 1250 °C. XAFS (XANES/EXAFS) spectra (Y-K, Zr-K edges) of studied samples were recorded at SSTRC, Novosibirsk. It was shown that from the yttrium side, the XANES spectra of both samples were almost identical. On the zirconium side, the XANES spectra have minor differences. It can be

assumed that the charge state and the nearest environment of yttrium also practically does not change depending on the composition of the samples. For zirconium, with the charge state unchanged, some changes in the nearest oxygen environment appear to occur due to the composition of the samples. It was found out that the curves of the radial distribution of atoms (RDFs) obtained from the EXAFS spectra of the studied samples have a number of characteristic features. Only the first coordination spheres of the Me-O and Me-Me types are observed, but long-range coordination spheres (more than ~0.45 nm) are practically absent, which may indicate distortions of the long-range order in the structures. The local yttrium arrangement is stable when the composition of the samples changes, which may indicate the formation of clusters that include only Y and O elements. The local zirconium arrangement depends on the composition of the samples, since there are some differences in the RDFs curves. Thus, the amplitudes of the peaks assigned to the coordination spheres Zr-O and Zr-Me are significantly reduced (by more than 25%) for the Y,Mg- modified sample in comparison with those for the Y- modified sample, which indicates distortions of the original fluorite structure. The observed changes in the Zr-O and Zr-Me distances (more than 0.05) are greater than the changes due to differences in the cell parameters for the compared samples. Using the model of statistical solid solution with a fluorite structure, it is suggested that the presence of Y-O clusters prevents refinement of structures.
The work was carried out in the framework of the RFBR project no. № 19-03-00530. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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X-RAY PHOTOELECTRON SPECTROSCOPY AND NEAR EDGE X-RAY ABSORPTION FINE STRUCTURE SPECTROSCOPY STUDY OF SYNCHROTRON RADIATION EFFECTS ON FLUORINATED GRAPHITE INTERCALATED N2O4

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Description

Fluorinated graphite (FG) attracts the attention of researchers due to a wide range of physicochemical properties, which is promising for its use as an element base of microelectronic devices (LED elements, gas sensors, etc.), and also as a cathode for lithium-ion batteries. More importantly, recent studies have shown that intercalated systems based on graphite and its derivatives can be used as a nanoreactor. In these devices, the layering of graphite and its screening effect allows you to purposefully change the reactivity of molecules and regulate the activity of functional groups on the surface. In addition, the subsequent thermal or photochemical treatment of fluoride graphite intercalated compound (FGIC), including irradiation with high-intensity light, can lead to a significant restructuring of the electronic structure of the system, which opens up new possibilities for using FG.

For the purpose of a detailed analysis of the mechanism of processes occurring on the surface of FGIC under the influence of thermal and photochemical effects, a comprehensive study of the electronic structure of intercalated N2O4 fluorinated graphite C2F0.8-0.9 before and after continuous in situ illumination with polychromatic photon beam of high intensity (zero-order light from the dipole beamline of BESSY II synchrotron radiation facility). X-ray photoelectron spectroscopy (XPS), near-edge X-ray absorption fine structure (NEXAFS), and Fourier transform infrared spectroscopy (FTIR) are used for this.

Thus, the effect of synchrotron radiation on the atomic and electronic structure of FGIC C2F0.8-0.9 N2O4 has been studied. It was found that in the initial samples of N2O4 on the surface, the FG is in an equilibrium mixture with various nitrogen-containing functional groups NO2, NO,

NO3, N2. Thermal and photochemical effects on FGIC lead to defluorination of the sample and the formation of defects, on the edge of which CF2 and CF3 bonds arise. In addition, the FG matrix recovery in progress with partial removal of the intercalate.
This work was supported by RFBR grant № 18-29-19073 мк.

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CURRENT STATUS OF THE STUDIES OF X-RAY DIFFRACTION ON TUNGSTEN DURING PULSED HEAT LOADS AT THE SCATTERING STATION «PLASMA» AT THE VEPP-4 SOURCE OF SYNCHROTRON RADIATION

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Description

Fusion plasma confinement at facilities based on a tokamak geometry of the magnetic field includes periodical transient heat loads to divertor plates. The divertor plates of ITER are seem to be covered by polycrystalline tungsten. The tungsten tends to crack in case of the pulsed heating. The reasons of the crack formation are deformations and mechanical stresses caused by the sharp rise in temperature of thin surface layer. The X-ray scattering station «Plasma» at the beamline 8 at the VEPP-4M source of synchrotron radiation was developed for dynamical measurements of deformations and mechanical stresses in tungsten during pulsed heating simulating by laser radiation. First results were carried out on the mosaic single-crystal tungsten. The observed evolution of the diffraction peak shape agrees with theoretical predictions based on calculations of deformation caused by pulsed heating. Deconvolution of the residual stress distribution show good agreement with theoretical model of distribution of the deformations in thin surface layer in the sample during pulsed heating. One of the most important cases was the observation of the bifurcation of the diffraction peak during the occurrence of the crack on the sample during sequential repeated irradiations of the sample. Moreover, the first experiments on the measurements of the diffraction on polycrystalline tungsten were carried out.

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HIGH RESOLUTION MONOCHROMATOR FOR SYNCHROTRON RADIATION BASED ON FLAT VLS-GRATINGS

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Description

We present the design of a high-resolution plane-VLS-grating soft X-ray and VUV monochromator of synchrotron radiation for the 125 – 4200 Å spectral range. A concave mirror is located at a distance of 28 m from a synchrotron radiation source. The mirror is set in a highly asymmetric scheme and focuses radiation at a distance of about 1350 mm. The VLS-grating is set close to the mirror and focuses onto the exit slit the radiation diffracted in the first external order. The frequency is scanned by rotation of only the plane VLS grating. Two replaceable VLS-gratings with line densities of 600 1/mm and 150 1/mm are planned for the 125 – 1000 Å and 900 – 4200 Å spectral ranges, respectively. The ruled area of the VLS gratings is 40x20 mm. The gratings and the mirror each operate for a deviation angle of 32˚, the total deviation angle being equal to zero. The resolving power obtained by numerical ray tracing is higher than 2000 in the entire spectral range. This work was partially supported by RFBR grant No.19-12-50059

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XAFS STUDY OF STABLE BIMETALLIC CATALYSTS FOR SELECTIVE HYDROGENATION OF FURFURAL

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Description

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AN ATTEMPT OF THE QUANTITATIVE ANALYSIS OF CYCLICAL CONSTITUENTS IN STRUCTURE OF SCANNING MICROFLUORESCENCE SIGNALS FROM HUMAN HAIRS

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Description

The distribution of some chemical elements along human hairs is proved to be an valuable indicator in a range of various cases. It may serve in order to use in medicine, toxicology, criminalistics, forensic, archaeologics, and so on [1]. However at the present any systematical studies focusing to analysing these distribution with submillimetrical and tens micron spacial resolution do not exist. We took an attempt to describe qualitatively as well as to test an possibility of the analyse in detail such distributions on the example of the limited sample (consisting of fragments of 5 human hairs). Our work was partitioned by two parts: panoramical and quantitative. The first part allowed to identify three main types of superposing legible pseudoperiodical cyclical components of elemental distribution for all studied hairs. The diapason of all crutial parameters of needed scanning experiments that is optimal for applied equipment for ability to process the results (cycles and correlation] between elemental signals) by statictical methods with a good quality was also found. The existence of an amount of strong limitations of these parameters are fully explained by the specifics of using synchrotron radiation sources of second generation. We can assume that this obstacle results in the existence of some principal limits for ability to process a detail analysis of human hairs (those are also characteristic for any case of applying a similar equipment). In the second part of this work we selected a concrete distribution of fluorescent signal from the sulfur with sufficiently acceptable relation «signal to noise». Two special mathematical methods of analysing time series were applied successfully for a detail analysis of the cyclical part of the signal. The algorithm «Hilbert-Huang transformation (HHT)» [2] found 4 pseudoperiodical constituents, the algorithm «Singular Spectrum Analysis (SSA)» [3] found 5 preudoperiodic constituents. The sum of all found components is equal initial signal despite of a normally distributed stochastic noise with very good quality. The shapes of the cyclical components differ from approximating cosines by 10-30 % in average (until 40-50 % for singular points) for different constituents. The small amount of determinated pseudoperiodical components may be explained by human methabolizm intraday cycles as well as the characteristic features [1] of the hair structure. The scanning experiments were carried out at Synchrotron and Terahertz Research (INP SB RAS, Novosibirsk) and the Kurchatov Complex of Synchrotron-Neutron Research (KISI, Moscow) using a confocal X-ray microscope. The work was carried out in the framework of the RFBR projects no. 19-05-50046. 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, using equipment supported by project RFMEFI62119X0022.

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STRUCTURAL STUDY OF MONO- BIMETALLIC CATALYTIC NANOSYSTEM BY XAFS

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Description

The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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A RANGE OF INTUITIVE DISCRETIZATION SCHEMES TO ACCELERATE ALGORITHMS FOR SOLVING DECONVOLUTION PROBLEMS WITHOUT LOSS OF ACCURACY

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Description

A discretized inverse problem of deconvolution with single- or multi-dimensional Gaussian function as the apparatus function [1] is found in a number of optical and spectroscopic applications. Because of its instability [1, p. 12; 2, p. 32-37], it is necessary to reduce it to some regularized analogue [1; 2, p. 47], after which it can be solved by common methods for solving linear systems of equations or optimization. The so-obtained result has a meaning of approximate solution, signal noise influence filtered by certain superimposition of special restrictions, either on the solution or on parameters of its search. The value of the key parameter of regularization method applied [2, p. 47], in turn, should be selected according to known principles. Proper selection [1, p. 55-61; 2, p. 66] of the key parameter reduces the signal noise contribution to the solution to the lowest possible level with maximum possible preservation of signal information and compliance of its a priori set properties, if any. Despite the uniqueness of result obtained by the chosen regularization method at specific implementations of signal noise and values of its key parameter, there remains the problem of competition of various regularized solutions. It consists in the fact that selection of different regularization methods, their auxiliary parameters, and implementation of signal noise can yield solutions that formally have comparable explanatory power, but differ in their features. An effective way to overcome this is the use of global optimization methods and genetic algorithms. Application of these methods radically increases the time required for calculations, and hence methods for further acceleration of solving the deconvolution problem, if possible, are in demand.

We have developed a number of techniques that may enable acceleration of solving discretized problems of deconvolution without significant loss of accuracy regardless of the regularization method. We considered specific examples to show that application of alternative schemes for improving discrete approximation of deconvolution problem and reducing its dimensionality (involving non-standard methods of interpolation and taking edge effects into account [1, p. 35], as well as breaking the separation problem into many equivalent subproblems) makes it possible to accelerate computing processes, at least when obtaining solutions of a certain class.

The work was carried out in the framework of the state assignment for Budker INP SB RAS and RFBR project no. 19-05-50046. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.
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REGULARIZATION APPROACH FOR SPECIFIC ADVERSE EVENTS IN PROCESSING ELEMENTAL MAPS OBTAINED USING MICRO-XRF

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Description

Micro-XRF is a promising method to study elemental composition of samples and objects of various nature with spatial resolution of tens of microns to tens of nanometers [1]. Application of polycapillary optics for focusing and (optionally) collecting enables conduction of studies on synchrotron radiation (SR) sources of the second and higher generation, the minimum possible spatial resolution limited to values of 10 to 25 microns (effective width of the focus of X-ray lenses, depending on the energy of transmitted radiation) [1]. At a sufficiently high signal-to-noise ratio and small scanning step, one can attain subfocus resolution (i.e., its further reduction by a factor of 2-3 [2]) via processing chemical element distribution maps using deconvolution methods [3]. However, at operation on secondgeneration SR sources, this method is applicable for processing maps only for matrix and minor elements (with relative concentration of not less than one percent) [4]. We have developed a regularization approach for situations with signal noise of medium grade. This approach correctly takes into account a priori specific information and is aimed at identifying the most general properties of composition and morphology in micro-areas less than 15 microns in size. It was tested and showed a good result for two characteristic cases of practical importance, which arose in processing of a series of maps resulting from studies of geological and cosmic samples (e.x., [4-5] and so on) using micro-XRF.
The work was carried out in the framework of the state assignment for Budker INP SB RAS and the RFBR projects no. 19-05-50046, 18-03-01251. The work was partly done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.
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THE FIRST RESULTS OF MEASURING XAFS SPECTRA IN THE SOFT X-RAY RANGE AT KOSMOS STATION

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Description

XAFS spectra were measured near the K edges of the absorption of phosphorus, sulfur, and L III absorption edges of molybdenum and niobium (2100 - 2700 eV). The measurements were carried out using an upgraded Si (111) dual-crystal monochromator in normal incidence geometry. The monochromator device is described. The main difficulties arising in the course of obtaining spectra are discussed. It is shown that the spectral resolution of the monochromator allows one to obtain XAFS spectra, the quality of which is sufficient to decipher the structure of the sample. The measurement was carried out with a partial funding from the Russian Science Foundation (project No. 18-03-01061).

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DIAMOND MICRO-CRL FOR COHERENT X-RAY IMAGING AND MICROSCOPY

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Description

We demonstrate the capabilities of ion-beam lithography (IBL) for the manufacturing of the X-ray refractive micro-optics. With the help of IBL, the hardest of current materials – diamond – was milled, and micro scale diamond lenses were produced. Lenses have a rotationally parabolic profile with radii of parabola apexes less than 5 μm. As has been confirmed with SEM and AFM, shape profile errors of fabricated lenses were < 200 nm, while the surface roughness was estimated to be 30 nm. Single lenses were stacked in the CRL within one technological process with high alignment precision that has been further verified by acquired X-ray radiograms. The optical performance of the CRL was successfully tested at a third-generation synchrotron, where the lenses provided diffraction-limited focusing of X-ray radiation and demonstrated intensity profiles with Gaussian distributions at every measured longitudinal position (along the optical axis) downstream of the CRL.

This research was supported by the Russian Science Foundation (Project No. 19-72- 30009).

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X-RAY REFLECTO-INTERFEROMETER BASED ON COMPOUND REFRACTIVE LENSES FOR THIN-FILMS STUDY

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Description

Compound refractive lenses (CRLs) have been widely used for more than 20 years on leading synchrotrons and free-electron lasers for hard X-ray beam transport, collimation and focusing [1-2]. The combination of coherent compatible optics and new coherent sources increased opportunities for the development of new research methods.

In this abstract, we demonstrate a new X-ray interferometer based on compound refractive optics (CRL) for thin-film structures study [3]. The idea of a reflecto-interferometer is to use a very simplified experimental setup, where a coherent monochromatic X-ray beam, focused by CRL, impinges on a thin film at a grazing angle. This converging fan of radiation incoming on a sample surface provides a range of grazing angles. For each grazing angle, the rays reflected from the front and rear boundaries of the film will interfere, and as a result, the diffracted

intensity in the range of exit angles equal to the angular range of the incident fan will generate an interference pattern representing fringes of equal inclination. The capabilities of the new reflecto-interferometer were demonstrated at the ESRF ID06 beamline using X-rays from 10 to 20 keV. The Si3N4 membranes of thicknesses in the range from 100 to 1000 nm were studied. Experimentally obtained reflecto-interferograms correspond well with calculated ones, and the distance between fringes correspond to the thickness of the tested membranes. While the interference pattern in rather wide angular range is recorded in one shot, the proposed approach has a very good temporal resolution, which is limited to a few milliseconds, depending on the X-ray flux and the sensitivity of the detector. The high spatial resolution of the interferometer was demonstrated on interferograms recorded from an 8 nm-thick gold strip deposited on an Si3N4 membrane. It was shown that the interference pattern is very sensitive even to small deviations in the thickness of the layer. In addition, this reflecto-interferometer can be easily adapted for use with the MetalJet Excillium micro-focus laboratory source, which has GaKα emission line at 9.25 keV. As a result, a series of interference patterns for test sample - free-standing thin-film membrane thick of 500 um were observed.
The new X-ray reflecto-interferometer opens a wide range of opportunities for the analysis of thin-film and multilayer systems. The recording of the interference pattern in a single shot allows a fast in-situ analysis of solid and liquid materials including organic and biological films. The proposed method has significant advantages compared to classical X-ray reflectometry, providing information on the thickness and density of layers or structures in real time which allows research with a fundamentally new spatial and temporal resolution.
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CONCEPTION OF VACUUM SYSTEM FOR SRS «SKIF»

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Description

Requirement for deep molecular rarefaction inside low aperture beam pipe in presence of high intensity Synchrotron Radiation together with very tight magneto-optical system makes performance of vacuum system for modern high brightness Synchrotron Radiation Sources (SRS) quite challenging. To avoid emittance blow-up its beam pipe must be as smooth as possible along beam propagation. It relates to all components like flange connections, pumping ports and compensators also. In addition, the vacuum system must be stable over years against inevitable micro-leaks and suitable for possible modifications of other systems, which require its air venting. The paper presents a conception of the SRS SKIF vacuum system fitting the set of requirements. A simplified model for estimation and optimization of a scenario for the vacuum system conditioning is also described.

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CHARACTERISTIC OF THE BiTeCl ELECTRONIC STRUCTURE BY RESONANT PHOTOEMISSION

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Description

The aim of this work is an experimental study of the electronic interaction in the BiTeCl compound and its effect on the formation of the electronic structure. The used method of resonant x-ray photoemission spectroscopy (RPES) allows distinguishing the contributions of the

various components to the valence bands. We can study not only the ground state, but also the characteristics of excited two-particle states, the reaction to external action, and the relaxation processes of the electronic system. BiTeCl has a hexagonal crystal structure of alternating layers of chlorine, bismuth and tellurium atoms. The crystal has no inversion symmetry due to the continuous stacking order of the three atomic layers. The weak bonding between the Te and Cl layer provides a natural cleaving plane in the (0001) plane. The BiTeCl crystal was grown based on BiCl3–Bi2Te3. The telluride compound was obtained by fusing stoichiometric amounts of elemental Bi and Te at 600 ◦C. BiCl3 was prepared by the evaporation of a saturated solution of Bi2O3 in HCl acid. The charge was then sealed in a growth quartz ampoule under a pressure of 10−3 Torr. After heating to 430 ◦C at a rate of 20 ◦C h−1 followed by 1 day of soaking at this temperature the melt was crystallized by a modified Bridgman method [1]. According to our x-ray diffraction analysis a major part of the aggregate consisted of the BiTeCl phase, which was selected for the RPES measurements.
The experiments were carried out at the Russian–German laboratory of the BESSY II synchrotron (Berlin). The RPES spectra were obtained using synchrotron radiation with 150–900 eV photon energy range. The energy resolution was 0.1 eV. The perfect working surface was prepared by cleaving the samples directly in the ultrahigh vacuum chamber of the spectrometer. The main regularities that appear when the excitation energy and the photoionization cross-section change were established.
The reported study was funded by RFBR, project number 19-29-12061 and was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme “Spin” No. AAAA-A18-118020290104-2 and AAAA-A19-119081990020-8).

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BEAM-SHAPING REFRACTIVE OPTICS FOR COHERENT X-RAY SOURCES

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Description

The most advanced X-ray sources, such as third-generation synchrotrons and free electron lasers (XFEL), are capable to generate high brightness coherent radiation, especially in the hard X-ray region. The availability of such beams facilitates the development of a new generation of X-ray optics, whose optical properties allow going far beyond simple collimation and focusing functions. This optics makes it possible to form amplitude and phase of wave front with almost complete freedom, using the most outstanding properties of synchrotron and X-ray laser radiation such as brightness, monochromaticity, and coherence. Like in visible light optics, beam-shaping functions can be implemented in an X-ray regime based on both diffraction and refractive optical elements. For example, the beam-shaping optics based on diffraction optical elements (DOEs) allows realizing almost any complex optical transformation. However, due to the high penetrating power of X-rays through DOEs their use is significantly limited in the hard energy range. In addition, since many unknown beam parameters must be defined in advance, the design of such beam-shaping optical elements is a challenging task. As for the beam-shaping elements based on refractive optics [1], they are deprived of the disadvantages which are inherent in DOEs. This optics allows for some beam transformations, and the possibilities of its applications cover various areas of modern X-ray optics, such as interferometry and coherent diffraction, phase-contrast microscopy and imaging, and ultrafast and nonlinear optics studies. For example, one of the most vibrant demonstrations of the beam-shaping optics is a special class of refractive optical elements that have axial symmetry and are capable to convert a point-like source to a narrow axial straight line segment. These optical elements are called axicons.

Recently, we demonstrated an X-ray parabolic refractive axicon lens as a novel type of X-ray beam-shaping element [2]. Under coherent X-ray illumination, the parabolic axicon generates Bessel-like beam propagated along the optical axis in the near field and ring-shaped beam in the far field. The optical transformations produced by axicon can be used in areas requiring special illumination, as well as extended focused beams, for instance, in diffraction and imaging techniques, in metrological applications, as well as for source diagnostics and beamline alignment. Moreover, such beam-shaping capabilities can significantly simplify some existing experimental layouts or lead to completely new optical schemes for X-ray techniques based on synchrotron and XFEL sources. Most recently, we proposed an optical scheme of phase-contrast microscopy technique based on the axicon optics [3]. Due to the unique optical properties of the parabolic refractive axicon lens, the new approach turned out to be more efficient for visualization of weakly absorbing samples as compared with the traditional microscopy technique. In addition to new X-ray axicon refractive optics, it is also worthwhile to consider other beam-shaping elements, called interferometers, whose optical functions are well known and successfully used. These devices allow realizing the paraxial optical schemes of interferometry based on the coherent properties of modern X-ray sources. Recently, we demonstrated bilens and multilens interferometers based on refractive optics which under coherent illumination generate an array of mutually coherent beams focused at some distance [4-5]. The size of the focal spots is restricted to the diffraction limit and can be less than tens of nanometers. When the beams overlap they produce a steady interference pattern of fringes in the far field. The proposed interferometers can be used in a wide X-ray energy range while maintaining high efficiency. The field of applications of their optical functions is not limited only to the interferometry techniques and can be extended in the area of beam diagnostics and beam conditioning. Moreover, such lens systems open up new opportunities for the development of phase-contrast imaging technique, which was recently demonstrated [6].

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X-RAY PHASE-SENSITIVE IMAGING TECHNIQUE BASED ON A BILENS INTERFEROMETER

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Description

Nowadays, the continuous evolution of synchrotron radiation sources has resulted in a dramatic increase of brilliance and degree of spatial coherence with respect to older designs. The availability of such intense coherent X-ray beams has triggered the development of wave

splitting interferometers similar to the classical double-slit Young's experiment [1-4]. The bilens interferometer consisting of two parallel compound refractive lenses (CRL) and characterizing by high efficiency even in hard X-rays is a remarkable demonstration of such optical devices [5]. In this work, the phase-sensitive X-ray imaging technique based on the bilens interferometer is developed [6]. The essence of the method consists of scanning a sample, which is set upstream of the bilens across the beam of one lens of the interferometer by recording changes in the interference pattern using a high-resolution image detector. The proposed approach allows acquiring the absolute value of a phase shift profile of the sample with a fairly high phase and spatial resolution. The possibilities of the imaging technique were studied theoretically and experimentally using fibres with different sizes as the test samples at the ESRF ID06 beamline with 12 keV X-rays. The corresponding phase shift profile reconstructions and computer simulations were performed. The experimental results are fully consistent with theoretical concepts and appropriate numerical calculations. Future improvements and applications of the interferometric imaging technique are discussed.

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METROLOGICAL APPROACH FOR DIAGNOSTICS OF X-RAY REFRACTIVE LENSES

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Description

Optical systems based on compound refractive lenses (CRLs) with rotationally parabolic profile [1] are amongst the most advanced optical components at the novel synchrotrons worldwide [2]. Methods and technologies of their production one of the most rapidly progressing areas of modern synchrotron instrumentation techniques. Manufacturing of CRLs is closely related to the analysis of technological errors affecting on quality of their optical characteristics. The most important problem is the geometric deviations of the CRL refractive profile from the calculated shape [3]. Therefore, in addition to the improvement of lens manufacturing methods, the development of metrological diagnostic methods which provide accurate measurements of the geometric characteristics of the parabolic profile of the CRL are also required.

This work presents a comparison of various methods of metrological studies of profiles of X-ray refractive lenses. Application of the regression analysis allows to assess the adequacy of the of proposed model of geometrical description of the lens profile and coaxial alignment of the refracting surfaces which determine the quality of the optical system for x-ray imaging. The

developed a comprehensive laboratory metrological approach allows controlling the quality of the profile shape of refractive lenses and thus significantly improve their quality characterization, by a proper adjustment of the CRL production process.

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MATHEMATICAL MODELING OF THERMAL LOADS OF X-RAY ADAPTIVE OPTICS MATERIALS

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Description

The paper presents the results of a study of the thermal loads of materials used in the production of x-ray optics. The development of new types of x-ray studies and the transition to the fourth generation of synchrotron radiation sources, which is realized by reducing the emittance of undulator sections, requires advanced studies of the thermal stability of the first components of the optical line of the beam. An increase in the radiation power density is a critical problem for the design of the optical elements of the undulator section; this is especially important for crystalline monochromators with relatively high angles of incidence. However, other optical elements — windows, lenses, slits, and zoom — are exposed to thermal loads. Therefore, it is important to consider the effect of thermal loads on materials of adaptive x-ray optics to predict not only cooling modes, but also thermal deformations. To this end, studies have been conducted on the interaction of X-rays with the main materials used in the production of X-ray optics - aluminum, beryllium, diamond and UHMW (ultra high molecular weight polyethylene).
The occurrence of thermal gradients occurs due to the absorption of X-rays by the surface of the material (radiant heat transfer) and volume absorption (according to the Burer-Lambert law). The problem was solved numerically by the finite element method in the ANSYS Workbench software package. In the framework of the task, the heat flux arising from the interaction of X-ray radiation with the surface of the substance was set as the boundary condition of heat transfer of the second kind. The shape of the heat spot was chosen in the form of a circle with a Gaussian character distribution of the density of thermal radiation. The interaction of X-rays with a plate of finite size and thickness was considered. As part of the problem statement, 3 loading modes with a characteristic X-ray wavelength were selected: 1, 0.5, and 0.25 angstroms.
The results of the calculations showed that the use of UHMW as a material for x-ray optics requires a very careful selection of operating modes, preference should be given to modes with a very low power density of the radiation load. The main heat load is associated with the surface absorption capacity of the material, combined with low thermal conductivity, leading to the appearance of a surface heat source that can literally burn through the material.
The best calculated thermal stability results were shown by diamond plates. In addition to excellent thermal conductivity, diamond has a low coefficient of volume attenuation of intensity, leading to low temperature gradients of the established temperature regime.
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EXPERIMENTAL IMPLEMENTATION OF X-RAY POWDER DIFFRACTION BY POLYCHROMATIC SYNCHROTRON RADIATION IN THE RANGE OF 20-30 KEV

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Description

The aim of the work is to develop a method that allows X-ray phase analysis using a wide synchrotron radiation (SR) spectral band (polychromatic radiation). This will make it possible to increase the number of photons in the primary beam by 2-3 orders of magnitude and, accordingly, reduce the time for determining the composition of the sample to nanoseconds.The relationship between the angular dependence of the scattering intensity of polychromatic radiation and the angular dependence of the scattering intensity of monochromatic radiation by an object is described by the Fredholm equation of the first kind and is an incorrect task. The solution of this equation in the case of significant experimental errors (which is inevitable in experiments with extremely high time resolution) is quite problematic. The idea of the method is to form a sharp short-wavelength boundary in the SR spectrum and approximate the X-ray diffraction pattern from the polycrystalline sample by the sum of Gaussian peaks, which allows one to determine the intensities and interplanar distances from polychromatic X-ray diffraction patterns using the procedure of minimization by peak parameters. Computer model experiments showed that in this case, the initial values of the peak parameters to minimize are determined with sufficient accuracy for a successful procedure, and the errors in determining the interplanar distances and their corresponding intensities are equal in order of magnitude to the errors associated with traditional experiments. The purpose of this work is the experimental implementation of the proposed method, debugging it on test samples and using fast processes to study. The work is aimed at methodological support of the fundamental task - obtaining previously inaccessible information about the atomic structure of matter during fast processes (explosion, solid-phase reactions). The results obtained will allow us to determine such process parameters as pressure, temperature, density and phase composition in the local region (several microns), as well as the dynamics of their changes in real objects. To date, obtaining direct structural information about the state of a substance during fast-moving processes and the dynamics of its change has been impossible. This hindered the development of the theory of fast-flowing chemical reactions and processes occurring in matter during the passage of the front of shock and detonation waves. The use of polychromatic synchrotron radiation (SR) opens up new possibilities and will allow to obtain previously inaccessible information on the kinetics of phase formation in explosion products after passing through a detonation wave. Synchrotron radiation, as a source of x-ray radiation, has a number of unique properties, the main of which are a large flux intensity, which allows the use of a very short exposure time (<1 ns), high periodicity in time (5-250 ns) and a small angular divergence. This compares favorably with SR from ordinary x-rays and allows one to obtain a multi-frame picture of the density distribution in shock waves and in a detonating explosive with good resolution when registering radiation passing through a substance. In addition, the registration of SR rays deflected by a small angle makes it possible to extract information on density fluctuations in the measurement zone, which in carbon-containing explosives can be associated with the synthesis of condensed carbon phases - ultrafine diamonds or low-density graphite-like substances.

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IN SITU XRD STUDY OF THE REDUCTION OF MIXED MN-CO OXIDE

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Description

The reducibility of oxides is an essential characteristic of catalyst of different reactions. First of all, it is important for oxidation reactions following the Mars-van Krevelen mechanism. In this

mechanism, a weakly bound surface oxygen atom is added to forming the oxygenated compound, leaving behind an oxygen vacancy on the surface. Then, the molecular oxygen react with the surface, dissociate and refill the vacancy. In this case, reducibility of oxide catalyst measures the tendency of oxide to lose oxygen or to donate it to an adsorbed species. Secondly, reduction can be an activation stage of Fischer-Tropsch synthesis, stream reforming and water-gas shift reaction. The catalysts activation leads to transformation from oxide state to metallic, depending on the reductive conditions the state of active sites can be changed significantly. Mn-containing oxides can effectively catalyze the oxidation of hydrocarbons, CO and chlorcarbons. Cooperative utilize of Mn and another oxide leads to synergetic effect – increase in catalytic activity as compared with simple oxides. In double metal oxide catalysts, the formation of mixed oxides is possible. The purpose of this work was to elucidate influence of redox properties of solid solutions on the catalytic performance. A series of catalysts based on mixed Mn-Co oxides with different molar ratios of cations have been prepared by coprecipitation. Reduction mechanism of Mn-containing catalysts with hydrogen was studied by a TPR-H2, in situ XRD, and in situ XPS, XANES. It was shown that the mechanism of reduction of Mn-Co oxides with hydrogen differs significantly from the processes occurring on simple oxides. The reduction of Mn-Co oxides occurs in two steps: (Mn,Co)3O4 transforms to (Mn,Co)O solid solutions, then the reduction of solid solutions (Mn,Co)O to metallic cobalt Co and MnO proceeds. Correlations between the redox properties and the catalytic activity in the CO oxidation reaction have been found.

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DEPENDENCE OF THE SPECTRAL AND LUMINESCENT PROPERTIES OF POLYMETHYL METHACRYLATE ON ITS MOLECULAR WEIGHT

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Description

A line of polymethylmethacrylate (PMMA) samples was synthesized using synchrotron radiation of the VEPP-3 accelerator and the high-energy electron beam of the ILU-6 accelerator. The study was carried out during the in situ synthesis of PMMA in the recording of luminescence spectra and their kinetics. An experimental study was also made of the luminescence of PMMA samples with a molecular weight in the range 0.2 · 10^6 - 6 · 10^6 under excitation by an SR beam in the range of 3 - 60 keV. It was found that with an increase in the molecular weight of PMMA, the maximum of the luminescence band of PMMA shifts toward the long-wavelength direction (redshift), and the luminescence decay time decreases. An increase in the luminescence bandwidth with increasing molecular weight is also observed. These effects are explained by the ordering of the polymer structure and increase in density, which leads to a decrease in interatomic distances and, consequently, to a shift in electronic levels and a change in their width.

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COMPARISON OF EXPERIMENTAL DATA OF 3D DENSITY OF THE EXPANSION ZONE OF TATB DETONATION PRODUCTS OBTAINED ON THE SYNCHROTRON RADIATION OF VEPP-3 WITH COMPUTER SIMULATION

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Description

Unique installations were made - an experimental synchrotron radiation station at the VEPP-3 / VEPP-4 accelerator complex: “Explosion”, “Investigation of the extreme state of matter”. According to the characteristics of the experiments, the station “Investigation of the extreme state of matter” has no analogues in the world. The new stations made it possible to obtain unique data on measuring the 3D density of the expansion zone of the detonating TATB.
In experiments on measuring the density of the zone of expansion of detonation products, a difference was found between computer simulation data and data obtained in experiments using synchrotron radiation. The new data allowed to modernize the codes for calculating the detonation parameters and take into account the condensation process of the solid nano - phase during the detonation of the used detonating systems.
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DEVELOPMENT OF PHOTON DIAGNOSTIC METHODS FOR SYNCHROTRON RADIATION SOURCES

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Description

Synchrotron radiation is the unique electromagnetic radiation, allowing the detailed study of the internal structure of materials using various non-destructive methods. As is known, such radiation is characterized by exceptional brightness and coherence, due to the choice of a specific wavelength or energy, synchrotron light is used in many diffraction methods [1].
Existing technology in particle accelerators led to the ultimate characteristics of the synchrotron radiation source. Further improvement of the storage ring, namely an increasing the electron density and an increasing the brightness of light, becomes difficult [2]. Today, 4th generation synchrotron sources considered diffraction-limited, since such sources have an electron beam emittance less than a photon beam emittance [3]. The transition to synchrotron sources with an ultra-small electron beam opens up new prospects in X-ray diffraction methods and coherent imaging. However, the determination of extremely small source parameters (for example «SKIF» [4]), requires a special approach and tools. Therefore, the diagnosis of such sources becomes an important task. The interest in the diagnosis of synchrotron sources is because this tool allows you to accurately determine the parameters of the generated X-ray beam. We present a source imaging experiment carried out with different detection methods at the ESRF beamline.
Photon beam diagnostics of a synchrotron radiation source can be divided into two directions: the direct source imaging method and the interferometric approach. The direct imaging method allows you to get an enlarged image of the source using Compound Refractive Lens (CRL) [5-6], Fresnel zone plate (FZP) [7], or pinhole camera [8]. The use of interference methods gives a complete image of the phase structure of the photon beam. The proposed diagnostic methods are applicable both for the 3rd generation of synchrotron sources and for the 4th generation.
This research was supported by the Russian Science Foundation (Project No. 19-72-30009).

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DISCOVERY OF THE SCALE EFFECT OF THE DEPENDENCE OF THE MASS OF SOLID DETONATION PRODUCTS ON THE MASS OF EXPLOSIVES IN "IN SITU" EXPLOSIVE EXPERIMENTS ON SYNCHROTRON BEAMS VEPP-4

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Description

A unique installation, the only one in the world, was commissioned - an experimental synchrotron radiation station at the VEPP-4 accelerator complex: “Investigation of the extreme state of matter” [1]. According to the characteristics of the conducted experiments, the station has no analogues in the world. The new station made it possible to obtain unique in situ data on the dynamics of the formation of detonation products of large explosive charges (up to 200 grams) of TNT - RDX.

The investigated explosive charges were cast TG samples ($\rho \approx 1.7$ g / cm3) with a diameter of 20, 30, 40 and a length of 55 mm. Initiation was carried out by the EDV-1 electric detonator through a plane wave generator (20 mm in diameter) and an intermediate charge of P-84 with a length of 5 mm and a corresponding diameter. After the electric detonator, a contact sensor was installed to stop the recording of the detector.

The experimental data obtained in this work are already used to take into account the carbon condensation energy behind the chemical reaction zone during detonation of TG charges. They are also important for constructing physical models of detonation and testing early models of the development of detonation processes.

In these experiments, a scale effect was discovered - a nonlinear dependence of the mass of solid detonation products on the mass of explosives. At small charges (10 -50 grams), the amount of solid detonation products linearly depends on the initial explosive mass. With large masses of 50 - 150 grams, a deviation from the linear dependence is observed. This is a large-scale effect - a deviation from linear dependence.

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DEVELOPMENT OF AN APPROACH TO MINIMIZE THE EFFECTS OF X-RAY GLITCHES

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Description

The construction of 4th generation synchrotron sources will make it possible to obtain a fully coherent high-energy x-ray beam with extremely low emittance and high brightness. The use of effective refractive optics already at the radiation output (front-end) is necessary to realize all the possibilities and fully reveal the potential of new diffraction-limited sources. X-ray refractive lenses (hereinafter CRL) [1] satisfy the above requirements. Monocrystalline diamond is considered to be an ideal material for CRL, mainly because of its stability in flow and high reflectivity in the hard X-ray range. Being universal for a wide range of applications, diamond CRL, nevertheless, have a feature for application in spectroscopic experiments, which was noted in a recently published article [2], which reported on the observation of intensity modulation at certain energies in the transmission spectrum. This issue is well known in X-ray spectroscopy and is called “diffraction loss” or “glitch” [3]. In paper [2, 4] X-rays were propagating through lenses, while the transmitted intensity was measured at different energies. Use of compound refractive lenses, that were perfectly aligned by stacking in a single plate, gave us strong diffraction losses, reducing the outgoing signal by maximal value of 40%. The magnitude of the effect was then minimized down to ~ 10% by use of CRLs compiled from individual lenses with different crystallographic orientation. At the same time, X-ray glitches did not affect any focal spot’s size or shape while only arousing the darkening of the focal spot at exact energies of X-ray glitches [4]. Despite X-ray glitches, monocrystalline X-ray optical materials are preferable than polycrystalline ones. While single crystals only uniformly reduce the outgoing intensity (i.e., gain factor of the lens), polycrystalline materials introduce speckles and distortions to the transmitted wave front. Such negative influence of the inner material limits the resolution and optical efficiency of X-ray lenses. In [5-6], it was found that the spatial position of the incident X-ray beam (relative to the lens aperture) most strongly affects the intensity and position of the glitches. The value of the glitch intensity strongly depends on the thickness of the material of the test sample, which is associated with the effect of attenuation (extinction) i.e. as the thickness of the material increases, the fraction of incident radiation diffracts, which causes a decrease in the intensity passing through the lens. Glitches become more pronounced with increasing thickness of the material through which the x-rays pass. Although glitches are always present in the transmission spectrum of single-crystal materials, based on the data obtained above, attempts were made to develop approaches to minimize or, ideally, get rid of glitches in the spectrum of single-crystal optical elements. An important result of the proposed work is a theoretical model, which was confirmed by the experimental results and which allows predicting the position and strength (intensity) of glitches if the crystallographic orientation relative to the x-ray beam is known with sufficient accuracy. Therefore, performing calculations for a precisely positioned single-crystal lens with a known crystallographic orientation, it is possible to choose specific energy intervals where the effect of glitches will have a minimal effect. The results and assumptions made it possible to start developing a method of getting rid of glitches at each energy using a small lens flap, which is calculated on the basis of a program that can determine the lens orientation solely from the spectrum of glitches and on the basis of an analytical approach that allows you to refine the orientation of the crystal and, probably , will allow the use

of crystalline lenses for experiments in which it is necessary to change the energy of the incident beam. How to avoid glitches (practical guidance). First current orientation and cell parameter of the lens has to be determined. For this energy of several glitches (at least 3) have to be measured with high precision. Then the found energies can be fitted using proposed approach (by tilting possible K0 directions and comparing the resulting spectrum to the measured one). This will allow to assign hkl indexes to the observed glitches. Next step is to calculate analytically the exact direction of the incident beam and cell parameter This will allow to predict with high precision all glitches for current orientation. Next multiple glitches spectra for different small tilts can be calculated, so for each energy a tilt with no glitches at that energy can be selected. During the energy scan the lens has to be tilt into precomputed orientations. The glitches are rather sharp, so the tilt required to shift a glitch is small. Therefore the efficiency of the lens shouldn't suffer. The method might require small increase in the lenses thickness to have possibility to tilt the lenses. Thus, by performing the sequence of actions indicated in the developed approach, the negative impact of glitches can be avoided.
This research was supported by the Russian Science Foundation (Project No. 19-72-30009).

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STUDY THE DIAMOND THIN MEMBRANES BY X-RAY REFLECTOR-INTERFEROMETERY AT THE ESRF BEAMLINE ID10

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Description

Today, the combination of new generation X-ray sources with modern optical elements gives a strong impetus to the development of new research methods, and to improve the classical methods. One such method is X-ray reflectometry (XRR). Despite the widespread use for thin-film structures study, XRR has a strong limitation related with the size and surface quality of the samples. Refractive optics is the most dynamically developing kinds of X-ray optical elements [1-2]. CRLs quickly gained popularity among synchrotron sources users due to their ease of operation and the possibility of application in a wide range of energies [3-4]. In this work, a new

X-ray reflecto-interferometer (XRI), based on CRL, was demonstrated to study thin-film structures using the synchrotron X-ray source [5]. Due to the CRL focusing properties, X-rays incident on the sample surface contain the necessary range of angles for the formation of an interference pattern in one shot. The capabilities of the new XRI were demonstrated at the ESRF ID10 beamline (Grenoble, France). The Si3N4 and diamond membranes with thicknesses 100 and 200 nm were studied using X-rays of energy 22 keV. Experimentally obtained reflecto-interferograms are in good agreement with calculated ones, and the distance between fringes in the interference patterns corresponds to the thickness of the tested membranes The new XRI opens wide horizons both for rapid thin-film and multilayer analysis and for studying the dynamics of processes on the surface and in the depth of the sample, as well as for studying complex structured and biological samples.

This research was supported by the Russian Science Foundation (Project No. 19-72- 30009).

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THE INFLUENCE OF INTERNAL BERYLLIUM MICROSTRUCTURE AND IMPURITIES ON THE CRL X-RAY OPTICAL PROPERTIES

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Description

Novel fourth generation and updated synchrotron radiation sources require highest quality X-ray optics resilient to extreme thermal and radiation loading while preserving their coherence and brilliance. And refractive optics is the best candidate for this task due to its extensively employed at synchrotrons and X-ray free-electron lasers. Refractive lenses are used as condensers, micro-radian collimators, low-band pass filters, high harmonics rejecters, beam-shaping elements. Two-dimensional beryllium lenses are and remain the driving force in the development of Fourier optics, coherent diffraction and full-field imaging techniques. However, the development of new coherent techniques such as phase-contrast imaging and coherent diffraction microscopy demanded to revise the requirements for surface quality and internal structure of X-ray optic materials [1-3]. It is worth noting that almost all beryllium grades, used for X-ray optics manufacturing, are sintered materials, which have inevitably internal micro- and nanograined structure and relatively high beryllium oxide (BeO) and other heavy elements concentration, which leads to strong small- and ultra-small angular X-ray scattering and additional losses of intensity [4]. The influence of the beryllium microstructure and impurities on the optical properties of the compound refractive lens was studied and successfully demonstrated for the first time in the microbeam and coherent full-field hard X-ray microscopy mode [5]. The paper includes recommendations on beryllium refractive lenses and beryllium windows manufacturing processes by using different beryllium grades for various applications of X ray optics. We are confident that there is a reasonable choice of beryllium materials suitable for coherence related techniques allowing to use the full potential of novel X-ray sources.

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INVERSE COMPTON SCATTERING AT COLLISION OF ELECTRON AND PHOTON BEAMS WITH OBLIQUE FRONTS

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Description

Inverse Compton scattering dubbed “light undulator” is a known source of x-ray radiation, bright and intense. Among the perspective directions of research one of the most significant is idea of Debus with co-authors: to use the laser pulse with skew front to increase the time of interaction of the electron and photon beams. The corresponding calculations were performed within classical electrodynamics. Here, we calculated this process in the terms of luminosity within quantum electrodynamics. Our results show that the condition suggested by Debus et al. for the maximal intensity will not result in the number of the scattered photons compared with the conventional collinear orientation of the fronts.

The study was supported by RFBR, grant 19-29-12036.

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GENERATION OF SMITH-PURCELL RADIATION FROM AN ARRAY OF SUB-WAVELENGTH PARTICLES

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Description

Smith-Purcell radiation is emitted by an electron moving near a periodically inhomogeneous target. The main features of Smith-Purcell radiation is monochromaticity and relation between the wavelength of radiation and the observation angle. As during generation there is no direct scattering the electrons on the atoms of material, this type of radiation can serve as a tool for non-invasive beam diagnostics. Here, we report on the recent progress in theoretical investigation of Smith-Purcell radiation from two-periodical arrays consisting of small particles. Such targets are referred as metasurfaces or photonic crystals as well. Second period in direction perpendicular to the electron trajectory opens new possibilities for the diagnostics of relativistic electron beam, including simultaneous measuring the two emittances for the electron beams with asymmetric cross-section.

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TRANSMISSION HARD X-RAY INTERFEROMETER-MICROSCOPE (15-35 KEV) AT VEPP-4 STORAGE RING FACILITY AS A PROJECT

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Description

A new Transmission Hard X-ray Interferometer-Microscope (THXIM), which is based on X-ray refractive lenses and diffractive gratings, was developed for 15-35 keV photon energies to set up at the second front-end of VEPP-4M storage ring. The synchrotron radiation (SR) path from the bending magnet source to the experimental hutch is 17 m. The THXIM block sequence on the

SR beam course within the 6.5 m hutch distance is the following: 1) The forvacuum block includes horizontal and vertical slits, a multilayered X-ray mirror monochromator, an SR beam position detector and a blocker absorbing the direct beam. 2) The block of the X-ray refractive condenser lens in the air atmosphere. 3) The block of a research object and the X-ray refractive objective lens with X-ray diffractive gratings is in the air environment. 4) At the end of the beamline station, the air block of the THXIM detector is disposed, which includes an X-ray scintillator (a 100 μm thin, 1 cm large area, CdWO4 crystal) and an optical microscope with a planapochromate objective, inclined mirror and a CCD camera. Between 2, 3 and 4 blocks, forvacuum tubes for the beam inflights are disposed. We develop inclined X-ray lithography with SU-8 and PMMA resist, as well as photo- and e-beam lithography and galvanoplastics technologies of gold, nickel and aluminum microstructures in order to create X-ray refractive lenses with high aspect ratios of 3D apex elements and X-ray diffractive gratings with nanometer range periods. The X-ray refractive long compound paraboloid objective lenses with 100 μm apertures and focal distances of several centimeters provide the THXIM resolution of dozens nanometers. The position choice for a THXIM research object within a local coherent zone, which is obtained by means of an X-ray refractive condenser lens with a long-length focal waist, is discussed.

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μ-XRF FOR THICK SPECIMENS

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Description

When studying samples without destruction by x-ray fluorescence analysis, the thickness of the investigated sample is limited by the depth of total absorption of the outgoing and excitation radiation. When analyzing complex geological objects containing high-Z atoms, the excitation energy can reach several tens of kiloelectronvolts, which can generate x-ray fluorescent light from a depth of several hundred micrometers. However, focused on the front plane of the sample the beam of excitation radiation is defocused at such depth, and its cross-section under the conditions discussed in the report can become significantly larger than the focus size. This effect is especially significant when the x-ray source is small, for example, for the SKIF synchrotron radiation source. Based on the geometric model of the actinic voxel, the conditions for optimal choice of the excitation energy and focusing conditions of the initial x-ray beam are determined.

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DETERMINATION OF THE STATE OF THE ACTIVE COMPONENT OF NANOCOMPOSITE MODEL METAL-CARBON CATALYSTS BY XAFS METHOD

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Description

This report shows the results of XAFS (XANES/EXAFS) research on the state and local structure of metals in the active component of model low-percentage metal-carbon nanocomposite catalysts containing nanoscale forms of Pt, Pd, Ru. It is a well-known fact that low-percentage catalytic nanosystems containing platinoids deposited on various carbon carriers are of great interest to researchers because of their practical significance; possibilities for varying catalytic properties and applications for a wide range of processes (hydrogenation, conversion of industrial substrates, debenzylation of amines, etc.).), low cost of final products, ease of disposal and recovery of expensive components from spent catalysts. Model samples were prepared from precursors of different nature, with varying methods of synthesis and formation of the applied component, recovery and activation modes. XAFS (XANES/EXAFS) spectra (Pt-L3, Pd-K, Ru-K) of studied samples were recorded at SSTRC, Novosibirsk. The lengths of interatomic bonds and the corresponding coordination numbers are established. Additionally XPS, TEM, XRD, XRF methods were applied to study chemical and phase compositions, morphology of the samples. Data obtained by different methods do not contradict each other. Possible variants of structural models are considered in detail. Correlations were found between the structure of the active component and the catalytic properties of the studied samples. The perspective of the proposed approach for the study of nanocomposite model metal-carbon catalysts containing platinoids is shown.
The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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STRUCTURAL STUDY OF BIMETALLIC CATALYTIC NANOSYSTEMS CONTAINING PRECIOUS METALS BY XAFS SPECTROSCOPY

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Description

This work presents the results of a study of the local structure of the active component of mono-, bi-metallic low-percentage (~1%) catalysts (containing Pt, Au, Pd, Ru) stabilized on oxide carriers using XAFS method (XANES/EXAFS). Studying the nature of nano-forms of noble metal stabilization is promising for creating effective catalysts for various applications, including catalytic systems for alternative energy applications. The development of synthesis methods can lead to a significant economic gain, due to the reduction of the metal content and optimization of the catalytic properties of the system. Model catalysts were prepared from mono-and bimetallic complexes, with varying synthesis methods: sol-gel, ion exchange, impregnation, reducing modes, and the nature of carriers. XAFS (XANES/EXAFS) spectra (Pt-L3, Au-L3, Pd-K, Ru-K) of studied samples were recorded at SSTRC, Novosibirsk. Genesis of the local structure of the active component was studied, including the study of oxidized precursors and catalysts after reducing and activation. It is established that depending on the background, it is possible to form various nanoscale forms of noble metals localized on the surface of the oxide carrier. Additionally, the samples were studied by XRD, XPS, XRFA, HRTEM. Variants of possible structural models are considered in detail.
The work was carried out in the framework of the RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk

FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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XAFS STUDY OF STABLE BIMETALLIC CATALYSTS FOR SELECTIVE HYDROGENATION OF FURFURAL

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Description

Today catalytic reaction of the selective hydrogenation of furfural is perspective way to create of motor fuel components and products with high added value. Unfortunately existing catalysts providing high conversion of the initial furfural have not sufficiently high selectivity for the target products (70-80%), which indicates the need to develop new significantly more active and selective catalysts with high stability. In this connection, the search for correlations between structural features and the charge state of metals in deposited bimetallic clusters and their catalytic activity and selectivity in the process of selective hydrogenation of various functional groups of the furfural molecule is an urgent research task. This presentation is devoted by a study of the state and local structure of the active component of Ru-Sb, Fe-Sb model catalysts catalysts for selective hydrogenation of furfural by XAFS (XANES/EXAFS). The catalysts were prepared by sol-gel from organic and inorganic mono- and bimetallic complex precursors. All XAFS spectra were recorded at SSTRC, Novosibirsk. The genesis of local structures and state metals for the prepared nano-structured catalysts were studied in detail. The interatomic distances and corresponded coordination numbers were determined. All possible structural models were discussed. The obtained XAFS results are in good agreement with XPS, XRD, EDX and HRTEM data.

The work was carried out in the framework of the RNF project no. 18-73-10216, RFBR projects no. 19-05-50046, 18-03-01251. The work was done at the shared research center SSTRC on the basis of the Novosibirsk FEL/VEPP-4-VEPP-2000 complex at BINP SB RAS, using equipment supported by project RFMEFI62119X0022.

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THZ NONLINEAR ELECTRONIC RESPONSE IN GAAS/INGAAS SEMICONDUCTOR NANOWIRES

Harald Schneider

Description

This presentation reviews some recent experiments using free-electron-laser-based narrow-band as well as tabletop-laser-based single-cycle terahertz (THz) fields for exploring electronic properties in semiconducting GaAs/InGaAs core/shell nanowires (NW) [1]. In undoped NW, charge carriers are optically excited by near-infrared pulses and probed by strong single-cycle THz fields up to 0.6 MV/cm. The photoexcited charge carriers exhibit a pronounced plasmon resonance, which undergoes a systematic redshift and a suppression of its spectral weight, which indicates a drop of the electron mobility at the highest fields to about half of the original value [2]. In n-type NWs, intense narrowband THz excitation causes a nonlinear plasmonic response, which manifests itself by a similar pronounced red shift of the plasma resonance. This nonlinearity is investigated by scattering-type scanning near-field infrared microscopy on individual NWs. For NW doped with Si to a concentration of 9x10^18 cm^-3, a spectrally sharp plasma resonance, located at a photon energy of 125 meV for weak excitation, undergoes a

power-dependent redshift to about 95 meV [3]. In these experiments, the observed behavior is attributed to a pronounced increase of the average electron effective mass caused by transient carrier heating and electron intervalley transfer. The results quantify the nonlinear transport regime in GaAs-based nanowires and show their high potential for development of nanodevices operating at THz frequencies.

[1] L. Balaghi et al., *Widely tunable GaAs band gap via strain engineering in core/shell nanowires,* Nature Comm. **10**, 2793 (2019)
[2] R. Rana et al., *Nonlinear terahertz field-induced charge transport and transferred-electron effect in InGaAs nanowires*, Nano Lett. 20, 3225 (2020)
[3] D. Lang et al., *Nonlinear plasmonic response of doped nanowires observed by infrared nanospectroscopy,* Nanotechnol. **30**, 084003 (2019)

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MULTICHANNEL THZ TELECOMMUNICATION BASED ON MODE DIVISION MULTIPLEXING (MDM) APPROACH

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Description

The present talk is devoted to the use of beams with orbital angular momentum (OAM) [1] for development THz multichannel systems based on the mode division multiplexing (MDM) approach. The work [2] shows the results of the feasibility study of organizing a multichannel terahertz (THz) communication system based on controlling the transverse-mode composition of a coherent beam of terahertz radiation. In [1,2], however, it was only a question of changing the transverse mode composition without changing the polarization state of the illuminating beam. In the long run, the development of methods for simultaneous control of the transverse mode composition and polarization state of a terahertz beam will allow developing multichannel terahertz telecommunication systems with high information capacity. In the work [3], the authors designed, produced, and examined a subwavelength axicon for converting linearly polarized terahertz radiation into a cylindrically polarized beam. In the present talk perspectives of application of terahertz non-uniformly polarized beams for telecommunication are also considered.

This work was supported by the RF Ministry of Science and Higher Education under the government project of the FSRC “Crystallography and Photonics” and by the Russian Foundation for Basic Research (grant 19-07-00423). The experiments were performed at the Shared Research Center SSTRC based on the Novosibirsk FEL.

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[2] Y.Y. Choporova, B.A. Knyazev, N.D. Osintseva, V.S. Pavelyev, K.N. Tukmakov, “Two-channel terahertz communication based on spatial mode multiplexing, Proceedings of 44th International Conference on Infrared, Millimeter, and Terahertz Waves”, IRMMW-THz, 2019.
[3] S.N. Khonina, K.N. Tukmakov, S.A. Degtyarev, A.S. Reshetnikov, V.S. Pavelyev, B.A. Knyazev, Yu.Yu. Choporova, “Design, fabrication and investigation of a subwavelength axicon for terahertz beam polarization transforming”, Computer Optics, vol. 43(5), pp.756-764, 2019.

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CONCEPTUAL DESIGN OF THE "FAST PROCESSES" BEAMLINE AT THE SRF SKIF 4TH GENERATION SYNCHROTRON

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Description

"Fast Processes" is one out of six 1st priority beamlines that are planned for construction within the project SRF SKIF (Shared Research Facility "Siberian circular photon source") [1]. The beamline would include two independent instruments installed at a wiggler source, i.e., Dynamic processes and Plasma. The beamline is designed to meet a wide range of research and technological challenges related to processes occurring in nano- and microsecond timescales. The current conceptual design of the beamline aims at a complex approach to structural studies of various objects relying on high-brightness synchrotron radiation beams. The beamline would implement X-ray diffraction, small-angle scattering, and radiography techniques with a high temporal resolution, with a typical delay between frames down to 2.8 ns and exposures of about 50 ps. The assortment of scientific problems to be solved at the beamline includes studies of detonation processes; impact of explosion and shock waves on structural materials; dynamic endurance and fracture emergence; influence of laser irradiation and plasma on a variety of substances. The aforementioned synchrotron-based techniques will allow us to track structural changes along the detonation and shock-wave front, detect the formation of nanoparticles from explosion products (e.g., nanodiamonds), and elucidate the phase composition and local structure of substances subjected to extreme dynamic impacts.

[1] http://srf-skif.ru

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TRENDS ON MONTEL X-RAY OPTICS AND PINHOLES FOR SYNCHROTRON BEAMLINES

Jörg Wiesmann, Andreas Stricker, Frank Hertlein, Uwe Heidorn, Christopher Umland (Incoatec GmbH)

Description

Different kinds of X-ray mirrors are required for beam alignment, guidance or monochromator applications. Therefore various types of optics with coatings for energy ranges between 100 eV and 80 keV have been investigated.

We will show stripe multilayer coatings which are often used as Double Crystal Multilayer Monochromators (DCMM) for example in tomography beamlines. The optics consists of up to 5 different coating stripes, optimized for each energy range.

We will also present results of a 50 cm laterally graded multilayer optics, developed for special mini-synchrotrons with a deviation to a specified film shape of less than 0.2 %.

We will present new developments of Montel Optics for synchrotron applications. Different types of these two-dimensional optics are used at DLS, NSLS and APS and Riken, for example in an analyzer system for inelastic scattering. One new 230 mm Montel Optic for 11215 eV was delivered a few months ago to ESRF for BL ID20.

Parasitic aperture scattering causes loss in data quality especially in SAXS and GISAXS applications. Various measurement results will be presented showing the improvement of data quality with scatterless pinholes. These pinholes are either made of Germanium for energies < 11.2 keV or of Tantalum for energies > 11.2 keV and are available with diameters from 2 mm down to 20 µm and below.

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