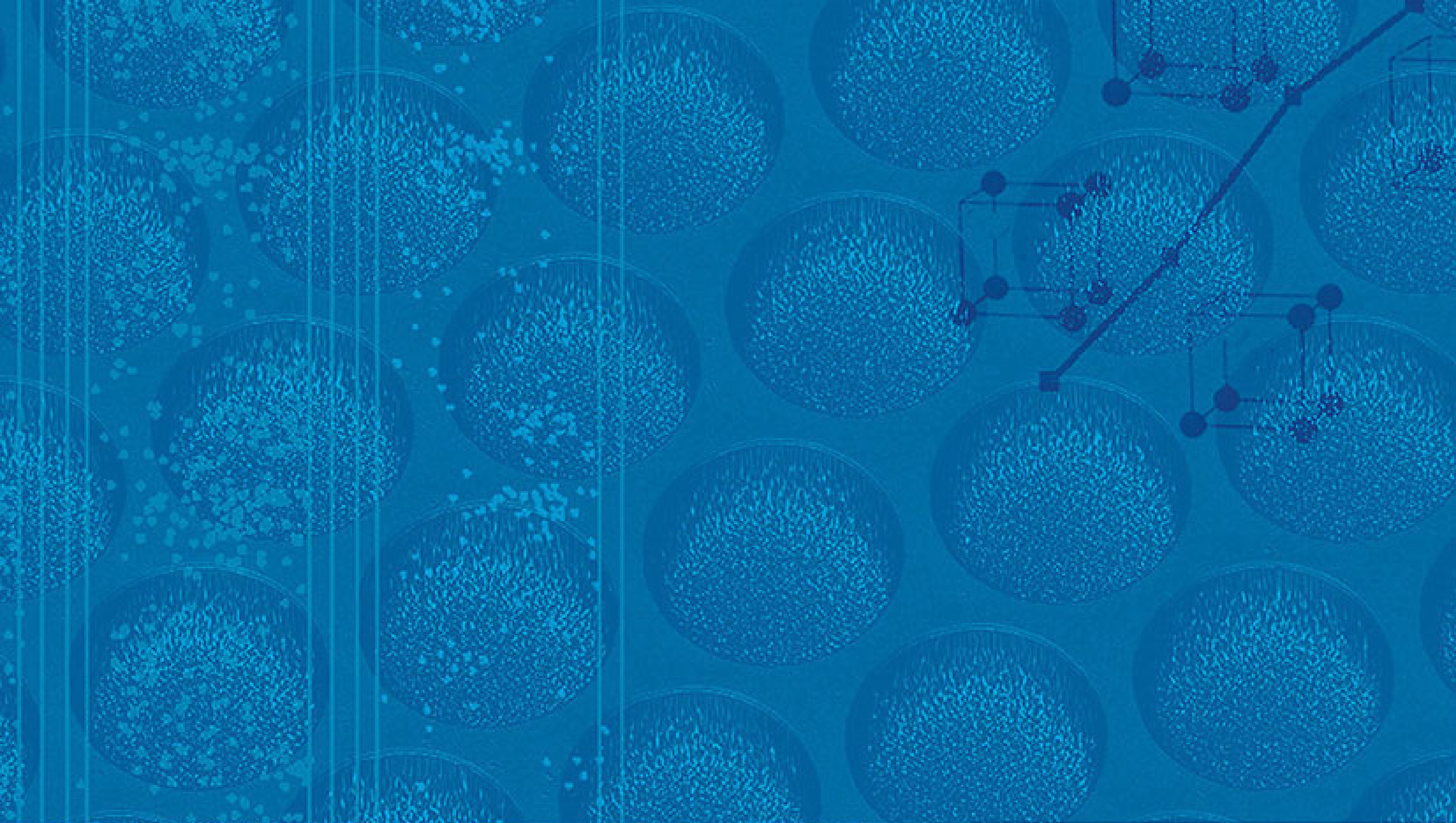

HELMHOLTZ-RUSSIA JOINT RESEARCH GROUPS (HRJRG)

3.03.2014

RUSSIAN FOUNDATION FOR BASIC RESEARCH
RFBR

Deutsches Wissenschafts- und Innovationshaus – Moskau
Deutschland Land der Ideen

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HELMHOLTZ ASSOCIATION OF GERMAN RESEARCH CENTRES

The Helmholtz Association is the largest German scientific organisation which is made up of 18 national centres which perform top-rate research in 6 major fields: Energy, Earth and Environment, Health, Key Technologies, Structure of Matter, Aeronautics, Space and Transport. The centres have more than 35,600 employees and an annual overall budget of €3,76 billion. The work of the Helmholtz Association follows the tradition of the great natural scientist Hermann von Helmholtz (1821–1894).

More than 11,249 scientific publications every year and around 400 new patent registrations, 2,000 cooperation projects with business and industry – the Helmholtz Association shows excellent results in both basic research and application. The Helmholtz Association provides an excellent infrastructure for research with large-scale facilities, such as particle accelerators, super computers and research ships, some of which are globally unique.

As a strong member of the global scientific community the Helmholtz Association works with national and international partners representing science and research as well as business and industry.

Russia is one of the key strategic partners of the Helmholtz Association. There are more than 200 cooperation projects between Helmholtz centres and Russian institutions. The Helmholtz Moscow Office was established in 2004 in order to strengthen co-operation between Russian scientists and researchers of Helmholtz Centres and to initiate new partnerships. It is the first point of contact for Helmholtz researchers who wish to cooperate with Russian partners, and for Russian scientists who need special information and contacts of their potential partners in the Helmholtz research centres.

RUSSIAN FOUNDATION FOR BASIC RESEARCH (RFBR)

Russian Foundation for Basic Research is a self-governed nonprofit federal state organisation to provide targeted diversified support to leading groups of scientists in Russia. RFBR supports fundamental research in all directions of natural sciences by selecting projects on a competitive basis after their comprehensive evaluation.

RFBR is conducting annually different domestic and international calls for the scientists from more than 4000 different Russian organisations like research institutes of the Russian Academy of Sciences, universities, research units of large state and private companies residing in different regions of Russia. The principal part of the RFBR funds (over 50%) is directed towards financing initiative (bottom-up) scientific projects performed by small groups of scientists (up to ten persons) or individual scientists.

The Foundation sees its mission in developing the powerful intellectual potential for the modern Russia. Also, it is looking for effective forms of integration of the Russian researchers into the world's scientific space.

RFBR is an active participant of the international cooperation programs and projects. The geography of international RFBR competitions reflects already active cooperation with more than 40 partners from 28 countries, among which European countries predominate, along with countries where fundamental research in natural sciences is conducted intensively. The closest and most fruitful ties are with the partner organisations from CIS countries, Germany, France, China, India, US, Japan, Taiwan and some others. Special attention is given to international projects leading to innovation breakthroughs in different fields as well as to multilateral projects.

Sampling in Listvyanka, outflow of Lake Baikal into Angara river.
Image by T. Luckenbach (UFZ)

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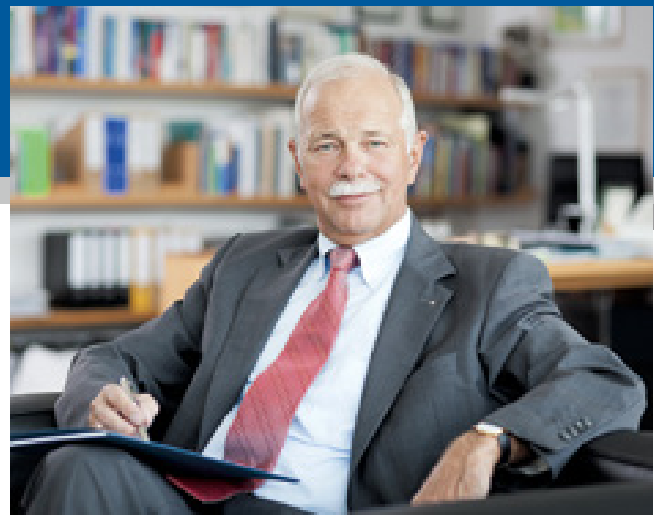

DEAR COLLEAGUES,

It is with great pleasure and pride that I am able to present to you the results of the 32 projects funded so far as Helmholtz-Russia Joint Research Groups by the Helmholtz Association and the Russian Foundation for Basic Research (RFBR).

The Helmholtz Association contributes to shaping our future by performing strategic research towards solving grand challenges and thus creating wealth for society and industry through the transfer of knowledge and technology.

We contribute to solving grand challenges by performing top-rate research in strategic programmes in the fields of Aeronautics, Space and Transport, Earth and Environment, Energy, Health, Key Technologies as well as the Structure of Matter.

The Helmholtz Association is globally recognized for our large-scale facilities and scientific infrastructure, cooperating closely with national and international partners.

One of the key instruments in achieving our strategic goals is The Initiative and Networking Fund. Within the framework of the fund, projects such as Helmholtz Alliances and Helmholtz Virtual Institutes were initiated, thus creating the framework for top-flight research, assuring excellence and certainly promoting young researchers.

The establishment of the Helmholtz-Russia Joint Research Groups, a programme of joint financing in cooperation with the RFBR, is one of the most successful instruments for supporting the work of outstanding young scientists in Russia and Germany.

Our association's investment in this project amounts to around EUR 12,5 million. We are pleased to see that the applications presented cover all fields of our expertise. We are also deeply satisfied to see that the Helmholtz Association's key programmes were of such high interest for young Russian scientists. This shows us once again that we are on the right track with our activities.

We are pleased to have the RFBR as our reliable partner contributing to the overall success of this programme and look forward to further expanding and developing our cooperation in the future.

I wish all project participants much success for their work and the further expansion of our joint research efforts.

Yours,

Prof. Dr. Jürgen Mlynek
President of the Helmholtz Association

DEAR READERS,

This publication aims at informing on the collaboration between the Russian Foundation for Basic Research (RFBR) and the Helmholtz Association started in 2007. After 7 years of our partnership its objective remains the unchanged: to obtain outstanding results from the activities of the Helmholtz-Russia Joint Research Groups (HRJRG) as also to help the scientists from Russia and Germany to establish fruitful and creative links.

As we entered the 21st century, all economic, social and scientific challenges have become global. This is why the RFBR has set international cooperation at the heart of its agenda. To make this cooperation more optimal and effective, the RFBR is continuously looking for new foreign partners across the world, first of all in the countries like Germany, where research funding and performing agencies are traditionally promoting and nourishing basic research.

Through its collaboration with the Helmholtz Association, the RFBR intends to realize a policy of excellence for the benefit of the scientific community in Russia and to focus on the fundamental research startups based on the available mega-science facilities. Of special importance is to have early career scientists involved in the projects supported by the RFBR and the Helmholtz Association and to encourage knowledge transfer to the applied research and innovation sector of our countries.

The Helmholtz Association is our privileged partner, generously contributing to the HRJRG funding and enjoying broad publicity in Russia due to high activity of its local outfit – Moscow bureau. We are proud to share this activity by attending the scientific events initiated by the Helmholtz Association or even to jointly hold them like we did this time announcing German-Russian Workshop envisaged to investigate our bilateral collaboration story – its experience, solutions and prospects.

We are convinced that the RFBR-Helmholtz partnership has a bright future and will add a lot to the further development of the Russian-German scientific ties.

Academician Vladislav Panchenko
RFBR Board Chairman

DEAR READERS,

The „Deutsches Haus für Wissenschaft und Innovation Moskau (DWIH)" – German Center for Research and Innovation Moscow – forms a part of the recently established new branch of Foreign Research Policy of the Federal Republic of Germany and is to present the efficiency and capability of German research and science abroad.

This concerns both research realized on the level of universities and of the well-known German Research Centres, among them the Helmholtz Association. The DWIH Russia as a forum enables presentation of innovation research, including its economic implementation and enhances a fruitful dialogue between German and Russian scientists as well as the demonstration of its innovative products of German enterprises.

Furthermore, the DWIH Russia particularly cares for young Russian scientists who will represent the next generation of prospective researchers. Thus, we warmly welcome the generously conceived "Helmholtz-Russia Joint Research Group" program, which aims at the support of young Russian scientists in Russia itself. We are delighted to contribute to this idea in a moderate, but due way. This programme represents a form of partnership between Russia and Germany, which falls in line with the DWIH policy in Russia and – even more important – it will be a milestone on the common way to future cooperation which benefits either side.

Dr. Gregor Berghorn
Head of the DWIH Moscow

HRJRG – A JOINT PROGRAMME OF THE HELMHOLTZ ASSOCIATION AND THE RUSSIAN FOUNDATION FOR BASIC RESEARCH

The Agreement (MoU) signed between the RFBR and the Helmholtz Association in 2006 opened a new track of cooperation between German and Russian scientists involved in the fundamental (basic) research. The parties of the Agreement aimed to start up practical joint R&D supported by a research funding agency like the RFBR and a research performing agency like the Helmholtz Association. It was mutually understood that the decision made was right. The RFBR got one more partner in Germany highly experienced in promoting multidisciplinary targeted (goal-oriented) research developing into one of the most dynamic areas of the RFBR recent activities. Accordingly, the Helmholtz Association entered into an agreement with an organization in Russia which operates in complete consistency with rules and principles applied by other leading science foundations both in Germany and globally. By mid-2000s the very nature of German-Russian scientific cooperation had, over the prior ten or so years, undergone a steady transformation from a donor-recipient model to a partnership model. Therefore, the partnership established was based on the principles of bringing in and going global as well as on international standards of reciprocity, mutual benefit and reasonable sharing of funding needed.

The RFBR and the Helmholtz Association common interests to make their bilateral cooperation a success helped them to develop a unique programme of supporting collaboration between young scientists from Russia and Germany. It resulted in launching of 32 research projects selected out of 101 proposals received for evaluation during five calls held in 2007–2012. The impressive number of proposals showed how great was the interest of call participants in their collaboration within the framework of the Helmholtz-Russia Joint Research Groups (HRJRG). The competition was very strong with the average success rate 32 per cent. Those who were lucky to be awarded with grants faced an obligation to present not only final reports but convincing results confirming high level and fruitful outcome of their joint research activities in 3 years. Hundreds of investigators were engaged totally in the HRJRGs, all of 18 Helmholtz centers were represented among the German researchers while Russian participants represented about 50 different Russian research organizations like RAS institutes, universities and some other.

According to the preliminary data about 500 publications has been produced by all 32 HRJRGs so far. This number includes also joint (co-authored) publications mostly published in prestigious science magazines and other national and international media with a high impact factor. Other impacts, however, are also significant. The HRJRG-207 sparked further development of a spectroscopy method (called Hilbert spectroscopy) aimed at detecting liquid explosives by using electromagnetic radiation. Other successes which are in the pipeline prove that RFBR-Helmholtz cooperation is in a position to generate tangible results. The subjects of research vary from medical subjects, such as cancer and diabetes studies, through energy efficiency studies to global change of basic environmental conditions worldwide. The most popular applications subjects for the joint research were in Earth and Environment (26) and Structure of the Matter (23), followed by Health (18), Key Technologies (14), Energy (12) and

Space (8). The largest number of projects supported was in Structure of Matter (8), then Earth and Environment and Health (6 each), Energy and Key Technologies (5 each), Aeronautics, Space and Transport (2).

Prospects of future cooperation are quite bright. Further success of RFBR-Helmholtz partnership is based on a number of factors.

First, the partnership has built a substantial number of networks (research teams within the framework of HRJRGs) eager and able to continue their collaboration. Many databanks with scientific and management information were established. More investigators from both sides were put on a "waiting list" after their proposals failed to be supported during the first round of RFBR-Helmholtz cooperation in 2007–2013.

Second, the challenges to perform top-rate research in line with the Helmholtz Association six strategic fields are impressive and appealing. Such fields of fundamental research as Aeronautics, Space and Transport, Earth and Environment, Energy, Health, Key Technologies, Structure of Matter are open for exploration without any limits.

One more factor favorable for future cooperation is availability of Helmholtz large-scale (mega-science) facilities, both existing and under construction, including those shared by Russia. The unique scientific installations are providing unprecedented opportunities for a cutting-edge joint research. Harmonization of this cooperation is possible through opening of access to similar facilities already available in Russia.

Finally, a very promising form of cooperation wasn't tested by two partners so far. This is joint participation in international multilateral programmes. The perspective is broad, but they could initiate its own programme, inviting other parties they can find in many countries among their common foreign partners.

Until now RFBR and the Helmholtz Association have invested quite a substantial amount of money in their joint programme. But the outcome already produced can hardly be measured in monetary terms.

By publishing this brochure we provide all the 32 Helmholtz-Russia Joint Research Groups with an opportunity to represent directly their projects and research results. At the moment of publication, 26 of 32 projects have been already completed and 6 are still in progress.

We wish all HRJRG participants success and look forward to expansion of the RFBR-Helmholtz cooperation forms.

Dr. Elena Eremenko
Head of Helmholtz Moscow Office

Dr. Alexander Sharov
Head of RFBR International Relations Department

ENERGY

HRJRG-011

ACTINIDE NANO-PARTICLES: FORMATION, STABILITY, AND PROPERTIES RELEVANT TO THE SAFETY OF NUCLEAR WASTE DISPOSAL

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The joint project between Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal and Lomonosov Moscow State University aims to develop a molecular-level understanding of the formation, stability, and properties of nano-sized actinide containing colloids relevant to safe spent nuclear fuel (SNF) and high-level radioactive waste (HLW) disposal, thereby filling conceptual gaps in the source term and transport models used in long-term assessment for deep geological repositories. Colloid-mediated transport is a key factor in radioactive nuclide migration. Plutonium and uranium migrate in colloidal form in the subsurface environment kilometers from the site where nuclear waste has been recently. Radionuclide-containing nano-particles can form in near-field repository conditions upon dissolution of SNF, HLW glass, canister and backfill materials in corrosive fluids (elevated pH, ionic strength, temperature, and radiation fields). The negative effect of such actinide-containing nano-particles on repository safety is evident, however little is known about mechanisms of their formation, their stability, or their transformation to pseudo-colloids. These factors certainly play a role in important open questions concerning long-term behavior of SNF and HLW forms such as effects of radiolysis on AnO_2 alteration and the mechanism and extent of actinide incorporation into secondary phases.

Wet chemical methods were used for preparation/generation of actinide containing nano-particles under varying conditions in combination with the analysis of actual samples from contaminated sites. They were characterized with advanced spectroscopic and microscopic methods. The project have been divided into interrelated research tasks, defined as work packages (WP): characterization of the structure and reactivity of actinide eigencolloid nano-particles generated under different conditions (pH, Eh, ionic strength, solution composition), synthesis and spectroscopic characterization of well-defined actinide oxides and oxyhydroxides nano-particles, investigation of the interaction of eigencolloids with ground water colloids, modeling physico-chemical processes of nano-particle formation, experimental development of techniques with nano-scale resolution, characterization of actinide nano-particles in samples from contaminated sites.

For the first time the monodispersed actinide and lanthanide oxides nano-particles have been synthesized by embedding them into the pore structure of mesoporous SiO_2. They were characterized by advanced microscopic and spectroscopic methods like HR-TEM, EXAFS and HEXS. Measured interplanar distances and calculated lattice parameters for synthesized nanosized CeO_{2-x} and ThO_2 samples differ from their bulk crystalline counterparts. We obtain with our synthesis CeO_{2-x} particles containing both Ce^{4+} and larger sized Ce^{3+}. The lattice parameter for these ceria nanoparticles is found to be larger than the bulk value due to the presence of Ce^{3+} with its larger ionic radius. The presence of Ce^{3+} was established by means of high resolution X-ray emission spectroscopy (HRXES), applied to the investigation of nanoparticles for the first time. The ThO_2 nanoparticles exhibit a decrease in interplanar distances, as one might generally expect of these nanoclusters. However, the lattice distance decrease for our particles is remarkable, up to 5%, indicating that contact with the surrounding silica matrix may exert a bond distance shortening effect such as through significant external pressure on the particle surface. Analysis reveals Pu to be correlated with the pond water colloidal stable organic matter with an experimentally determined particle-size of about 1–2 nm.

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Fig. 1. The attendees of Russian-German Symposium on Actinide nano-Particles, Moscow, May 2009.

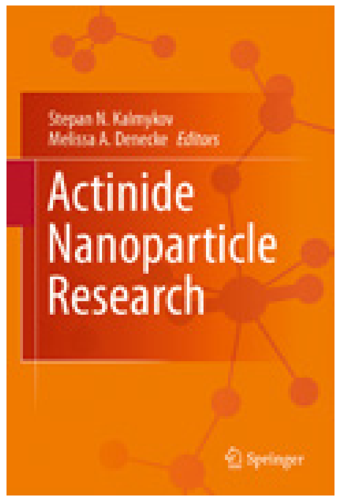

Fig. 2. The book published as a result of this Symposium.

In 2009 we conducted "Russian-German Symposium on Actinide nano-Particles" in Moscow (see Fig. 1) with about 60 attendees from Russia, Germany and other countries. As a result, the book "Actinide nanoparticle research" was published covering all the major aspects of formation, stability, properties and environmental behavior of actinide nanoparticles (Fig. 2).

List of publications:

1. O.N. Batuk, St.N. Kalmykov, E.V. Zakharova, M. Klimenkov, V.V. Kriventsov, Uranium dioxide behavior in hydrothermal oxidizing conditions, Speciation, techniques and facilities for radioactive materials at synchrotron light sources. Actinide XAS 2008 Proceedings of the 5th Workshop Saint-Aubin, Fance. 15–17 July 2008 Nuclear Science NEA/NSC/DOC(2009)15 OECD Nuclear Energy Agency 2009
2. O. Batuk, D.V. Szabo, T. Vitova, D. Schild, M.A. Denecke, S. Kalmykov, SYNTHESIS AND ELECTRONIC STRUCTURE OF CERIUM AND ACTINIDE DIOXIDE CLUSTERS Russian-German Symposium on Actinide Nanoparticles, p. 20, May 2009, Moscow, Russia
3. D.N. Batuk, S.N. Kalmikov, E. Shirshin, Ya.V. Zubavichus, URANIUM(VI) AND PLUTONIUM(V,VI) INTERACTION WITH AMORPHOUS SILICA NANOSPHERES, Russian-German Symposium on Actinide Nanoparticles, p. 40, May 2009, Moscow, Russia
4. O. Batuk, M. Bouby, S. Kalmykov, M.A. Denecke, H. Geckeis, CHARACTERIZATION OF Pu CONTAMINATED SUBSURFACE WATER SAMPLES FROM THE MAYAK SITE, Russian-German Symposium on Actinide Nanoparticles, p. 41, May 2009, Moscow, Russia
5. Actinide nanoparticle research, ed. by S.N. Kalmykov, M.A. Denecjke, Springer, 2011
6. O.N. Batuk, D.V. Szabo, M.A. Denecke, T. Vitova, S.N. Kalmykov, Synthesis and characterization of thorium, uranium and cerium oxide nanoparticles. Radiochim. Acta 101, 233–239 (2013)

HRJRG-013

HIGH DOSE IRRADIATION DAMAGE OF RAFM STEELS

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Introduction

The Helmholtz-Russia Joint Research Group – 013 had been working between February 2008 and December 2011. The following three institutions were involved in the implementation of the project:

- Karlsruher Institut für Technologie (KIT, IAM, Karlsruhe, Germany)
- Ulyanovsk State University (UISU, Ulyanovsk, Russia)
- Research Institute of Atomic Reactors (RIAR, Dimitrovgrad, Russia)

The main objective of the project was a development of phenomenological modelling tools for description of low temperature irradiation induced hardening and embrittlement of RAFM steels.

Reduced Activation Ferritic/Martensitic (RAFM) 7-10%-Cr-WVTa steels are primary candidates for application in first-wall and blanket structures of a future fusion power plant. Although RAFM steels exhibit clearly better irradiation performance as compared to the commercial martensitic steels, the low temperature hardening induced by neutron irradiation accompanied by embrittlement and reduction in toughness and ductility remains the main obstacle for their application. The designated project was aimed at understanding of the high dose neutron irradiation damage in RAFM steels and its influence on the steels' mechanical properties. The specific goals of the project were: I) Understanding of the irradiation induced changes in the microstructure within proper physical models allowing description of primary defect (interstitials, vacancies) formations and their evolution (defect clusters, dislocation loops, etc.); II) Correlation of the irradiation induced changes in the microstructure with the changes in the mechanical properties. Identification of the dominant hardening/embrittlement mechanisms in RAFM steels; III) Development of the models for prediction of the irradiation induced hardening/embrittlement of the RAFM steels by taking into account microstructure evolution as well as application and adaptation of already existing material hardening models to RAFM steels.

Work Results

The quantitative TEM analysis of the neutron irradiation induced microstructural defects including defect clusters, dislocation loops, voids, bubbles, etc. has been performed in specimens irradiated up to 32 dpa at 330 °C. The microstructural data were used for correlation of the irradiation induced changes in the microstructure to the changes in the tensile yield stress, see Fig. 1. The dislocation loops/defect clusters were proven to provide the dominant contribution to the total hardening. The estimation of hardening showed, however, that the defects visible in TEM alone are not sufficient to explain the tensile hardening. Implementation of other complementary techniques, e.g. Small Angle Neutron Spectroscopy, is proposed for quantification of defects with sizes below 1 nm.

Simulation of atomic displacement cascades up to 20 keV was performed in Fe-10at.%Cr binary alloy at 600 K in terms of the molecular dynamics by using improved interatomic potentials [Tikh2009]. Additionally, the role of 0.1 at.% carbon was investigated in Fe-9at.%Cr system [Tikh2011]. The dependence of "surviving" defects amount on cascade energy was studied. The cascade efficiency obtained for damage energy in the range from 10 to 20 keV is ~0.2 NRT, that is slightly higher than for pure α-Fe. The results on size and amount of vacancy and interstitial clusters generated in displacement cascades were obtained. Carbon at the concentration under study is found not to affect the number of surviving defects and the cascade efficiency. At PKA energies of 15 and 20 keV, the presence of carbon slightly decreases the fraction of point defects forming clusters. The evolution of the displacement cascades near Cr-rich

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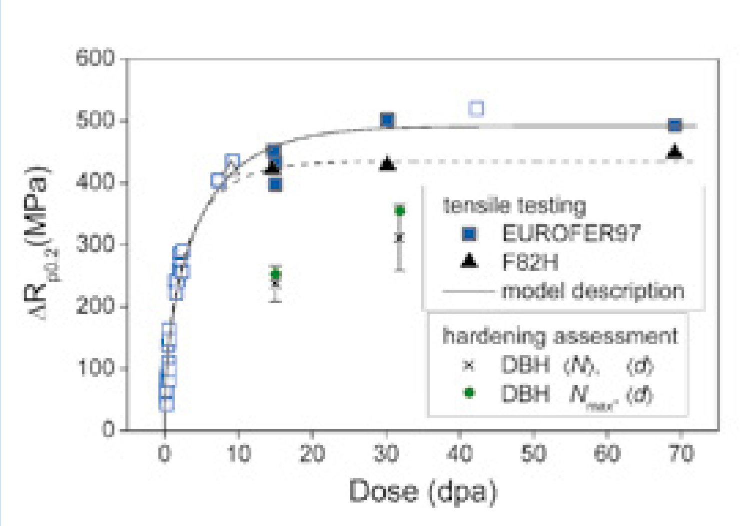

Fig. 1. Irradiation hardening vs. irradiation dose for EUROFER97 and F82H steels for T_{irr} = 300–335 °C and T_{test} = 300–350 °C [Gaga2011a]. The full symbols represent KIT results, the open symbols are from literature. The solid line is a model description of hardening [Gaga2011a]. The estimated hardening by dislocation loops using the Dispersed Barrier Hardening model is shown by solid circles and crosses [Weiß2012]. The crosses are calculated by using average loop density and average loop size, whereas circles are calculated by using the maximum loop density and an average loop size.

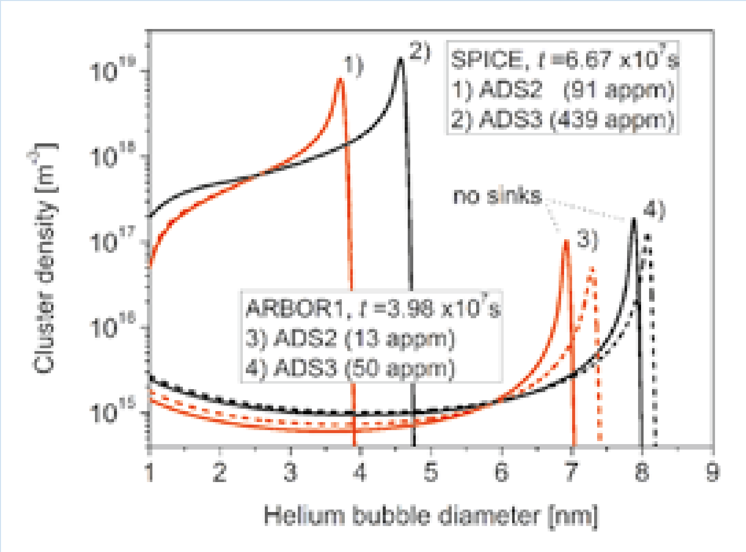

Fig. 2. Simulations of final bubble size distributions in SPICE (13.6dpa/250°C) and ARBOR1 (22.4dpa/330 °C) irradiation experiments [Deth2012a]. Produced helium contents in neutron irradiated boron doped steels ADS2 and ADS3 are indicated in parenthesizes. While continuous lines show simulation results without taking sinks into account, dashed lines present simulations considering grain boundaries and line dislocations as sinks for helium.

nanosized precipitates in Fe-9at.%Cr matrix has been investigated as well [Tikh2011b]. The main obtained result is an ability of small Cr precipitates (1 nm) to dissolve directly in the displacement cascades.

A rate theory model was developed for description of homogeneous nucleation and growth of helium bubbles [Deth2010a], [Deth2010b], [Deth2012a], [Deth2012b]. The size distribution of the helium bubbles was obtained for different helium production rates and helium contents. A diffusion governed growth of helium clusters was shown to yield a homogeneous bubble distribution which is in a good qualitative agreement with the investigated microstructure. The simulations were performed under the assumption of single mobile defects with effective diffusivities as the fitting parameter. The designated helium diffusivities were taken to be close to helium-di-vacancy diffusivities, as the vacancy mediated diffusion mechanism is believed to be the dominant diffusion mechanism under neutron irradiation at low temperatures, where vacancy supersaturation overwhelms the thermal vacancy effects. Furthermore, the influences of the helium diffusivity, bubble surface energy, and helium-to-vacancy ratio in the bubbles and helium solubility on the evolution of helium bubble microstructure have been studied parametrically. Fig. 2 shows the cluster size distribution after SPICE and ARBOR1 irradiations [Deth2012a].

A model of a phase equilibrium for binary alloys containing particles of the second phase of arbitrary size was developed in terms of the regular solution theory [L'vov2011]. The model was applied for calculation of the dependence of phase composition of Fe-Cr binary alloy on sizes of containing nanoscale clusters [Svet2011]. Iron content in nanoscale iron-chromium clusters was proven to be above the content predicted from phase diagrams.

The kinetic model of cluster formation was developed [Svet2011]. The model was applied for calculation of second phase particles evolution in Fe-20 at.%Cr alloy (Fig. 3a-c). The iron-chromium clusters generated during the nucleation process may be considered quasi-equilibrium, i.e. their composition is defined only by the cluster size.

Modelling of formation of second phase particles in alloys based on Fe-XCr (X=10, 12, 14, 16 at. %) has been performed [Svet2011b]. The developed model, which takes into account radiation enhanced diffusion, allows quantitative conclusions about cluster and matrix composition change under neutron irradiation, and also allows calculation of the dependence of average size and cluster concentration on damage doses up to 10 dpa for Fe-Cr alloys of different compositions. The diffusion coefficient of Cr atoms under irradiation was estimated to be seven orders of magnitude higher than the corresponding thermal diffusion coefficient at a temperature of 300 °C.

Summary
The results obtained within the HRJRG are of great scientific importance for understanding of high dose irradiation damage in RAFM steels. The post-irradiation mechanical and microstructural examinations and the correlation between the microstructure and mechanical properties allowed us to gain a deeper insight into the radiation damage phenomena. The developed modelling tools allows us to predict the evolution of the radiation defects e.g. defect clusters/ dislocation loops, helium bubbles and precipitates under neutron irradiation conditions. The performed MD simulation of displacement cascades allows more accurate determination of effective displacements by taking into account the point defect recombination during cascade evolution.

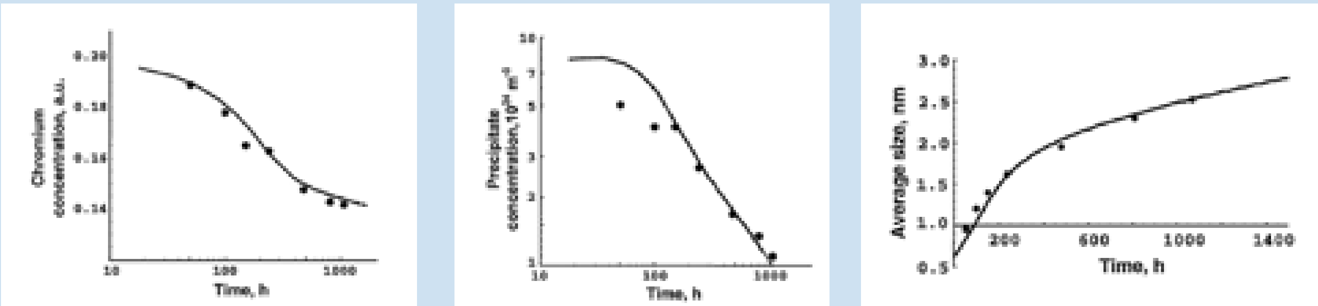

Fig. 3. Concentration of Cr in alpha-iron matrix (a), cluster concentration (b), and average size of α'-phase precipitates versus annealing time at T = 773 K (c). Points represent experiment taken from literature, solid lines represent our calculation [Svet2011].

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[Gaga2011a] E. Gaganidze et al., Mechanical properties and TEM examination of RAFM steels irradiated up to 70 dpa in BOR-60, J. Nucl. Mater. 417 (2011) 93-98.

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HRJRG-022

HYDROGEN ISOTOPES RETENTION IN FIRST-WALL MATERIALS FOR ITER AND FUSION POWER REACTORS

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The rising energy demand of mankind and the lack of natural fuel resources forces to search for alternative energy sources. A very promising solution is to use energy from the fusion reactions of the hydrogen isotopes D and T. In order to demonstrate the possibility of obtaining energy from fusion reactions with magnetic confinement, the ITER experiment was internationally agreed and is currently being built in Cadarache, France.

Tungsten, beryllium and carbon fibre composites (CFCs) were initially foreseen as plasma-facing materials (PFMs) for ITER. The accumulation of hydrogen isotopes in the PFMs and the diffusion and permeation of hydrogen through the materials are of a great importance due to the radioactivity of tritium and for the plasma fuel balance.

The HRJRG-022 investigated the behaviour of hydrogen isotopes in tungsten and CFC during 4/2008 – 3/2011. At the time of application, experimental data on hydrogen behaviour in tungsten were scarce, and the theoretical understanding was limited. The HRJRG-022 strongly contributed to the general understanding of hydrogen behaviour in tungsten by providing experimental data on hydrogen retention in and diffusion through tungsten, and by developing a theoretical model describing the hydrogen-tungsten interaction. Tungsten shows a unique behaviour unlike many other metals due to the creation of additional trapping sites by hydrogen-induced stress in the material, which creates dislocations and may result in blistering. A theoretical model describing the formation of ion-induced trap sites was developed, and its parameters were adjusted to fit the experimental data. This allowed to determine basic material parameters, such as natural and ion induced trap densities, the recombination coefficient at the surface, and effective diffusion coefficients. The model was used to extrapolate to the tritium inventory in ITER and predicted inventories well below the maximal allowed limit.

Impurity layers (for example, carbon or beryllium layers) at the surface can increase the trapped inventory by decreasing the outdiffusion of implanted hydrogen. The effect of impurity layers on hydrogen retention and permeation was studied experimentally for carbon, boron and alumina layers (which were used as proxy for beryllium). It could be shown, that an increased permeation is only observed in a very narrow range of impurity layer thicknesses, while for realistic thicker layer thicknesses the permeation is decreased by impurity layers.

The HRJRG-022 played an important (and often a leading) role in the worldwide activities to understand hydrogen behaviour in tungsten. These combined efforts, together with experimental data obtained at the tokamak experiment ASDEX Upgrade, finally led to the decision of ITER to replace CFC by tungsten in the DT operational phase. The results obtained by the HRJRG-022 made an important contribution to this decision.

While the interaction of ions with CFC was studied intensively in the past, the interaction of hydrogen gas with CFC was studied much more scarcely. The HRJRG-022 showed quantitatively, that CFC is transparent for hydrogen gas, and that the transport of hydrogen gas through CFC can be described by a conductivity. Surface amorphous hydrocarbon or tungsten layers can only reduce the conductivity, but do not fully inhibit it. These results are especially of relevance for the JET ITER-like wall experiment, where tungsten layers on CFC are used as PFM. This experiment started operation in 2011.

The work is succeeded in the HRJRG-216, where the interaction of hydrogen with advanced materials for a future DEMO reactor is the main topic.

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Hydrogen retention in and permeation through tungsten

Measurements of deuterium retention in different tungsten grades have been done for various irradiation temperatures, incident ion energies and fluences up to $2\times10^{25}m^{-2}$ at the Garching ion beam facility, at the LENTA device in the Kurchatov Institute in Moscow, and at the MEDION device at MEPhI (Moscow). An experimental ultra-high vacuum installation for thermodesorbtion (TDS) measurements was developed and build at MEPhI. The experimental procedure allows a minimal deuterium background signal.

A model including deuterium implantation, diffusion, trapping and second order desorption was used in order to understand the deuterium inventory and release kinetics in W. A trap production mechanism due to ion implantation was developed and included in the model. Calculations show that the formation of additional high-energy traps in W at moderate temperatures is, probably, connected with the movement and agglomeration of vacancies. Although the vacancies are immobile at implantation temperatures of 400–500 K, the stress-induced field can initiate their movement and growth.

Calculations indicate the presence of ion-induced and natural defects in polycrystalline W which act as trap sites for deuterium. Trap energies were found to be 0.85 ±0.05 eV, 1.45 ±0.05 eV, and about 2 eV. All trapping sites can exist in W as intrinsic defects and as ion-induced traps. Ion-induced traps are produced in W during implantation by the stress field induced by the incident ion flux for low-energy ions and by both stress and atomic displacement damage for high-energy ions.

Deuterium permeation through 50 µm and 400 µm thick tungsten foils was investigated during simultaneous ion irradiation and gas loading from the front side of the sample by measuring deuterium signals at the sample back side in the temperature range 550–650°C. The experimental results were compared to calculations with the TMAP 7 code. High-energy traps with an activation energy of about 2 eV and concentrations of 1–30 ppm were found to strongly influence D diffusion in W at the investigated temperatures. These observed high energy traps may be surfaces of pores and cracks in the tungsten material.

120–170 nm thick carbon layers were deposited on the front side of 50 µm thick tungsten foils, and the permeation through this layered system was measured at incident ion energies of 200 eV. The permeation flux was close to zero for the first five hours of implantation, while the lag time for pure tungsten was only 15–20 minutes at these conditions. During that time the film thickness decreased from 120 down to about 65 nm. Then, the permeation flux started to increase and reached a maximum at a remaining carbon thickness of 10–20 nm. Subsequent bombardment finally totally removed the carbon film from the surface and led to a decreased permeation at a steady state level. Therefore, it can be concluded that a carbon film with a thickness larger than the implantation range suppresses the permeation, but long time irradiation (which modifies the film) can make it transparent for deuterium ions.

Hydrogen permeation through carbon-based materials

The gas-driven permeation of hydrogen through carbon-based materials (fine grain graphites, carbon-fibre composite in different directions) was investigated at room temperature as a function of membrane thickness and gas loading at pressures of 10^{-2} –10 Pa. It was shown that hydrogen penetrates through the materials due to diffusion of molecular gas through the system of open porosity, which connects the front and back surfaces of the membrane, and not due to hydrogen atoms diffusion through the bulk of the material. The obtained gas permeability for the materials investigated strongly depends on porosity. The gas driven permeation through graphite coated with different types of tungsten coatings with thicknesses up to 200 µm has been investigated. It was found that W coatings with thicknesses up to 3 µm are transparent for hydrogen gas penetration and do not influence the permeability, because the open porosity system of graphite remains open. Even a 200 µm thick layer of VPS-W has an open system of connected pores, which still connects the front and rear surfaces of the deposited layer.

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HRJRG-216

HYDROGEN BEHAVIOUR IN ADVANCED AND RADIATION-DAMAGED MATERIALS FOR FUSION APPLICATIONS

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In order to demonstrate the possibility of energy production by fusion the ITER experiment is currently being built in Cadarache, France, where tungsten and beryllium are foreseen as plasma-facing materials (PFMs) and austenitic steel as constructive material. In a next-step reactor (DEMO) more advanced plasma-facing and structural materials will have to be used. These advanced materials for fusion applications include tungsten-based materials, ferritic-martensitic steels and vanadium-based alloys. However, these materials are not yet available on a commercial scale, and very little is known about their properties and their interaction with hydrogen. This lack of materials and knowledge about their properties is a severe problem for the future development of fusion, especially for experiments beyond ITER such as DEMO.

Diffusion, retention in and permeation through materials are of a great importance due to safety reasons and for the fuel balance of a fusion reactor. The accumulation and permeation of tritium is currently one of the most critical unsolved safety issues for ITER, and this problem will get even more severe for DEMO.

During a fusion reactor operation it's PFMs and constructive elements are constantly damaged by plasma irradiation, thermal shocks and stresses, and neutron irradiation. This will strongly change the crystalline structures of the materials and their physical properties (thermal conductivity, ductile-to brittle transition temperature, strength, etc.). Due to the additional damage, the accumulation and diffusion of hydrogen isotopes in these strongly damaged materials may change significantly.

Experimental data on the influence of different types of damage on hydrogen accumulation and permeation in materials are very scarce, and the detailed theoretical understanding of hydrogen transport through damaged materials is by far incomplete. These data are strongly required especially for future fusion power reactors such as DEMO.

The main goal of this project is to study the influence of radiation damage of plasma-facing materials (tungsten and tungsten-based materials) and constructive materials (different types of steels, vanadium alloys) on hydrogen accumulation and permeation through materials, and to obtain a deeper understanding of the physics of the interaction of hydrogen with radiation damage. The behaviour of hydrogen in advanced fusion materials with improved properties is another question. These topics are a logical continuation of the previous project HRJRG-022.

Radiation damage in tungsten and its influence on deuterium retention

Tungsten retains only relatively small amounts of hydrogen isotopes, especially at elevated temperatures. However, radiation damage by fast neutrons can increase the retained amount to concentrations of about 1% H/W. In our investigations irradiation by MeV tungsten ions is used as proxy for neutron irradiation. The retention was investigated as function of tungsten grade, damage level, incident deuterium fluence, and sample temperature. It could be demonstrated, that the retention saturates at about 0.5 displacements per atom (dpa), i.e. at higher damage levels the retention does not increase further. The damage was investigated by scanning transmission electron microscopy (STEM) and positron annihilation Doppler spectroscopy. The irradiation creates dislocations, vacancies, and vacancy clusters, which act as trapping sites with high de-trapping energy for hydrogen. Annealing of defects with low trapping energy occurs in the temperature range between 300 and 700 K. Radiation-induced defects with high de-trapping energy are thermally stable at least up to 1.100 K. This conclusion was supported by scanning transmission electron microscopy data.

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In order to investigate deuterium transport in radiation damaged tungsten permeation measurements were performed. The defects had a strong influence on the permeation break-through time, which increased by at least one order of magnitude compared to undamaged tungsten. Good agreement between a trap-diffusion model and the experimental data could be achieved. This allowed a very precise determination of the trap energy.

Deuterium retention in advanced tungsten materials

Main drawbacks of tungsten are its poor thermo-mechanical properties. These can be improved by doping. A very promising class of materials are toughened, fine-grained, recrystallized tungsten-based materials doped with 1.1 wt% TiC and 3.3 wt% TaC. However, there is some concern that the additional defects may increase hydrogen retention considerably. Deuterium retention in these materials was investigated by irradiation by low-energetic deuterium ions and by exposure to deuterium gas. The TaC-doped material shows comparable deuterium retention as tungsten, while the TiC-doped material shows bulk deuterium concentrations more than one order of magnitude higher than that in pure tungsten.

Deuterium retention in reduced activation steels

Reduced-activation ferritic-martensitic steels (RAFMs), such as Eurofer or Rusfer, are foreseen as structural (and, to some extent, also plasma-facing) materials for future fusion reactors. Deuterium retention in these materials was investigated under exposure to deuterium gas. Neutron irradiation was simulated by tungsten ion irradiation, and pulse heat loads were applied in the QSPA-T facility at 0.5 MJ/m^2 with a duration of 0.5 ms. Deuterium retention in damaged and undamaged Rusfer in the temperature range of 300–600 K has a maximum at about 500 K for all investigated damage types. Typical values of deuterium bulk concentrations are of the order of only 10^{-3} atom%. Irradiation by heavy ions results in an increase of the deuterium retention by a factor of about two, irradiation of Rusfer with high heat fluxes or high-flux irradiation with a low temperature plasma at elevated temperature leads to a decrease of the retention in Rusfer.

Deuterium permeation through reduced activation steels

Gas driven permeation (GDP) through reduced activation steels was investigated in the temperature range of 573–973 K at pressures of 10^{-2} – 10 Pa, and plasma driven permeation (PDP) in the temperature range of 600–800 K. GDP through the membranes was shown to be limited by processes at the surface and the permeating flux was proportional to the input pressure at pressures 10^{-2} – 10^{-1} Pa. The diffusion limited regime was reached at pressures above 0.5 Pa. The permeation efficiency at PDP was estimated as 0.02–0.1 in the temperature range of 600–800 K.

Deuterium permeation and retention in low-activation vanadium alloys

V-Cr-Ti alloys have the advantage of a very low activation by fusion neutrons and have good compatibility with liquid lithium at high temperatures. This makes this class of materials attractive for fusion applications. The permeability of the V-4Cr-4Ti alloy was investigated by gas- and plasma-driven permeation. Diffusion, trapping and permeation of hydrogen isotopes in the material are generally very high. This renders the use of these materials problematic without additional permeation barriers.

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HRJRG-411

ODS-HITS: TAILORING NANOSCALED FEATURES IN NOVEL STEELS FOR HIGH-TEMPERATURE APPLICATIONS USING ION BEAM MODIFICATION

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Introduction

One of the most daunting challenges in reformation of the energy system in Europe and, in particular, in Germany is the availability of suitable structural materials which can withstand severe corrosion and thermo-mechanical loadings over long time periods. Novel high-temperature resistant materials are required for further advances in efficient energy production and conversion. One of the possible candidates is oxide dispersion strengthened steel (ODS) possessing excellent high-temperature creep, corrosion and irradiation resistance. Besides nuclear applications, this novel class of materials has a great potential for use as structural materials for concentrated solar power plants, jet engines, chemical reactors as well as for hydrogen production from thermolysis of water. However, to obtain the allowable maximum efficiency ODS steels should be optimized for their specific applications.

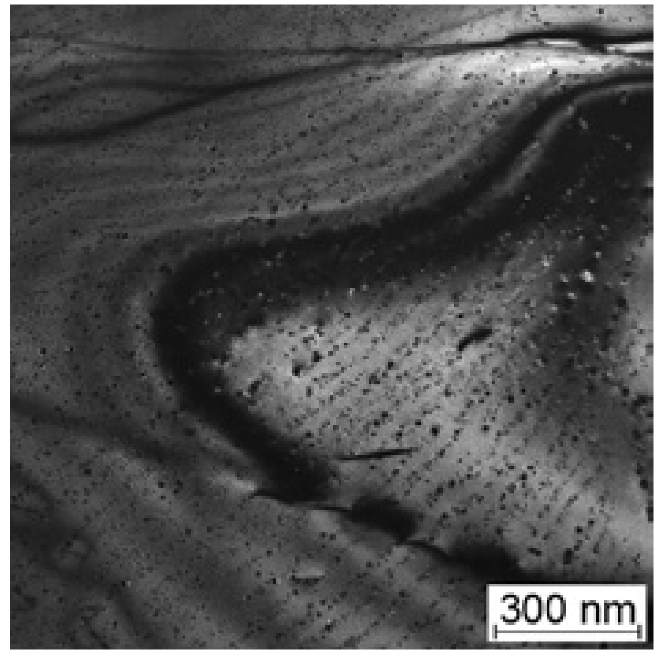

Figure 1: Ordered arrangements of ODS particles found in EUROFER ODS.
TEM picture by M. Klimenkov

Tailoring of ODS material properties for specific applications requires understanding of basic mechanisms of oxide particle nucleation and growth. Transmission electron microscope (TEM) studies of the ferritic-martensitic ODS steel developed at KIT [1] confirmed formation of a large number ($4 \cdot 10^{21}$ m^{-3}) of well-formed oxide precipitates with diameters of typically 4–15 nm (see Figure 1). Investigations on the same material performed at ITEP, Moscow, using Atomic Tomography Probe (ATP) have revealed even higher number density (~10^{24} m^{-3}) of smaller nanoclusters (1–4 nm) often invisible in TEM [2–4].

It is known that tiny oxide particles dispersed in the steel matrix impart excellent mechanical properties to ODS material, but their formation mechanisms and, hence, the ways to affect their composition and properties as well as spatial distribution are not yet well understood.

These nanoclusters are segregated arrangements of various solute atoms including oxide forming elements. We have tentatively identified the nanoscaled features as precursors of ODS particles able to grow into larger well-formed particle under high-temperature annealing. It was suggested that nanoclusters are

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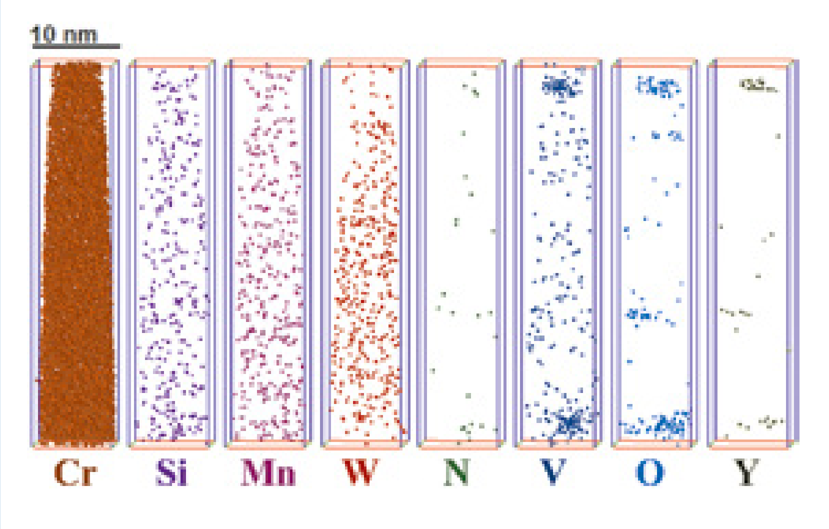
a.



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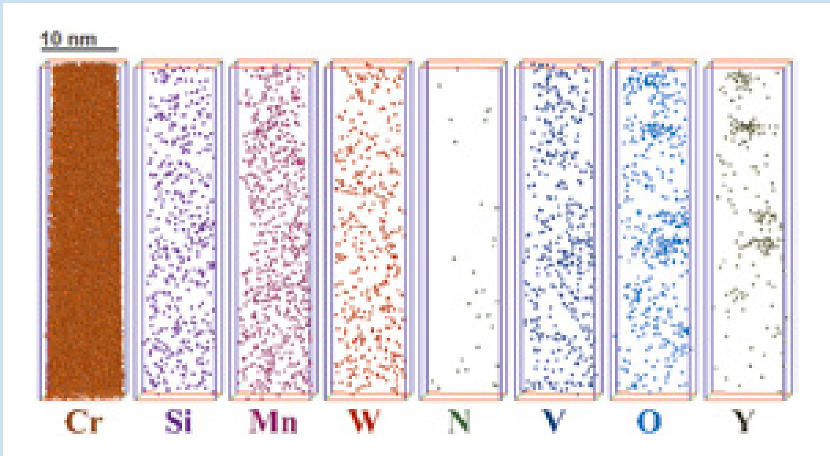

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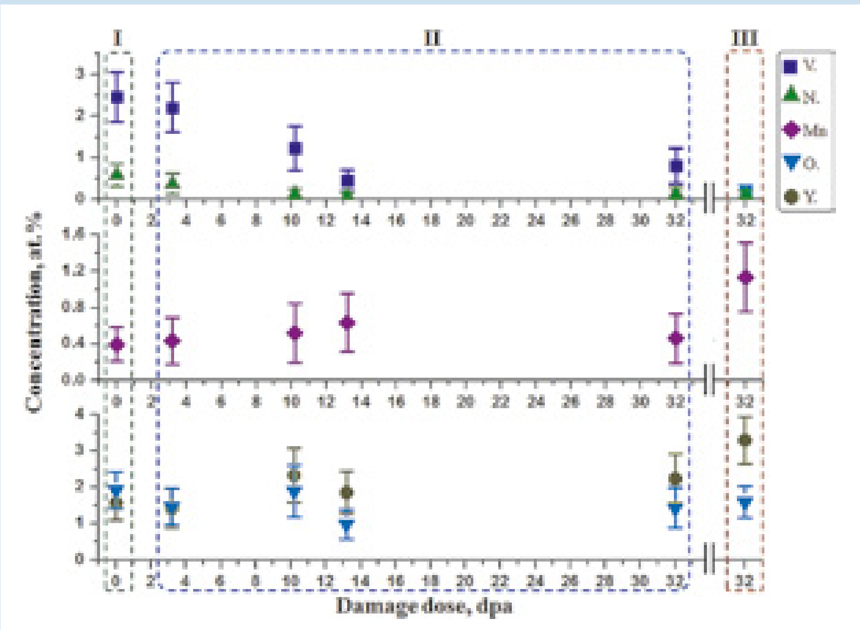

Figure 2: 3D atom map of the ODS Eurofer sample irradiated with Fe ions up to 3 dpa (a) and 32 dpa (b). Evolution of chemical element concentrations in nanoclusters: I – as received; II – irradiated with Fe ions up to given dose (see x-axis) at room temperature; III – neutron irradiated in BOR-60 reactor (T = 332 °C).

serving as nucleation centers for ODS particles, while their chemical composition is evolving during nanocluster growth. However, this hypothesis should be verified experimentally with a special attention on the role of various alloying elements in the nucleation of nanoclusters.

Thus an experimental program aimed at investigation of the role of various alloying elements in precipitation of nanooxides in ODS steels combined with extensive multiscale modeling focused on elucidation of the atomic scale mechanisms of nanocluster nucleation and growth was proposed.

This project is studying the process of nanocluster formation as well as their stability under ion irradiation, with a focus on the role of minor alloying elements (e.g. Ti, V, N). The innovative feature of this proposal consists in combination of ion beam modification and ATP investigation of nanoscaled objects in ODS steels as well as multiscale modeling.

Scientific basis

Yttrium oxide (yttria) is known as one of the most thermodynamically stable materials and is widely used for the production of oxide dispersion strengthened alloys. Unfortunately, it is not possible to produce yttria strengthened alloys by conventional metallurgy. Therefore presently nanoscaled-ODS alloys are produced mainly by mechanical alloying (MA) of a mixture of steel and yttria powders followed by powder densification at temperature around 1.000–1.200 °C and pressure ~100 MPa [5,6].

The final size, coherency with the matrix and spatial distributions of oxides strongly depend on the source powder chemical composition and parameters of the fabrication process. On the other hand, the oxide size and homogeneity of their distribution directly affect mechanical properties and irradiation resistance of ODS steels. Thus tailoring of oxide particle ensembles bears a strong potential for steel optimization to meet the demands of future advanced technologies [8].

Recent experiments revealed that yttrium dissolves, at least partly, in the steel matrix and precipitates later as nanoscaled yttria particles during mechanical alloying. This opens a possibility to govern size and spatial distribution of oxide particles and optimize mechanical properties of ODS material in a desired way.

It is well-known that steel properties may drastically depend on alloying elements even if their concentration is homeopathic (several hundreds of appm). This is especially true for nanostructured alloys like ODS steels. As was mentioned above, the number density of nanofeatures is essentially higher than that of grosser ODS particles. Hence, material properties can be largely influenced by this component of the microstructure. However, the mechanisms of alloying elements (Ti, V, N, Mn) influence on nucleation and growth of nanooxides at atomic scale are not yet revealed.

Results

The results of Atomic Probe Tomography (ATP) characterization of nanoclusters in ferritic-martensitic steel EUROFER ODS were jointly published by ITEP and KIT [2–4]. Tiny Y-O clusters enriched in vanadium and nitrogen were observed. After fast neutron irradiation up to 32 displacements per atom (dpa) at 320 °C the chemical composition of Y-O nanoclusters has markedly changed: Mn and Y enrichments within nanoclusters were detected, while V concentration was reduced (see Figure 2c-III).

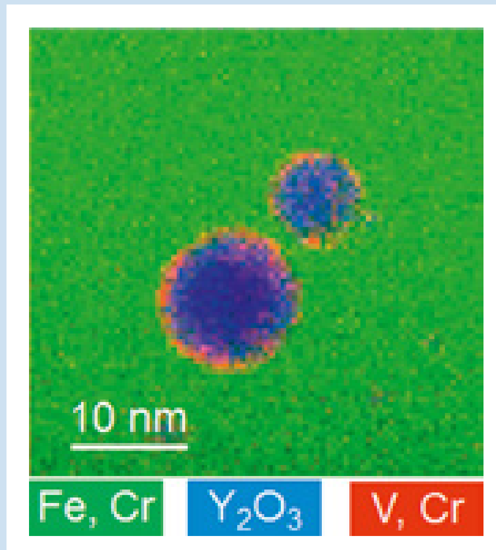

Figure 3: EDX element map of complex shell structure around small ODS nanoparticles [11].

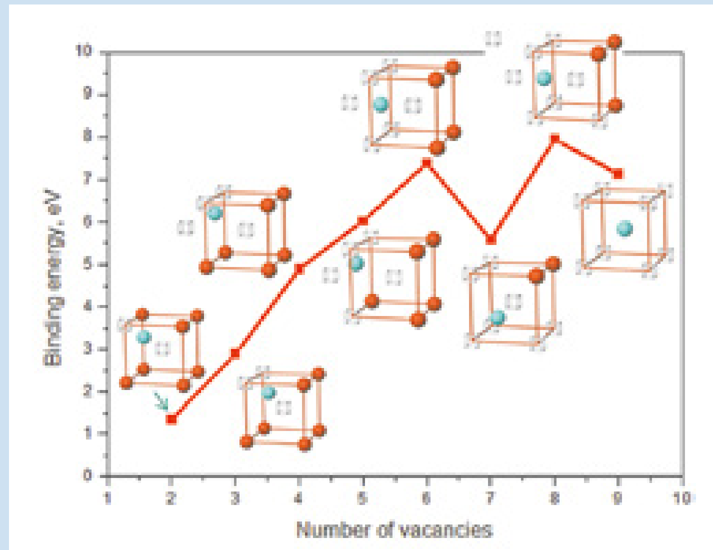

Figure 4: Binding energy of vacancy-yttrium clusters (2–9 vacancies) calculated by DFT method [18]. Colors are as follows: Fe – orange, Y – cyan, vacancy – gray cube.

These findings emphasize the role of minor alloying elements in formation and evolution of the nano-oxide clusters. Taking in mind that these clusters are supposed to be the seeds for oxide particle nucleation, it is important to understand the mechanisms of their formation and thus to propose the ways of knowledge-based tailoring of material properties.

Analytical TEM investigations of ferritic and ferritic martensitic steels have shown that ODS particles often possess a complex structure: yttria containing core and a thin V-Cr-O shell around (see Figure 3) [9,12].

Similar core-shell structures were observed by ATP studies of nanoclusters in EUROFER-ODS [2]. The core of nanocluster is enriched with Y, O, V and Cr. Some solute elements can be found in the nanoclusters, but not in the larger ODS particles investigated by TEM supposing temporary evolution (aging) of the cluster composition during its growth.

Pilot experiments performed at ITEP have shown similar composition changes after implantation of ATP needles with iron ions suggesting correlation between nanocluster nucleation during fabrication or aging and their evolution under ion implantation.

Low energy (150 keV) implantation is sufficient to penetrate a needle and produce damage and stopped ion profiles within the ATP needle. As the samples are not radioactive, the ion modified needles can be used for ATP studies immediately after implantation. The needles made of ODS steels were irradiated up to 32 dpa at room temperature. Changes of nanocluster chemical composition similar to that after neutron irradiation were found (see Figure 2c-II).

In the project the advanced modern approach of multiscale modeling is applied. As a first step ab initio calculations are performed to provide necessary information for simulation of nanoparticle nucleation and growth using atomistic kinetic Monte Carlo code.

The main objective of this modeling part is to study at the atomic scale the mechanisms of nanooxide nucleation, in particular, the energetics of Y-vacancy (see Figure 4), Y-O-vacancy complexes with a special focus on the role of alloying elements on nanocluster nucleation and growth.

This extended modeling program would not be possible without preliminary work performed in a long-term cooperation with other European and Russian research groups. Some essential results on Y-Y and Y-O interaction were already obtained [11–13] allowing us to concentrate mainly on the role of Ti in cluster nucleation and growth.

Outlook

The following results are expected to be obtained after the completion of the project:

- Recommendations for optimization of mechanical properties of ODS steels for high-temperature applications based on the experimental and theoretical understanding of ODS particle nucleation and growth
- Experimental database of nanocluster chemical compositions in dependence of the initial material composition, scheme of annealing and concentration of implanted elements
- Analytical and computer models of nanocluster formation will be suggested and confronted with the experimental results available earlier and obtained during this project.

Project results will be published in international journals and presented at international and national conferences. The knowledge obtained in this project will be used for accelerated development of novel materials and tailoring of ODS steel properties for specific applications.

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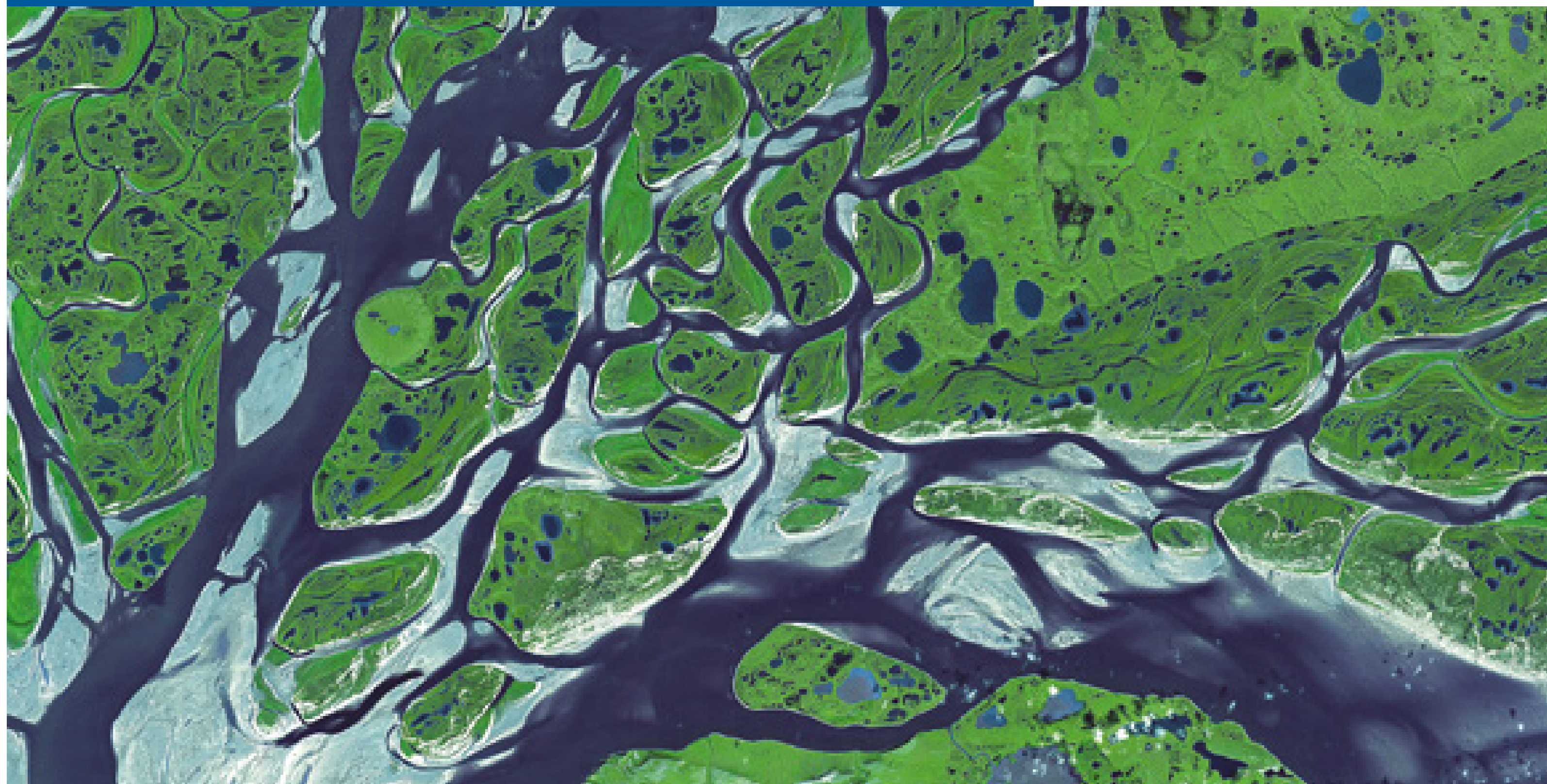
EARTH AND ENVIRONMENT



Lena-Delta pictured by NASA satellite. Image: HZG

HRJRG-025

ECOLINK PROJECT – GLOBAL CHANGE REQUIRES LARGE-SCALE SCIENCE

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Worldwide basic environmental conditions are currently changing dramatically. The changes include the increase of ecosystem exposure to toxicants due to intensified agriculture and industry, increasing demand for energy supply, and climatic changes that in turn increase demand for plant protection and disease vector control. To use chemicals safely, a key challenge is our ability to perform a reliable environmental risk assessment. This is the basis for an efficient sustainable landscape management accepted by the public.

The German-Russian project ECOLINK (2008-2011) aimed at understanding cross-Eurasian patterns in reaction of biological communities to chemical contamination and climate change. This international initiative is conducted by the Helmholtz Centre for Environmental Research – UFZ, Department of System Ecotoxicology, Leipzig and Institute of Systematics and Ecology of Animals, Novosibirsk. This project results supports future realistic predictions of ecological consequences of chemical contamination in conditions of global climate change.

The ECOLINK project employed an approach that is novel for ecotoxicology – establishment of the ecosystem level dose-response relationships depending on regional biotic characteristics and climate-related abiotic factors. In 2008 the unique cross-continental Europe-Asia mesocosm experiment was started and were run during two years. This unprecedented investigation was focused on reactions of freshwater plankton communities to pesticide contamination and climate-related environmental factors in Central Europe (UFZ, Leipzig) and Southwestern Siberia (ISEA, Novosibirsk). In this experiment similar series of model freshwater pond ecosystems have been installed on the territory of UFZ, Leipzig and in the Karasuk field research station (Southwestern Siberia, Russia). This system of the pond mesocosms in total includes about 300 little ponds and allows to manipulate basic climate-related abiotic factors (temperature, insolation etc) and therefore to investigate combined effects of toxicants and the climate-related factors. Besides, location of these ponds in two different regions allows to take into account basic faunistic, environmental, and phenological parameters.

Results of this experiment show that sensitivity of the biological communities can vary to the very pronounced magnitude, up to a factor of 100, and, furthermore, this variability can be reproduced and predicted, as it depends on the basic environmental factors. Therefore, community-level alterations in the sensitivity cannot be considered as an intrinsically unpredictable noise. The magnitude, direction, basic factors and mechanism that determine these alterations require further investigations. This implies that a transition is needed in the ecological risk assessment from the arbitrary-defined safety factors towards empirically based standards. Such a transition has a potential to significantly increase reliability of this ecological practice, which was repeatedly disqualified due to discrepancies between the field-observed effects and predictions based on the laboratory studies.

More generally, results of the project indicate that, ecotoxicology, as any applied ecological discipline, should be matched to scales relevant for management practices. So with pesticides applied at the field scale and generally regulated at the national or supernational scale, ecotoxicological investigations should cover these scales. There is a clear need to better incorporate ecological theory and new large-scale- oriented approaches to estimate and predict effects of contaminants across various spatial and temporal scales including the regional and bigger scales.

Mesocosms in Karasuk. Image by ISEA

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HRJRG-100

ASSESSING THE SENSITIVITY OF ARCTIC COASTAL DYNAMICS TO CHANGE

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In the context of the global climate change, and increased human activity in the high latitudes today, the Arctic represents an area of huge scientific interest because of the sensitivity of the landscapes to even minor changes in the modern world. One of the most illustrative examples are the coastal areas, which are the best accessible for both scientific research and industrial infrastructure and significantly affected by climate change. Coastal dynamics and different issues related to them (rates of coastal erosion, permafrost melting, sediment and organic carbon fluxes transferred to the Arctic Ocean, subaqueous permafrost development, etc.) play an important role in the understanding of modern trends of changes in the Arctic region, both natural and human-induced.

The present project has been focused on several different key sites on the coasts of the Pechora, Kara (fig. 1) and Laptev (fig. 2) Seas. Both natural undisturbed conditions (Buor Khaya Bay; Muostakh Island; Oyogosskiy Yar, Laptev Sea) and conditions of active oil and gas development (Varandey and Kharasavey industrial areas, Pechora and Kara Sea) have been analyzed. The rates of coastal retreat have been analyzed, the amount of the material input to the shelf has been made, calculations of wind and wave energy affecting the coasts have been performed. As a results of profile sampling, estimations of total organic carbon and other elements brought to the shelf from the destroyed cliff were made. Suspended inorganic matter distribution and fluxes have been analyzed. Mathematical simulation of degradation processes of the subaqueous permafrost within offshore have been made.

It was found that cryogenic processes in the Arctic region dominate among other exogenous shore processes, especially within the shore sections composed of high ice-content ground. The average speeds of shoreline recession are: 0.5 m per year for Pechora and Kara coast, 0.7 m per year for the Laptev Sea coast; 1.0 m per year for the East-Siberian Sea coast. Maximum speeds are 25 m per year. At the areas technogenic disturbances of lithodynamic regime coastal retreat rate are increased in 2 times or more. The total lost land area is about 15 sq km per year. Preliminary mass estimates of the material input to the shelf have been made: 58 mln. tons for Pechora and Kara Seas, 62 mln. tons for the Laptev Sea, and 90 mln. tons for the East Siberian Sea. This exceeds solid river discharge of the Laptev Sea and East Siberian Sea basins and is more than a summary shore input of the other Arctic Seas. It has been found that due to the warming in Arctic, the speed of shore erosion on the observed cites of the Laptev Sea has increased since 1999–2002, for Pechora and Kara Seas – since 2005. It increased significantly at the shore sites composed of high ice-content ground (so-called "Ice Complex").

The analysis of changing climate conditions included not only the temperature factor, but also one of the most important ones: the increase of ice-free period. The reduce of sea ice extent in the Arctic Ocean leads to the increase of the period of open water when the sea waves can directly affect Arctic coasts. The growth of this period and the increase of the distance between coastline and sea ice edge (so called "wave fetch") leads to the growth of wave energy, which is the main factor of coastal dynamics. Therefore, together with the warming action of waves and air due to temperature growth, mechanical abrasion also increases dramatically due to a longer wave fetch which allows the waves to gain more strength. Another consequence of the ice-free period prolongation is that the strongest autumn storms, during which the coast earlier could be already protected by growing ice, now can coincide with the period of open water, which will also lead to coastal destruction. The calculations of year to year variations of wave energy, made for the key sites of West and East sectors of Russian Arctic for 30 years period, showed that during the last "warm" years only insignificant increase of wave energy occurred in the coastal zone. This is since the increased wave fetch and longer ice-free period are partly balanced out by the decrease of wind. It has been found that, in general, typical thermal-erosion coast dynamics is determined by the combination and interaction of a number of environmental forcing factors. Among them, ice extent, together with thermal and wave energy, are determined as the most important.

Figure 1. Kara Sea shores with massive ice beds (photo by S. Ogorodov)

Figure 2. Laptev Sea shores with wedge ice complex (photo by M. Grigoriev)

To perform the project tasks, an analysis of sediment distribution, including organic carbon and many other components brought from destroying coasts to the coastal shelf to the depths of 10–15 m, was made on the basis of profile sampling of the bottom and coastal deposits near Kharasavey Cape (Kara Sea) and in the Eastern Buor-Khaya bay (Laptev Sea). The characteristics of organic matter distribution in the nearshore shelf zone adjacent to ice-rich coasts have been established. The coasts composed of Ice Complex supply a considerable amount of organic material, which comprises ca. 2–3 weight percent in average in these strata, to the sea. The destruction of Ice Complex plays an extraordinary important role in the budget of coastal sediment fluxes to the Arctic Ocean. The Laptev Sea coasts composed of Ice Complex supply 72% of mineral debris and 92% of organic carbon to its basin. These percent contents are yet higher for the East-Siberian Sea, corresponding to 78% and 98%.

Average volumes of organic carbon inputs from destroying coasts of the Russian Arctic seas were identified. They constitute 0.3 million tons per year in the White Sea; 0.6 in the Barents Sea; ca. 1.0 in the Kara Sea; 1.6 in the Laptev Sea; 2.4 in the East Siberian Sea; and 0.2 in the Chukchi Sea. The total volume of organic carbon brought by rivers is approximately 5 times greater than its input from coasts. Only the East Siberian Sea where the coastal output of organic carbon is almost 2 times greater than the river one, forms an exclusion.

Mathematical simulation of degradation processes of the subaqueous permafrost within offshore have shown that perennially frozen ground flooded by the sea can exist in a frozen state for a prolonged period of thousands or even tens of thousands years. Heat influence of the sea and diffusion of salts are the most important components of the degradation processes in upper horizons of the subaqueous permafrost. Herewith, influence of the thermal component is higher than the diffusion's one. The permafrost thaw front notably outruns the depth increment of the salt content leveling boundary. The average inclinations of the subaqueous permafrost upper table (for non-lithified coasts) within the offshore of the seas of Eastern Siberia have been evaluated. They vary over a wide range from 0.0002 to 0.1, comprising 0.011 in average. On the whole, the rates of degradation of the subaqueous permafrost upper table vary from 1 to 25 cm per year, while the rates of degradation at its lower table decrease to the first mm per year.

As a result of the project, we have analyzed and established the main factors controlling the change in the coastal dynamics in the Arctic today (temperature increase, ice-free period growth, lengh of wave fetch, wind-wave energy, exposition, cliff parameters and sediment composition, ice content, etc.). Complex integrated studies including many issues of the modern Artic coastal dynamics and establishing links between them are especially important because of the necessity of combined results of different approaches. Only comprehensive analysis of the modern processes will allow creating long-term forecasts of the evolution of the coastal processes in the key sites of the Russian Arctic under the influence of environmental forcing changes.

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HRJRG-110

SEISMIC TOMOGRAPHY ALGORITHMS FOR FUNDAMENTAL AND APPLIED PURPOSES

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In 2009–2011, the Russian Institute of Petroleum Geology and Geophysics (Novosibirsk) collaborated with the German GeoForschungsZentrum Potsdam in the framework of the joint Helmholtz-Russia Joint Research Group Project on the topic of developing seismic tomography algorithms for multiscale studying geological structures inside the Earth.

Seismic waves generated by artificial shots of earthquakes propagate through the earth and accumulate the information about the inner structures. Seismic tomography is an instrument which helps to decipher this information and obtain 3D models of the earth structures. This procedure is in some sense similar to the medical tomography, but it appears to be much more complicated because of several reasons. Within the project we have designed several seismic tomography algorithms and probed them with various datasets representing objects on completely different scales and properties. For example, in a case of a seismic experiment on scale of several tens meters, the seismic tomography revealed clear location of small-scale objects, such as water pipes. The same tool can be used in a large variety of applied tasks, such as engineering of buildings and archeology. On scales of kilometers, a similar algorithm makes possible studying the structures above tunnels which is important for monitoring the rock state and detecting the presence of any fracture zones. Within the project we have implemented the seismic tomography algorithm for studying the oceanic area in the Pacific coast close to the Chilean margin along the marine seismic profile executed by German colleagues from Geomar. As the result, we provided the detailed structure of the coupling zone between the subducting Nazca Plate and overriding South American continent down to the depth of a few kilometers. Very exciting objects for studying by means of seismic tomography are the volcanoes. Within the project we studied several volcanic areas such as Toba in Sumatra and Merapi in Java and detected deep traces of their feeding from depths of more than 100 km. On scales of hundreds kilometers we performed several studies which allowed us to solve some tectonic problems. One of them was related to the presence of deep earthquakes beneath Vrancea in Romanian Carpathian located within the continental area. Seismic tomography revealed a drop of colder material which falls down to the mantle, and it helped us to propose the mechanical explanation for this phenomenon. For regional scale areas of thousands kilometer size, the seismic tomography uses all available information on earthquakes from global seismological catalogues. Using millions seismic rays we reconstruct complex 3D structures in the mantle to the depths of many hundreds kilometers. In this way, within the project we have obtained valuable information on the shape of the subducting plates in western Pacific. Another example of using this method is the high-resolution model of the mantle beneath Europe which helps to understand puzzling interactions of the European and African lithosphere plates. These and many other results would be hardly possible without exchange of data and algorithms between the Russian and German scientists within the collaboration supported by the the Helmholtz Association and the Russian Foundation for Basic Research.

Joint publications within the HRJRG-project:

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HRJRG-221

THE IMPACT OF GLOBAL CHANGE ON ANCIENT ENVIRONMENTS: ARE STRESS TOLERANT INVADERS A THREAT TO THE LAKE BAIKAL FAUNA?

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Background of the project

Lake Baikal, the largest freshwater body in the world located in Eastern Siberia and UNESCO world heritage site, is inhabited by an extraordinarily diverse and unique endemic fauna. It is not clear, how the endemic fauna of Lake Baikal remains clearly distinct from a Palearctic freshwater fauna ubiquitous in the Northern hemisphere and why these faunas do not intermix. Lake Baikal is characterized by peculiar abiotic conditions (high oxygen content, low salt content, super-oligotrophic conditions, low content of organic matter) that have remained stable for millions of years and we hypothesize that the endemic fauna of Lake Baikal is highly adapted to these specific conditions. Lake Baikal species therefore outcompete potential invaders. However, the abiotic conditions of Lake Baikal have rapidly changed in the last decade as a result of global climate change and change of the chemosphere. In this project we aim to determine which shift of abiotic conditions, namely temperature regime and chemical stress, results in a situation outside the optimum for Lake Baikal endemic and non-endemic species. We thus test the hypothesis that a non-Baikal species is better capable of dealing with temperature- and chemical-related abiotic stress than Baikal endemics. If abiotic conditions of Lake Baikal are going to further progress – as it is predicted – they could provide a competitive advantage to non-Baikal species that may eventually replace Baikal-endemics and change the ecosystem.

Approaches

We examine stress-response capabilities and physiological performance ranges of the amphipod species that are endemic to Baikal in comparison to a non-endemic species that is regarded as potential invader species that could replace endemic species in Lake Baikal. Using high through-put sequencing technology we address the question which genes for cellular stress mechanisms endemic amphipod species possess and how expression of these genes responds to stress conditions, such as elevated temperature or toxic chemicals.

Furthermore, the physiological performance ranges of endemic and non-endemic amphipod species are examined.

Outcome so far

We sequenced the genome of one amphipod species endemic to Lake Baikal. The genome is surprisingly large, around three times larger than the human genome. DNA sequence comparisons with other genomes show that sequences are very dissimilar. The data are highly interesting as genome data for this taxon are not yet available (Rivarola-Duarte et al., 2014).

Looking at how endemic amphipod species from Lake Baikal deal with temperature stress we found big differences between the examined species: One is highly tolerant to elevated water temperature, whereas the other is not. The tolerance to temperature could be related to a highly potent stress response system that is highly developed only in the temperature-tolerant species (Bedulina et al., 2013). Indeed, physiological performance of this tolerant species at different temperatures resembles that of a non-Baikal amphipod species. These data enable important conclusions, which are: (1) a low stress response capability is not per se a phenomenon found in Lake Baikal endemics and (2) the sensitivity of species endemic to Lake Baikal to shifts in conditions is species-specific.

Researchers involved in the project:

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- Postdocs: Dr. Daria Bedulina, Dr. Marina Protopopova (Irkutsk State University)
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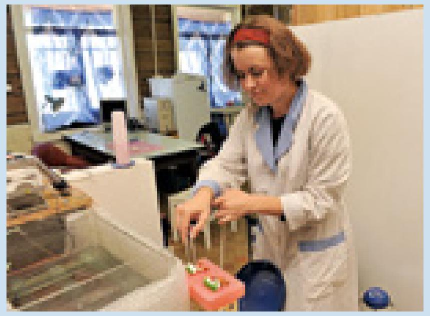
- Students: Hendrik Michael, Irene Fernandez Casas, Benjamin Knoll (UFZ)



Our studied species *Eulimnogammarus verrucosus* and *E. cyaneus*, endemic to Lake Baikal, and *Gammarus lacustris*, a potentially invasive species to Lake Baikal. Photos by V. Pavlichenko (ISU)



Dr. Daria Bedulina working in the field lab in Bolshie Koty at Lake Baikal. Image by T. Luckenbach (UFZ)

Lena Jakob working in the lab at Irkutsk State University. Image by Y. Lubyaga (ISU)

Lorena Rivarola-Duarte isolating RNA in Leipzig. Image by S. Schreiber (UFZ/IZI)

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HRJRG-308

EUROPEAN AND RUSSIAN EXTREME EVENTS: MECHANISMS, VARIABILITY AND FUTURE CLIMATE CHANGE

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The focus of our study is to investigate extreme weather and climate events (related to temperature, rainfall, droughts, storm winds, sea waves, air pollution, permafrost) over Europe and Russia in order to establish a link between changes in the intensity and frequency of extremes and global climate change.

Changes in the hydrological cycle

Global warming may become increasingly important in changing the hydrological cycle due to the exponential increase of the water-holding capacity of the atmosphere with temperature. Here we present estimates of possible changes in rainfall characteristics (amount, intensity, frequency) and runoffs of the major Eurasian river basins for the late XXI century. According to multi-model simulations, the mean annual runoff of all analyzed Siberian rivers is expected to grow by the late XXI century. This is mostly due to an increase in spring runoff because of an increase in winter precipitation and, accordingly, snow mass, as well as more intense snow melting in spring. On contrary, summer runoffs of the Yenisei, Ob, and Volga show a distinct tendency toward a decrease due to the appropriate changes in precipitation and evaporation. Mean rainfall and its intensity will increase for all analyzed watersheds with respect to multi-model simulations. The frequency of rainy days in the analyzed watersheds also will increase, particularly during winter, whereas the trends in the probability of summer precipitation are negative.

Wind-wave activity in the Arctic Ocean

Waves in the Arctic Ocean pose a new practical and research problem. Arctic marine navigation and other offshore and shelf activities become possible, but risks due to waves and associated storm surges and coastal erosion are likely to increase. Here we report modeling of 21st century waves in the Arctic by means of the third-generation wave forecast/hindcast model WAVEWATCH-III forced by winds and sea ice concentration produced within the regional model HIRHAM, under the anthropogenic scenario SRES-A1B. We find that significant wave height and its extremes will increase over different inner Arctic areas due to simulated reduction of sea ice cover and regional wind intensification in the 21st century (Fig. 1). The opposite tendency, with a slight reduction in wave height appears for the Atlantic sector and the Barents Sea. Our results extend the knowledge of wave climate to high latitudes in the Northern Hemisphere and demonstrate the wave response to a combined influence of wind and ice forcing in a climate-change scenario.

Arctic cyclones

Cyclones are key weather elements that make a major contribution to climate variability and also bring intense changes in wind, temperature and precipitation. Simulations with regional climate model HIRHAM forced by anthropogenic scenario SRES-A1B are analyzed to assess possible future changes in Arctic cyclone characteristics. Our model simulations show a slight decrease/increase in a cyclone frequency during warm/cold season by the end of 21st century. Noticeable changes were detected for the intensity and size of Arctic cyclones for the both seasons. Significant increase was found for the mean cyclone size and intensity, and frequency of weak cyclones during the cold season.

Potential link of Arctic sea ice with extreme winters in Europe and Russia

During the first decade of the 21st century, several anomalously cold winters were observed over the northern continents despite the highest rate of the global warming for the last two decades. The cold winter temperature, in particular over Europe and Russia, may not be fully explained by the North Atlantic Oscillation (NAO) variability. Atmospheric circulation anomaly accompanied the cold events often

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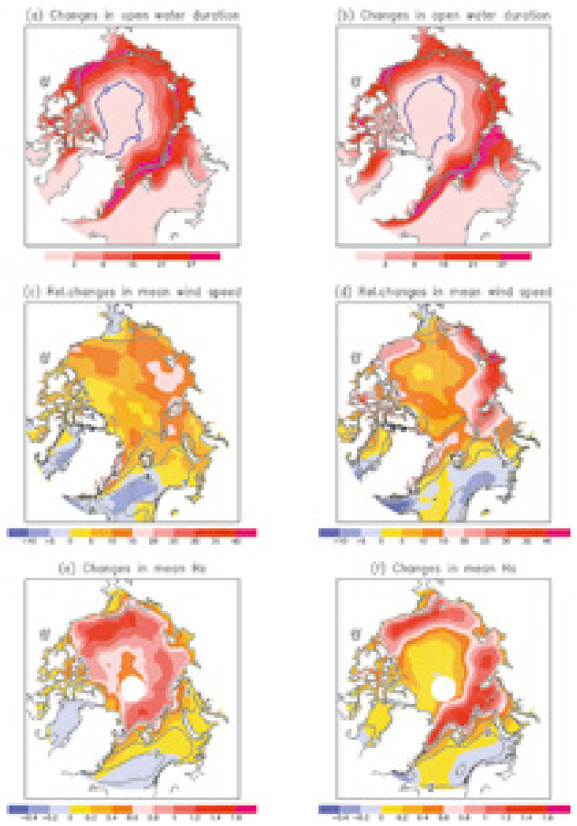

Figure 1.
(a, b) Simulated changes in the number of days with ice-free conditions;
(c, d) relative changes (%) in mean wind speed at 10 m height U_{10} (normalized to mean climatological U_{10} for 1980–1999);
(e, f) changes (m) in significant wave height H_s for the period 2046–2065 with respect to reference period 1980–1999, for September (a, c, e) and October (b,d,f).
Contours indicate: (a–b) the mean climatological locations of the multiyear ice boundaries (shown by null value isolines) for the periods 1980–1999 (black line) and 2046–2065 (blue line); (c–d) mean climatological U_{10} for 1980–1999; (e–f) mean climatological H_s for 1980–1999.

had a distinct structure with anti-cyclonic anomaly in the Barents Sea region. This suggests a possible impact from Arctic sea ice cover decline that accelerated in the last decade and was, in winter time, most pronounced in the Barents and Kara Seas. Idealized sensitivity experiments using artificially modified sea ice concentrations in the Barents and Kara Seas indicated a non-linear atmospheric circulation response to the BK SIC reduction that could in certain range produce cooling over the large continental areas. The current low sea ice concentrations may belong to that range. This motivates using realistic sea ice anomalies to infer about sea ice role in the observed recent weather anomalies.

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Changes in permafrost conditions

Possible changes in the soil thermal regime characteristics of the Northern Hemisphere are estimated using a model of the heat and moisture transport in the ground. For high latitude regions of Russia, the model estimated temperature trends in grounds (around 0.3C/10 years at a depth of 3 m) are quite consistent with empirical estimates for the past few decades. The largest areas with extreme values of the trend of ground temperature (more than 0.05C/year) in the 21st century at high latitudes of the NH were obtained using the estimates of climate changes according to calculations with the models CCCMA_CGCM3_1_T63 UKMO_HADGEM1.

Modeling the air pollution

The regional atmospheric modeling complex is based on the RAMS/CAMx numerical models of the atmosphere, that are widely used for regional studies of atmospheric pollution. Basic model parameters (the geographical boundaries of the computational domain, horizontal and vertical resolution of the computational grid, initial and boundary conditions, turbulent mixing coefficients in the boundary layer, etc.) were adjusted for the analyzed region. RAMS well reproduces vertical profiles of basic meteorological parameters in the lower troposphere. Comparison to CO observations at surface (monitoring station Zotino; 60°N, 89°E) showed that CAMx reproduces the seasonal effect of springtime biomass burning emissions in southern Siberia (about 15 ppb in intensive fire seasons).

The impact of a warmer Mediterranean Sea on Central European summer flooding

Central European weather and climate are influenced by the Mediterranean Sea which itself experienced a strong surface temperature warming during the last four decades. One phenomenon linked to extreme weather events are cyclones following the "Vb" pathway. These cyclones can carry large amounts of moisture from the Mediterranean to Central Europe and cause extreme precipitation events. Our results show that precipitation return levels in JJA show an increase along the Vb cyclone track, for daily as well as for five day persistent precipitation extremes. This increase can be attributed to the warmer Mediterranean Sea.

The Extreme Flooding of July 2012 in Krymsk, Russia, from a Climate Perspective

One of the most devastating meteorological extremes during recent years has been the extreme precipitation event along Russia's Black Sea coast, near the town of Krymsk, during the 6th and 7th of July 2012. The extreme precipitation was caused by a low pressure system that advected warm and moist air north-eastwards from the Black Sea. Sea surface temperatures in the Black Sea have exhibited a strong and continuous upward trend over the last decades, with warming exceeding 2K in some regions. As the Black Sea served as the principal moisture source for the observed extreme precipitation, we investigate the impact of the increased SSTs on the properties of the cyclone and the resultant magnitude of the precipitation. Our results suggest that such an extreme event would not have been possible without the current warmed SSTs. We find that the increased SSTs played an important role in amplifying the precipitation experienced near Krymsk, facilitating enhanced moisture fluxes and increasing instability within the planetary boundary layer.

HRJRG-404

STRUCTURAL PROPERTIES OF CARBONATE-SILICATE MELTS AND THEIR EFFECT ON FRACTIONATION PROCESSES IN THE DEEP EARTH INVESTIGATED BY SYNCHROTRON RADIATION, SPECTROSCOPIC, AND ION PROBE METHODS

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Intense experimental and field studies during the last decade provided evidence for importance of carbonate-containing melts for the evolution of the Earth's upper mantle and for modern industry. In currently active volcanism on the Earth's surface carbonate melts are confined to a single unique location – lavas from Ol Doinyo Lengai volcano, Tanzania. However, they are often associated with continental intra-plate volcanism, and they play an important role at deeper levels. At convergent tectonic plate boundaries subduction transports huge amount of carbonates from oceanic sediments down into the mantle. In addition, other deep sources of carbonatites are also possible. Finally, carbonatite magmatism is responsible for formation of deposits of industrially important rare earth elements (REE) and Nb.

Carbonatite and carbonate-silicate melts have very distinct physical properties compared to silicate melts, such as lower density and viscosity and very high electrical conductivity, which are a consequence of differences in their structural properties. In addition, carbonate-silicate melts in the upper mantle appear to be efficient diamond-forming media. This is proven both by findings of relics of such melts as inclusions in kimberlitic diamonds, as well as by numerous experiments on diamond synthesis. Nucleation and growth of diamonds in carbonate-silicate melts largely depends on solubility of elemental carbon in the melt, which, in turn, depends on its carbonate/silicate ratio, and thus, the structure of carbonate-silicate melts.

There are two poorly understood key aspects of the evolution of carbonate-silicate systems in the upper mantle: (1) transition from virtually pure carbonatitic melt to silicate-rich varieties with increasing temperature during partial melting of the mantle and (2) the possibility of liquid immiscibility between carbonate and silicate melts. The understanding of these processes critically depends on detailed information about atomic-level structure of the substances at relevant pressure-temperature (P-T) conditions. Laboratory experiments at high pressure and temperature have revolutionized the research on the deep Earth during the last century and provided a huge amount of information about the properties of minerals and their interactions in the interior of planets. We are now able to better interpret geophysical and geochemical observations and construct consistent models of the composition, inner structure and dynamics of planetary bodies. An ultimate boost in progress has been achieved by the use of hard-X-ray synchrotron radiation (SR) to study samples in situ at extreme P-T conditions using high pressure-high temperature (HP/HT) devices such as a diamond anvil cell. On the analytical side, major progress has been made in the development of ion beam or laser beam based techniques to achieve precise element concentrations as well as isotope ratios at very high spatial resolution.

The project consists of two interrelated tasks: investigation of samples quenched from HP/HT conditions and in situ studies of the most interesting compositions. Investigation of quench products is important for comparison with results of studies of natural samples encountered in the field. In addition, the range of analytical techniques applicable to these materials is somewhat more extensive than for in situ work. Importantly, relevant P-T-range is challenging for in situ spectroscopic and X-ray studies, since it requires combination of relatively high temperatures and relatively low pressures. The Russian partners focus mostly on investigation of quenched samples synthesized in large volume high pressure apparati and the German group focuses on in situ studies.

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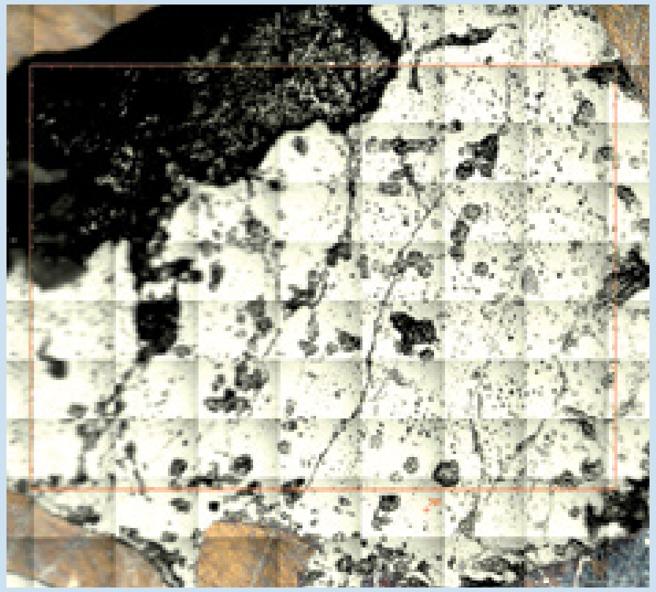
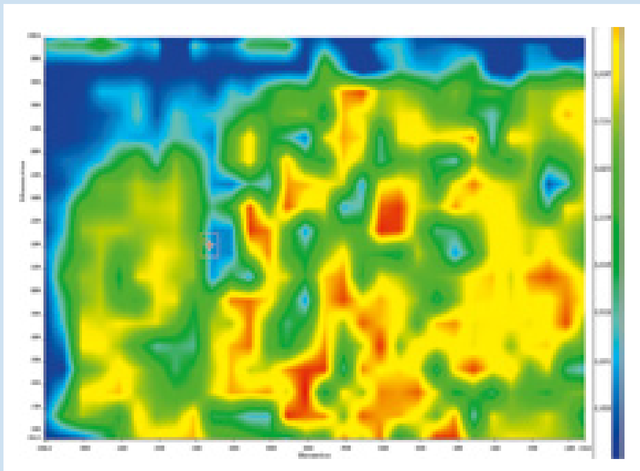
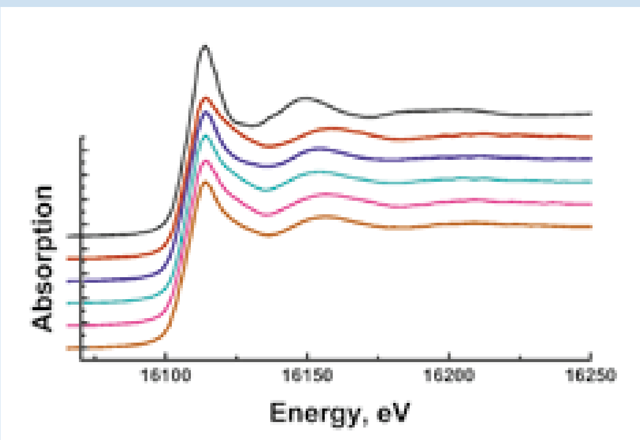
Structural properties of silicate, carbonate-silicate and carbonatite melts are investigated using X-ray diffraction/scattering and X-ray absorption spectroscopy using synchrotron radiation. Experiments with synchrotron radiation are performed at the Kurchatov Institute Moscow, at DESY Hamburg and ESRF Grenoble. Experiments at DESY and ESRF focus on those experiments that strongly depend on a small X-ray beam and high photon flux, whereas the facility at Moscow is used for measurements that are not critical in terms of beam size and flux or for test experiments. Where possible, X-ray diffraction experiments with synchrotron radiation are complemented by measurements using a laboratory X-ray source. Further insight to the structural properties is achievable by Raman and infrared (IR) spectroscopy. Particularly Raman spectroscopy is well suited to be combined with diamond anvil cells to perform experiments in-situ at HP/HT. Elements partitioning and isotopic fractionation between various phases is studied using electron microprobe and Laser-Ablation ICP-MS.

In summary, upon completion of the project we expect to gain important insight into structure, formation, exsolution and fractionation processes conjoint with carbonatitic melt systems. The results will advance our understanding of the relationship between structural properties and chemical behaviour in magmatic systems in general. They will also contribute to the development of reliable models for the interpretation of natural alkaline carbonatite systems.

Some examples of on-going studies are shown on figures below. Here we present an optical image of a carbonate-silicate melt quenched from HP/HT conditions (left) and map of carbonate distribution in this sample obtained using Infra-red microscopy (right). X-ray absorption spectra at Sr K-edge are shown in the bottom plate. The upper spectrum is $SrCO_3$ standard, the others shows Sr spectra for samples with variable silicate-carbonate ratio. Strontium behaviour is of interest on its own, but here it also serves as a proxy for Ca due to similarity in their geochemical behaviour.







Examples of on-going studies: an optical image of a carbonate-silicate melt quenched from HP/HT conditions (left) and a map of carbonate distribution in the sample obtained using Infra-red microscopy (right). In the bottom plate X-ray absorption spectra at Sr K-edge are shown.
Images by A. Shiryaev.

HEALTH

Image by HZI / Bellhäuser

HRJRG-006

MOLECULAR PATHOGENESIS OF BILATERAL BREAST CANCER

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Breast cancer (BC) is a leading oncological disease in women, which affects 1 out of 10 females. Up to 7% of BC patients develop this disease in both breasts, known as bilateral breast cancer (biBC). During the last decades, genetic pathways of unilateral BC have been intensively studied. However, only scarce information is available on the molecular pathogenesis of the bilateral form of this disease. Unilateral BC may often arise sporadically (i.e. without evident involvement of predisposing factors), while biBC is likely to accumulate in subjects with a high degree of BC susceptibility. Arising in the same body, bilateral carcinomas share key components of natural history and tumor pathogenesis, such as the genetic background, environmental factors and metabolic peculiarities. Therefore, revealing common genetic alterations in both left and right tumors is of great importance for the identification of risk factors predisposing to BC development. At project start, only a few studies in the literature were devoted to the molecular pathogenesis of bilateral breast cancer. Since April 2008, Russian and German scientists have been working together on investigating essential pathways of breast cancer pathogenesis and on identifying new genetic biomarkers of breast cancer susceptibility.

The Russian scientists identified the molecular subtypes of biBC. An accurate classification will potentially aid individualized clinical biBC treatment, as it may provide a basis for predicting overall prognosis, responses to chemotherapy as well as for selecting and designing novel therapies. A comparison of tumor pairs provided insights into the role of the genetic background and/or environmental factors in determining the pathogenetic variant of biBC. Profiling gene mutations in both tumors, the data pointed to an independent clonal origin of biBC. Moreover, biBC tumors showed significant accumulation of multiple alterations compared with unilateral BC, indicating increased mutagen exposure or impaired genome stability. In addition, the Russian group developed a novel design of epidemiological study, which is based on the "comparison of extremes" (e.g. biBC patients versus elderly tumor-free females), and is potentially suitable for rapid, large-scale screening of candidate BC-associated gene polymorphisms.

The Helmholtz group set out to determine the regions of profound genomic instability in biBC tumors, focusing on examining high-risk DNA damage loci, known as common fragile sites (cFSs). In recent years, cFSs have become of increasing interest in cancer research, as their tendency to breakage has been associated with genomic instability already in the premalignant stages of tumour progression. Therefore, identifying cFS genomic sequences is a matter of great importance in cancer genomics, since DNA alterations at cFS loci may serve as potential biomarkers for early cancer diagnostics and as targets for individualized therapies. Researchers from the Helmholtz group identified the genomic architecture and genetic information of previously uncharacterized cFSs associated with cancer and other human chronic disorders. Analyses of DNA copy number changes within cFS genes in biBC samples revealed a higher incidence of instability within cFS genes in biBC tumors than in unilateral samples. Taking into account that cFS activation is a prominent initiating event in the generation of DNA damage in different tumor types, identified cFS sequences may serve as targets to develop new diagnostic DNA biomarkers for uni- and biBC. The obtained data provide new insights into genomic alterations in biBC that so far have escaped molecular characterization.

During the period of project implementation several Russian scientists visited the Helmholtz group in Heidelberg to establish a detailed research plan and perform experimental work. In June 2009, six Helmholtz scientists met their colleagues in Saint Petersburg, where young and principal investigators from both groups exchanged the latest results and discussed further steps. The results obtained in the study have been presented in 18 publications of peer-reviewed international journals, strengthening the positions of both research groups in the national and international context. Data and experience obtained from the pilot studies of both groups contribute to the understanding of several aspects of the molecular pathogenesis of biBC and highlight the necessity to detect the full repertoire of somatic and germline genomic alterations in biBC tumors. Currently, the Russian and German research groups continue to collaborate using next-generation sequencing technologies to identify risk-modifying genetic alterations at the single nucleotide level in biBC.

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HRJRG-024

DERIVATION OF GERM LINE COMPETENT RAT ES CELLS FOR GENE TARGETING

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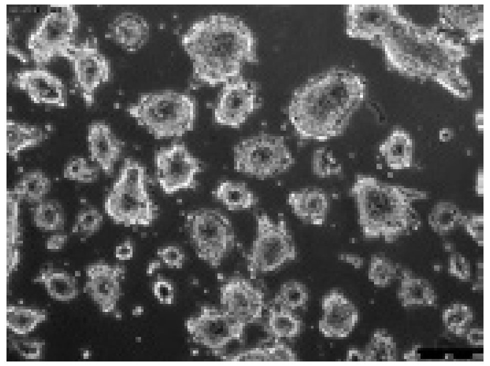
Project achievements

The rat represents an important animal model that, in many respects, is superior to the mouse for dissecting behavioral, cardiovascular and other physiological pathologies relevant to humans. We set in this Helmholtz-RFBR joint project (2007–2010) to derive induced pluripotent stem cells from rats (riPS) because it would open the opportunity for gene targeting in specific rat strains, as well as for the development of new protocols for the treatment of different degenerative diseases. During the course of this project we developed an improved lentivirus-based hit-and-run riPS derivation protocol that made use of small inhibitors. We demonstrated that the excision of proviruses did not affect either the karyotype or the differentiation ability of these cells. We showed that the established riPS cells are readily amenable to genetic manipulations such as stable electroporation. Finally, we proposed a genetic tool for an improvement of riPS cell quality in culture. These data prompt iPS cell-based gene targeting in rat as well as the development of iPS cell-based therapies using disease models established in this species.



Cultured rat iPS cells obtained during the course of the project. Image by Inst. of Cytology RAS and MDC Berlin.

Future joint activity

The collaboration between Dr. Natalia Alenina and Dr. Alexey Tomilin established during the course of this joint project has remained very active and productive. The two labs are jointly studying molecular mechanisms of stem cell maintenance as well as developing new tools that would ensure rapid and safe transfer of pluripotent stem cells to clinics. To this end, we have recently implemented into to stem cell field a novel generation of human artificial chromosomes (HAC) vectors (alphoid^{TetO}-HACs). We were the first who successfully transferred the in vitro assembled alphoid^{TetO}-HACs into the ES cells and then showed its stable maintenance and expression within most tissues of living mice. The use of HACs holds tremendous promises for gene therapy and iPS/ES cell-based regenerative medicine and, as before, Dr. Alenina and Dr. Tomilin will keep working together to jointly address some critical issues of biomedicine.

List of publications:

1. Liskovykh M., Chuykin I., Ranjan A., Safina D., Tolkunova E., Minina J., Zhdanova N., Dyban P.A., Mullins J.J., Kostyleva E.I., Chikhirzhina E.V., Bader M., Alenina N., Tomilin A. (2012) Generation of rat-induced pluripotent stem cells: Reprogramming and culture medium. Cell and Tissue Biol 6(2): 115–121.

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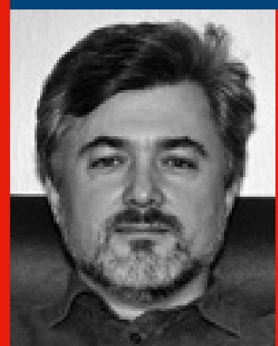

HRJRG-102

DEFINING LIFE/DEATH DECISION IN THE CROSSTALK BETWEEN DNA-DAMAGE-INDUCED APOPTOSIS AND DNA REPAIR

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Apoptosis is a certain form of programmed cell death (PCD) playing a key role in the development and homeostasis of multicellular organisms. Defects in the apoptotic pathway can lead to multiple human diseases, such as neurodegenerative diseases, autoimmune diseases, AIDS and cancer. In mammalian cells apoptosis can be induced by either extra- or intracellular stimuli, triggering the extrinsic or intrinsic pathway, respectively. The extrinsic pathway is triggered by the stimulation of death receptors (DR) on the plasma membrane. DR stimulation leads to the formation of the death-inducing signaling complex (DISC) and initiator caspase-8 activation. The intrinsic pathway can be triggered by chemotherapeutic drugs, irradiation or DNA damage and results in mitochondrial outer membrane permeabilization (MOMP), release of cytochrome C into the cytosol and initiator procaspase-9 activation. Both pathways eventually lead to the activation of effector caspases leading to the apoptotic phenotype including chromatin condensation, nuclear fragmentation, membrane blebbing, cell shrinkage and formation of apoptotic bodies. In order to better understand those signaling decisions, numerous systems biology studies of apoptosis have been conducted. Systems biology is a relatively new field with the ultimate goal to understand biological processes in their entirety, and it involves the combination of experimental procedures with mathematical modeling.

In the current project we addressed signaling pathways of apoptosis, DNA damage, caspase activation and analyzed these signaling pathways using the approaches of systems biology and systems medicine. We have combined the expertise of both Russian and German sides. Our studies provided new insights into the mechanisms of the life and death regulation on the qualitative and quantitative levels, apoptosis initiation and caspase activation, function of the key enzymes of DNA repair machinery, the crosstalk of life and death decisions in apoptosis and DNA repair. Special attention has been given to the determination of the CD95 DISC stoichiometry, molecular determinants of DNA repair signaling, novel methods of analysis of the composition of the high molecular weight platforms and using mathematical models of apoptosis for the development of novel anticancer therapies.

Mathematical modeling of apoptosis and DNA repair allowed determining and supporting quite some molecular paradigms. One of the key questions that was unclear for a number of years is whether caspase inhibitor c-FLIPL could also activate caspase-8 at the DISC. Only mathematical modeling was capable to predict the exact concentrations of the DISC components when c-FLIPL could play an activating role (Fricker et al., 2010, J Cell Biol). These predictions were successfully confirmed by experimental data. Remarkably, a new mechanism of apoptosis signaling has been discovered in the course of this project using biochemical analysis, mass spectrometry and mathematical modeling. Namely, we have determined the stoichiometry of the CD95 DISCs and found that caspase-8 outnumbers FADD at the DISC forming the so-called caspase-8 chains (Schleich et al., 2012, Mol Cell). Using mathematical modeling we further analyzed the dynamics of the chain formation and found that the DISC is a very dynamic system and its stoichiometry, i.e. length of the caspase-8 chains, is defined by the strength of CD95 stimulation. This finding adds another layer of complexity in caspase-8 activation and regulation of apoptosis in extrinsic signaling.

The non-apoptotic signaling features of CD95 have gained increasing interest, and, consequently, the concept of switching the phenotypes between apoptotic and non-apoptotic signaling also attracted our

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German researchers of HRJRG-102.
From left to right: Inna Lavrik, Nicolai Fricker, Kolja Schleich, Petra Richter, Jennifer Hölzel, Claudia Weber, Selcen Öztürk.
Image by DKFZ

Russian Researchers of HRJRG-102. First row: Pavel Pestryakov, Natalia Lebedeva, Ekaterina Maltseva, Yuliya Krasikova.
Second row: Mikhail Kutuzov, Yuliya Maksyutova, Ekaterina Belousova, Anna Shtygasheva, Emmanuel Crespan, Nadegda Dyrheeva. Image by NIBOCH

5 Selected publications based on HRJRG-102 funding:

1. Schleich K, Warnken U, Fricker N, Oztürk S, Richter P, Kammerer K, Schnölzer M, Krammer PH, Lavrik IN. 2012. Stoichiometry of the CD95 Death-Inducing Signaling Complex: Experimental and Modeling Evidence for a Death Effector Domain Chain Model. Mol Cell. 47:306–319.
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3. Lebedeva N, Rechkunova N, Ischenko A, Lavrik I. 2013. 12: 1037–1042. The mechanism of human tyrosyl-DNA phosphodiesterase 1 in the cleavage of AP site and its synthetic analogs. DNA repair. 12: 1037–1042.
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5. Neumann L, Pforr C, Beaudouin J, Pappa A, Fricker N., Krammer PH, Lavrik IN*, Eils R*. 2010. Dynamics within the CD95 Death-Inducing Signaling Complex Decide Life and Death of Cells. Mol Syst Biol. 6: 352.

attention. The challenging question is how stimulation of death receptors could also result in the induction of NF-κB and MAPK pathways, e.g. non-apoptotic pathways. Our ODE models of CD95-induced apoptosis found that DISC formation also leads to the induction of NF-κB and MAPK pathways (Neumann et al., 2010, Mol Syst Biol, Kober et al., 2010, Cell Death and Dis). Intriguingly, caspase-8 activity and the concentration of c-FLIP play an important role in NF-κB and MAPK induction. Thus, our systems biology studies have demonstrated that the amounts of the main regulators of DR-induced apoptosis procaspase-8 and c-FLIP at the DISC also play a key role in the induction of non-apoptotic signaling.

Taken together, our research programme has provided new insights into the mechanisms of life and death in the cell and initiated a number of leading edge research projects that have been successfully finished or will be accomplished in the near future.

HRJRG-116

GENETIC SUSCEPTIBILITY TO TUBERCULOSIS

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Abstract

Tuberculosis (TB) is one of the world's most threatening infection diseases. Resistance to treatment and an increasing rate of TB-HIV co-infections underline the need for new strategies to fight this disease. For a better understanding of the pathology and the host response, animal models are important. The group of Alexander Apt in Moscow at the Central Institute for Tuberculosis established a unique mouse model consisting of a resistant (A/Sn) and a susceptible (I/St) strain. This resource was used for a state-of-the-art joint analysis together with the department Infection Genetics at the Helmholtz Centre for Infection. We performed genome-wide gene expression arrays to study the transcriptome of whole lungs after high dose infection with Mtb H37Rv. The expression analyses revealed a family of cysteine protease inhibitors as a potential key player in the defence of Mtb. Moreover, we could identify major differences e.g. in antigen presentation, T cell and NK cell activation between susceptible and resistant mice. In summary, these studies contribute to a better understanding of the host factors that are involved in the resistance and susceptibility of the mammalian host to Mtb.

The results of this collaboration have been published in:
Shepelkova G, Pommerenke C, Alberts R, Geffers R, Evstifeev V, Apt A, Schughart K, Wilk E. Tuberculosis (Edinb). 2012 Dec 28. doi:pii: S1472-9792(12)00207-7. 10.1016/j.tube.2012.11.007.

Scientific results

1. Regulation of immune responses to M. tuberculosis infection is more complex in TB-resistant A/Sn compared to TB-susceptible I/St mice

To monitor the global transcriptome patterns in the two mouse strains, gene expression was assessed using Agilent 4x44K whole genome microarrays. Genes that changed their expression level at least two-fold compared to non-infected controls with a p-value of ≤0.1 were considered as differentially expressed genes (DEG). Altogether, 1,627 DEG were identified in our analysis. 675 (41%) DEG changed their expression after infection of mice from both strains (summarized in the left panel before, separate for up-an down-regulated genes in the right panel), whereas 249 (15%) genes were differentially regulated exclusively in I/St (127 upregulated, 122 downregulated) and 703 (43%) only in A/Sn mice (349 upregulated, 354 downregulated). Thus, substantially more genes changed their expression levels after TB challenge in resistant A/Sn mice compared to susceptible I/St mice, indicating a more complex response to infection in the resistant strain. Also, in a comparison of all gene expression changes, generally higher activation was observed for A/Sn compared to I/St mice (Fig. 1A, scatter plot of fold-change of expression levels after infection).

Signaling pathway impact analysis (SPIA) and evaluation of overrepresented gene ontology (GO) terms revealed a more pronounced activation of innate and adaptive immune mechanisms in infected resistant A/Sn mice compared to susceptible I/St mice.

A significant overrepresentation of mast cell related and FcεRI signaling GO terms were found in resistant A/Sn but not I/St mice. Also, GO terms specific for γδ T cells were significantly overrepresented in A/Sn but not in I/St mice. Furthermore, SPIA and GO term analysis clearly indicated a stronger activation of adaptive immune responses in resistant A/Sn mice. In contrast, 'neutrophil homeostasis' and 'positive regulation of nitric oxide biosynthetic process' were found to be significantly activated in susceptible I/St but not in A/Sn mice. In addition, SPIA demonstrated

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a stronger activation of NK cells in the resistant strain. A slight downregulation, not meeting the criteria of DEG, of Klra8 and Ncr1 NK cell-specific marker genes was revealed in I/St mice (Fig. 1B) supporting the data obtained by SPIA, namely a stronger activation of the NK cell mediated cytotoxicity in infected A/Sn mice. T and B cell specific marker genes were moderately upregulated in mice of both strains, but to a somewhat higher extent in A/Sn (Fig. 1C). After M. tuberculosis infection, numerous B cell-specific markers showed either no regulation or even a small decrease of expression in I/St but a slight increase of expression in A/Sn mice (Fig. 1D). Remarkably, in addition to a stronger activation of the B cell receptor signaling pathway compared to I/St, infected A/Sn mice upregulated numerous immunoglobulin genes (Fig. 1E). Overall, a stronger and more versatile activation of the immune response was observed in TB-resistant A/Sn mice.

2. Susceptible I/St mice demonstrate an increased activation of granulocyte responses after infection

Most cytokines and chemokines were similarly regulated in both mouse strains. However, some genes were differentially regulated: Ccl5 and Il1b showed a strain-specific upregulation in A/Sn mice, whereas I/St mice showed an increased expression of Cxcl11 and selective significant upregulation of Ccl20. In addition, we found an exclusive upregulation of Il11 in I/St mice, confirming results from our earlier studies. Furthermore, GO term analysis revealed an enrichment of granulocyte-associated responses, especially nitric oxide production and the granulocyte-specific genes Mmp8 and Ngp were considerably upregulated, in I/St mice. In contrast, no significant changes in mRNA expression were observed for the type 1 cytokines TNF-α, IFN-γ and CCL5.

Taken together, these expression changes suggested a more profound infection-induced neutrophil influx and more neutrophil-related activity like nitric oxide biosynthesis in the lungs of susceptible compared to resistant animals. Indeed, pathological examination of the lungs for neutrophilic inflammation confirmed this finding.

3. Cystatin type 1 genes are upregulated in susceptible I/St mice

The most prominent infection-induced upregulation in susceptible I/St mice was observed for the cysteine protease inhibitors type 1 (stefins)-encoding genes. Interestingly, all members of the stefin gene cluster on chromosome 16 were upregulated, whereas the expression levels of the chromosome 10 gene encoding cystatin B, another type 1 stefin, did not change after infection. Gene expression of type 2 cystatins located on chromosome 2 also did not differ between A/Sn and I/St mice, except for the Cst7 gene, whose expression increased postinfection stronger in A/Sn compared to I/St mice.

Discussion

The present study was the first report analyzing gene expression patterns of the host response to M. tuberculosis at the level of the whole lung. We report major qualitative and quantitative differences between the lung transcriptomes from infected TB-resistant A/Sn and TB-susceptible I/St mice. Our results suggest that resistant A/Sn mice showed a more complex response to M. tuberculosis than susceptible I/St mice. The chemokine CCL5 important for T cell migration to M. tuberculosis-infected lungs was not significantly regulated in either strain at two weeks after infection, at a time before the adaptive immune response is fully established. The analysis of cell-specific signature gene expression demonstrated that, following infection, T cell activation-related signals are increased in both mouse strains, confirming that I/St mice are not defective in T cell recruitment to the site of infection. However, the SPIA implied a reduced level of activation through the T cell receptor in I/St mice, which is in agreement with earlier data showing a diminished IFN-γ response in these mice at the later phases of

Galina Shepelkova in the lab. Image by Helmholtz Moscow Office

TB infection. Thus, more advanced phases of infection have to be studied to find out whether TB-susceptible I/St mice have a delayed or deficient T cell response to the bacterial pathogen or not. Whereas in A/Sn mice the expression of B cell-specific marker genes showed no or only marginal increase after infection, their expression in I/St mice clearly decreased. Although the B cell response hardly reaches its maximum at day 14 of infection, the B cell-related activity appeared to be more advanced in A/Sn mice. This observation, in turn, may explain the lower neutrophil influx to the lung in A/Sn mice, given the capacity of B cells to inhibit the recruitment of neutrophils to the site of infection.

In conclusion, with the exception of the apparently deleterious neutrophil response pathway, TB-susceptible I/St mice display a narrower pattern of gene expression regulation following TB infection compared to their more resistant counterparts.

Future outlook

The HRJRG contributed substantially to the collaborative research activities between the German and the Russian group. Without this programme, the scientific projects would not have been possible. The first contacts between the groups were made at a Helmholtz-Russian workshop in Moscow; the scientific meetings between the groups and the visits of the Russian scientists were essential for a successful completion of the research project. At present, there is no subsequent funding program available which would support the continuation of the joint research activities, but the principal investigators are regularly scouting the EU programs for such possibilities.

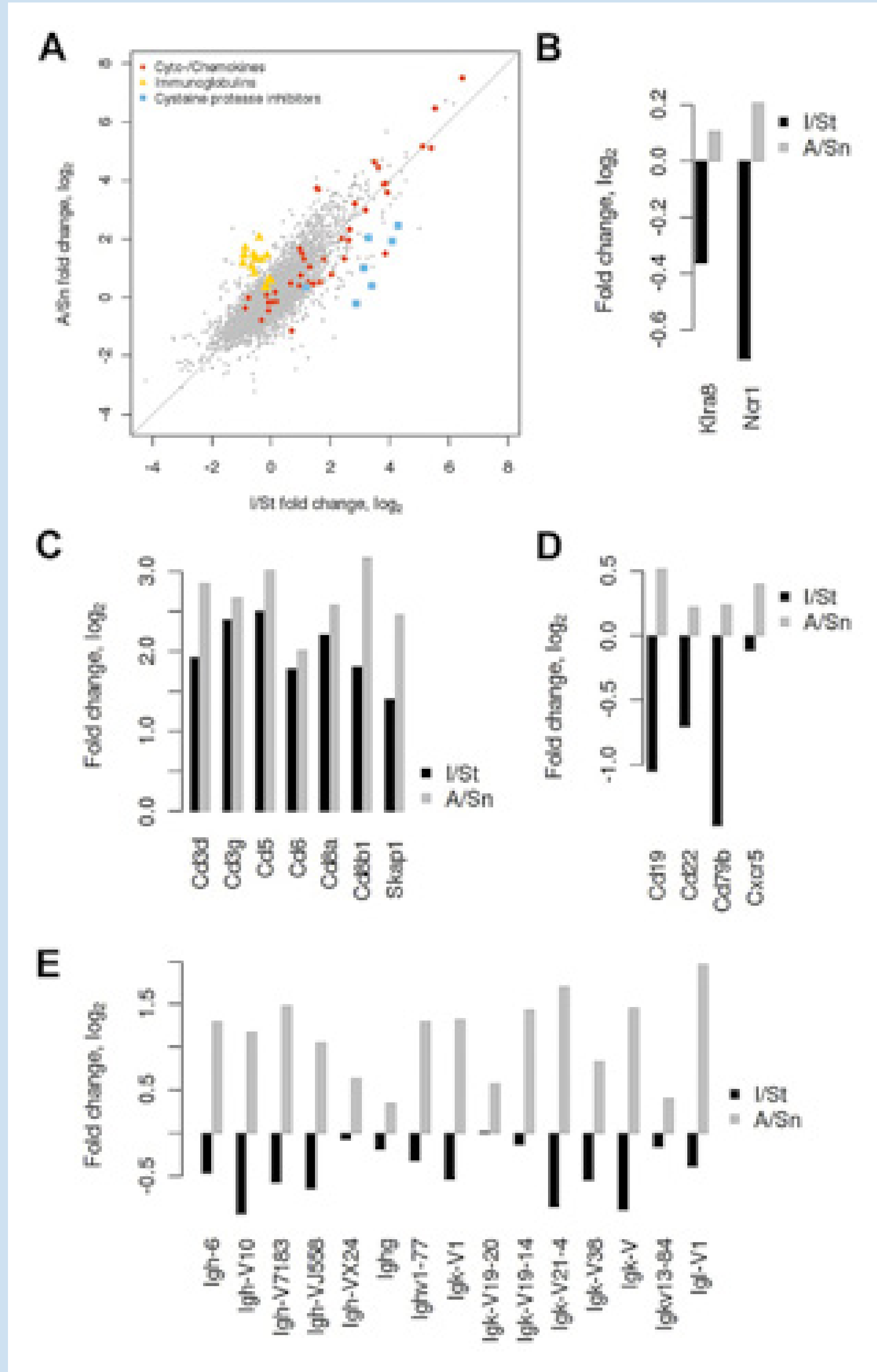

Figure 1: The expression of functionally associated genes varies between TB-resistant A/Sn and TB-susceptible I/St mice.

HRJRG-220

POSSIBLE BENEFICIAL EFFECTS OF TNF AND/OR LYMPHOTOXIN ABLATION IN CARCINOGEN-INDUCED AND SPORADIC CANCER, AS STUDIED IN MICE

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Our project is focused on studying the role of two closely related cytokines: Tumor Necrosis Factor (TNF) and Lymphotoxin (LT) in tumor development using several experimental mouse models relevant for human cancer. Initially TNF has been discovered as an anti-tumor factor, but it is now recognized as one of the mediators of immune regulation with key roles in host defense and inflammation. In certain experimental models TNF can play a pro-tumorigenic role, although the sources of such pathogenic TNF have not been identified. On the other hand, anti-TNF therapy proved to be beneficial in rheumatic and other autoimmune diseases.Whether such a therapy is also beneficial for cancer patients, is important to elucidate. There is a recently uncovered link between the LTalpha/LTbeta-->LTbetaR signaling axis and cancer. Our study unravels possible beneficial effects of TNF or LT ablation in several models of experimental cancer, which are relevant for human cancer, with specific focus on the cellular sources of pro-tumorigenic TNF and LT.

In the course of the study both sides contributed unique mouse models that complemented each other. In particular, crosses between cancer prone mice (generated in the laboratory of Prof. Thomas Blankenstein) and conditional immune-deficient mice (generated in the laboratory of Prof. Sergei Nedospasov) allow the analysis of auto/paracrine cytokine effects on cancer development. As a result of this successfully established collaboration, the research on newly generated mouse lines will be continued in both laboratories even after the current funding period.

In addition, German scientists contributed to educational courses at the newly established Chair of Immunology at the Faculty of Biology, Lomonosov Moscow State University in Moscow. The Russian partners, in particular the young investigators, have greatly profited from collaboration with the laboratory of Molecular Immunology at the MDC. Two of the undergraduate students from the Russian side visited the laboratory of the German partner as summer students in 2012. They have been introduced to and involved in all aspects of the work, including development of mouse models, experimental carcinogenesis, evaluation of mice (histological, immunological and molecular analysis), statistical analysis, discussion on the results and comparing them to those of the relevant literature in the filed.

To summarize, in line with one of the main goals of this joint collaboration, we have successfully established several mouse models of sporadic cancer in the laboratory of the Russian partner. This required extensive training and interaction between the young investigators and the students on both sides as a guarantee that these models can be used in the future. We are planning to complete the long-term mouse studies started during this project.

Selected publications of the project:

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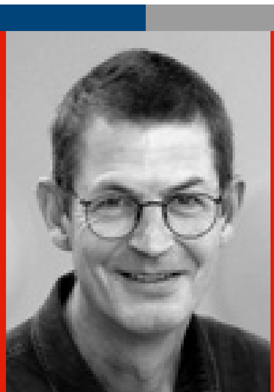

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HRJRG-310

GENETIC FACTORS INFLUENCE THE HUMAN METABOLISM

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The understanding of mechanisms controlling human health and disease, in particular the role of genetic predispositions and their interaction with environmental factors, is a prerequisite for the development of safe and efficient therapies for complex disorders, such as type 2 diabetes and cardiovascular disease. Over 100 years ago, Archibald Garrod predicted that inborn errors in human metabolism were 'merely extreme examples of variations of chemical behavior which are probably everywhere present in minor degrees' and that this 'chemical individuality [confers] predisposition to and immunities from the various mishaps which are spoken of as diseases'. Today we are able to conduct genome-wide association studies (GWAS) with a broad panel of metabolite concentrations in human body fluids. These studies identified a number of common genetic variants in genes coding for enzymes and transporter proteins that induce major differentiations in the metabolic make-up of the human population, thereby confirming Garrod's 100 year-old prediction. In combination with the increased knowledge about disease associated genetic loci, these so-called "genetically influenced metabotypes" can now be used to uncover new complex risk factors of common.

Metabolites are products of the metabolism, whose concentrations can be measured in human blood, urine or other body fluids. The levels of different metabolites quantify important biological processes, which can be either directly involved into pathogenesis of human diseases (such as e.g. cardio-vascular disease), or indicate disease predisposition, onset and progression. New high-throughput molecular biology techniques allow characterization of human metabolome by measuring simultaneously thousands of metabolites. At the same time, composition of individual genomes can be characterized by determining DNA sequence at millions of sites. To study genetic determinants of human metabolism, both metabolomic and genomic measurements are performed in a large number of people, and statistical association between genotypes and phenotypes is studied by use of genome-wide association scans. Effective analysis of these big data requires development and application of efficient statistical and computational approaches.

To study how genetic factors influence the human metabolism, within a Helmholtz-Russia Joint Research Group we intensified an already existing cooperation between the Institute of Genetic Epidemiology at the Helmholtz Zentrum München, German Research Center for Environmental Health (HMGU), and the laboratory of Recombination and Segregation analysis, Institute of Cytology and Genetics, Siberian Branch of the Russian Academy of Sciences (IC&G SB RAS). Both partners have a longstanding experience in the field of GWAS, and complement their competencies and research interests. In particular the analysis of metabolomic data is a major research focus of the Institute of Genetic Epidemiology (HMGU). In a variety of these projects it was possible to use the excellent data resource of the population-based KORA study (Kooperative Gesundheitsforschung in der Region Augsburg). The research focus of the laboratory of Recombination and Segregation analysis (IC&G SB RAS) is theoretical genetics and the development of methods for genetic epidemiology.

It is usually assumed that genetic effects are additive, i.e. the joint effect of alleles is a sum of their effects. In our project we aim to achieve better understanding of genetic control of human metabolome through modelling of genetic interactions within GWAS framework. Refined strategies include statistical modelling of allelic, epistatic, and gene-environmental interactions. We develop new

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Helmholtz-Russia Joint Research Group investigating the role of genetic interactions in the control of human metabolome. Picture taken during a meeting in Munich, Sept 2013. Standing, from left to right: Sodbo Sharapov, Yakov Tsepilov, Christian Geiger. Sitting: Konstantin Strauch, Janina Ried, Yurii Aulchenko. Image by MDC

statistical genetic methods, algorithms, and software, which have wide utility for the field of GWAS. In particular, we have developed methods to detect potentially interacting loci [1], methods for fast GWAS using mixed models [2], and genomic control for non-additive models [3]. As a next stage, we apply existing and newly developed methods to analysis of real KORA data, thus identifying novel loci for different metabolites. Through these analyses we obtain a deeper understanding of the biology of regulation of human metabolism, making a contribution to the molecular studies aiming to better diagnostics and therapy of a number of diseases related to metabolic disturbances.

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AERONAUTICS, SPACE AND TRANSPORT

Wind channel. Image by DNW

HRJRG-205

MARTIAN SATELLITE GEODESY, CARTOGRAPHY, AND FUTURE EXPLORATION

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In 1877, Asaph Hall, an astronomer at the United States Naval Observatory, discovered that Mars is accompanied by two satellites, Phobos and Deimos. Phobos has an odd shape (Fig. 1), which can be described as an ellipsoid, approx. 26 x 23 x 18 km in size, and is orbiting the planet at a distance of approx. 6000 km. Deimos has a size of approx. 16 x 12 x 10 km, moving at a much greater distance of about 20.000 km.

The origin of the two satellites has remained a mystery to the present day. The satellites may have been ejected from their parent planet early in history. Alternatively, Phobos and Deimos may represent captured asteroids from the distant asteroid main belt.

American, European and Russian space engineers have identified Phobos as a critical target for future space missions, from where recovering extraterrestrial samples may be comparably straightforward. In particular, Russian space scientists are planning a sample return mission to Phobos shortly after 2020. In the future, Phobos may be an important stop-point for future manned missions on their way to Mars. Efforts must begin today to prepare for these missions.

The Mars Express (MEX) launched by the European Space Agency (ESA) is currently the only Mars spacecraft to carry out Phobos flybys and make close-up studies of the object. During a mission of more than 10 years, MEX has returned new data on Phobos, including imagery, spectral data, and gravity field measurements. The image data are obtained by the HRSC (High Resolution Stereo Camera) including Super Resolution Channel (SRC), which has been developed and is operated by the German Aerospace Center (DLR) in Berlin. Our team benefits very much from these new data.

In 2011, we launched our Helmholtz-Russia Joint Research Group to study the geodesy and cartography of Phobos and Deimos and to prepare for Future Exploration of the Martian Satellites. Scientists and Phobos/Deimos experts from German Aerospace Center (DLR); Technical University Berlin (TUB); Moscow State University of Geodesy and Cartography (MIIGAiK), MIIGAiK Extraterrestrial Laboratory (MExLab); Vernadsky Institute of Geochemistry and Analytical Chemistry (GEOKHI) of the Russian Academy of Science teamed up for this effort.

We focused on the following projects:

1. Phobos and Deimos astrometric observations (Fig. 1) and new orbital modeling.
2. Establishment of a new geodetic control point network and a more detailed shape model.
3. Modeling of the Phobos' gravity field and studies of spacecraft motion near Phobos.
4. Production of orthoimages and a new Phobos topographic map (Fig. 2)
5. Studies in Phobos' surface geology, in particular mapping and statistical analysis of Phobos craters and grooves.
6. Joint data analysis: discussions of Phobos and Deimos origin, evolution, and fate.
7. Student education and training.

With the project coming to its conclusion by the end of 2014, we have updated the available data products for Phobos, and we have greatly improved our understanding in many areas of Phobos and Deimos science. Several students benefitted from this research and have prepared publications and theses. This project has been an excellent basis for further cooperation in space science between the team partners (Fig. 3) in Russia and Germany.

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Fig. 1: SRC image h7492_052.sr2 showing Phobos and the more distant (smaller) Deimos in a rare mutual event on 5th of November 2009.
Credit: ESA/DLR/FU (G. Neukum)

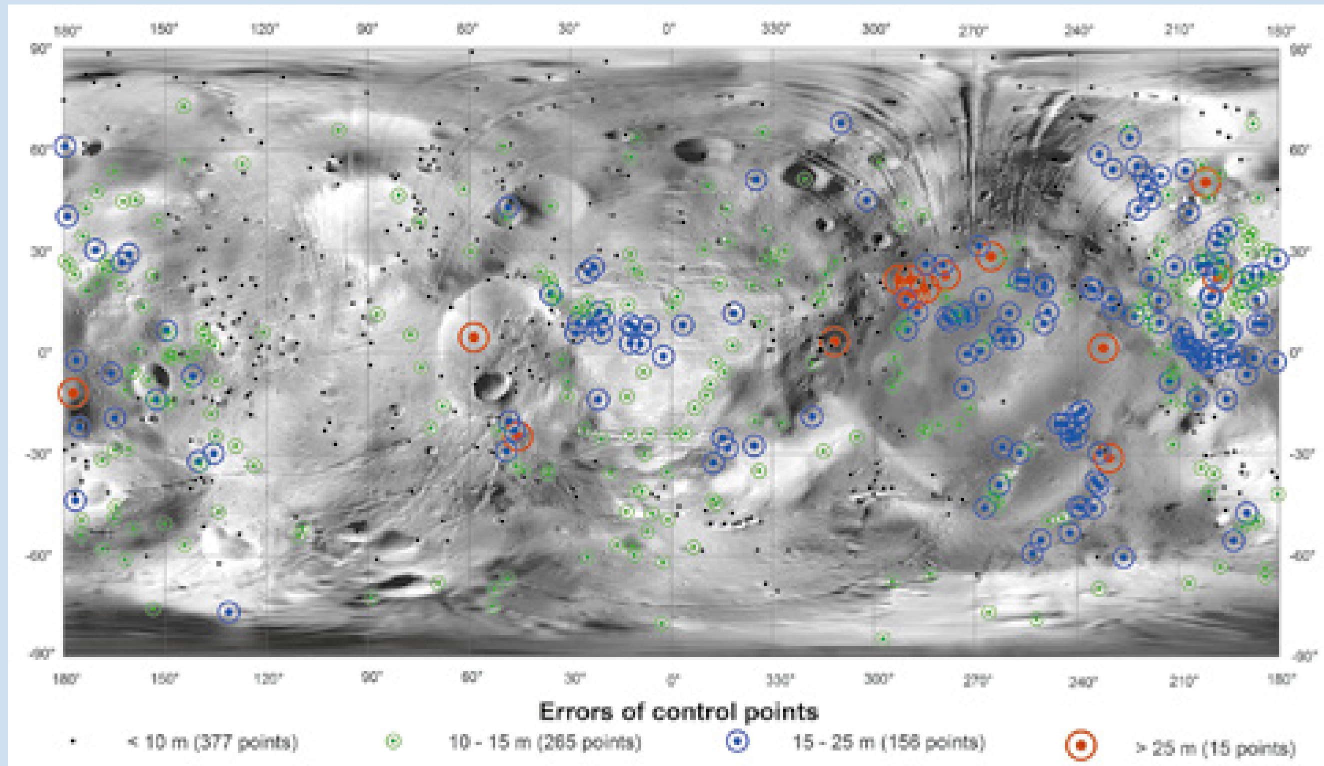

Fig. 2: MEX SRC-camera and Viking Orbiter images of Phobos were combined into a global orthoimage mosaic (20 m/pixel). The colored dots mark geodetic control points and their estimated positional accuracies. The mosaic was produced using the Russian commercial Photomod software, special edition (Credit: MIIGAiK, Rakurs™).

Fig. 3: Project Meeting at MIIGAiK, September 2013.
Back row (from left to right, respectively): Jürgen Oberst (Helmholtz Principal Investigator), Vadim Sizenkov, Vasiliy Dmitriev, Anatoliy Zubarev.
Center row: Dmitriy Zhukov, Irina Karachevtseva (Russian Principal Investigator), Valeriy Lupovka, Ljudmila Shishkina (Mitrokhina), Natalia Kozlova, Irina Nadezhdina.
Front row: Vyacheslav Patratiy, Alexander Kokhanov

List of joint publications:

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HRJRG-304

COMMUNICATION WITHOUT BLACKOUT FOR SPACE MISSIONS

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During interplanetary missions or re-entry flights to earth, the communication between spacecraft and control station on earth may interrupt. In the frame of the project „Communication Blackout Migration for Spacecraft – COMBIT" the scientists of two Helmholtz Centers – German Aerospace Center (DLR) in Cologne and Karlsruhe Institute of Technology (KIT) – develop in co-operation with the scientists of the IOFFE Physical-Technical Institute of the Russian Academy of Sciences in Saint Petersburg a new method to solve this problem. Since 2012 both the Helmholtz-Association (HGF) and the Russian Foundation for Basic Research (RFBR) have been funding the project in the frame of the programme of the "Helmholtz-Russia Joint Research Groups (HRJRG)".

When a vehicle enters the radio blackout phase, it loses all communication including GPS signals, data telemetry, and voice communication. Blackout occurs when the radio waves used for communication between ground stations and satellites are attenuated and/or reflected by the plasma layer that is created during hypersonic/re-entry flight. This phenomenon was well known at the beginning of space exploration when space capsule would experience several minutes of radio blackout during re-entry. Nearly 50 years later, hypersonic capsules still experience radio blackout during re-entry.

The so-called "radio blackout" is caused by the high temperature gas behind the bow shock in front of the spacecraft like Space Shuttle or re-entry capsules. Due to the high temperature gas properties change significantly. With increasing temperature first the vibrational mode of molecules is excited, which is followed by dissociation and atoms are produced. At temperatures above 5.000 K molecules and atoms ionize and a plasma layer consisting of ions and electrons is formed around the vehicle. In case of high concentration of charged particles this layer may reflect the radio waves and all communication including GPS signals, data telemetry, and voice communication to the spacecraft is lost.

The COMBIT team tries to solve the radio blackout problem by reducing the electron number density of the plasma layer. Such an approach would be successful because radio wave transmission is possible at radio wave frequencies greater than the plasma frequency, which is related to the electron number density of the plasma layer. This should be achieved by means of magneto-hydrodynamic (MHD) effects.
A combined magnetic and electrical field created close to the antenna should deflect charged particles in such a way that a local gas layer with low plasma frequency forms and the communication between the control station and spacecraft is guaranteed.

The COMBIT team consisting of ten scientists has a clear share of work. DLR is responsible for the design and conducting experiments in the arc heated facility L2K, which allows producing ionized hypersonic flow with a total temperature of several thousand degrees. At such temperatures the gas is composed of molecules, atoms, ions and electrons. The magnetic field inside the test model is created by a cooled superconducting magnet, which has been developed at the Institute of Technical Physics of KIT. The experts of IOFFE institute are in charge of physical modelling of the MHD process and numerical rebuilding of the experiments.

In L2K the ionized high temperature gas is accelerated to hypersonic speeds using a supersonic nozzle. Inside the extension part of nozzle and in the free stream the velocity increases but the temperature, pressure and density decrease. But in front of the model a bow shock forms and decelerates the flow. The shock heats the gas to temperatures at which the flow is ionized. The magnet is mounted

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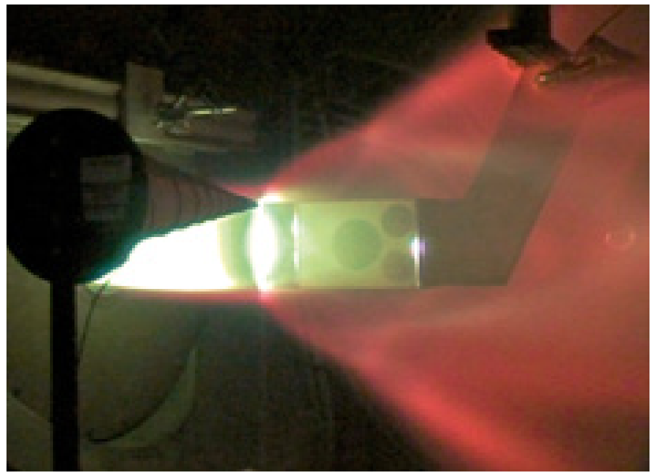

Preliminary Test in L2K: Flat plate model inside the ionized flow of L2K. Receiving antenna (left). Figure: DLR

in the middle part of the model. Two electrodes for producing an electrical field are integrated on the model surface upstream and downstream of the magnet. The sending antenna inside the model is placed close to the downstream electrode. Its signal has to pass the ionized flow before reaching the receiving antenna, which is placed outside the flow.

In L2K the ionization of the flow is weaker compared to the flight conditions with black-out effects. Therefore the experiments have to be carried out at higher intensity of the magnetic field, which cannot be realized with permanent magnets. Only cooled superconductive magnets are able to achieve magnetic field intensities beyond 2 Tesla on the model surface. The compact size superconducting magnet of KIT is cooled down to 4 Kelvin, i.e. minus 269°Celcius using Helium as coolant. Another very challenging requirement is the sufficient and reliable thermal isolation of the magnet from the high temperature environment of the flow.

The test configuration in particular concerning the location of the sender antenna inside the model has been defined based on the numerical simulation of IOFFE. Only a three dimensional, very complex simulation of the plasma flow with the magnetic and electrical fields is able to rebuild the correct test environment. This pre-test simulation is an important step for the preparation of the tests and understanding the results of experiments and post-test simulations with some possible improvements.

The HRJRG programme allows bringing together the Helmholtz and Russian institutions with long term experience in this field, in order to make a significant step in physical understanding of complex MHD interactions, improvement of experimental and numerical tools and finally increase its technological readiness level. Until now four progress meetings took place in an alternating way in Germany and Russia. These meetings and several teleconferences intensified not only the scientific but also personnel interaction in the team remarkably.

During preliminary tests it could be demonstrated that even in the weakly ionized flow of L2K the attenuation of the communication signal can be measured clearly. These tests showed also some positive effect of the permanent magnets with a magnetic field strength of 1 Tesla. The main tests with superconducting magnets are planned in early 2014.

HRJRG-304: Dr. Sergey Ponyaev (IOFFE), Nikolai Monakhov (IOFFE, Ph.D. student), Yuriy Kurakin (JSCC/IOFFE), Dr. Burkard Esser (DLR), Prof. Sergey Bobashev (IOFFE), Dr. Alexander Schmidt (IOFFE), Dr. Sonja Schlachter (KIT), Dr. Ali Gülhan (DLR), Dr. Wilfried Goldacker (KIT), Lars Steffens (DLR, Ph.D. student). Image by IOFFE

KEY TECHNOLOGIES

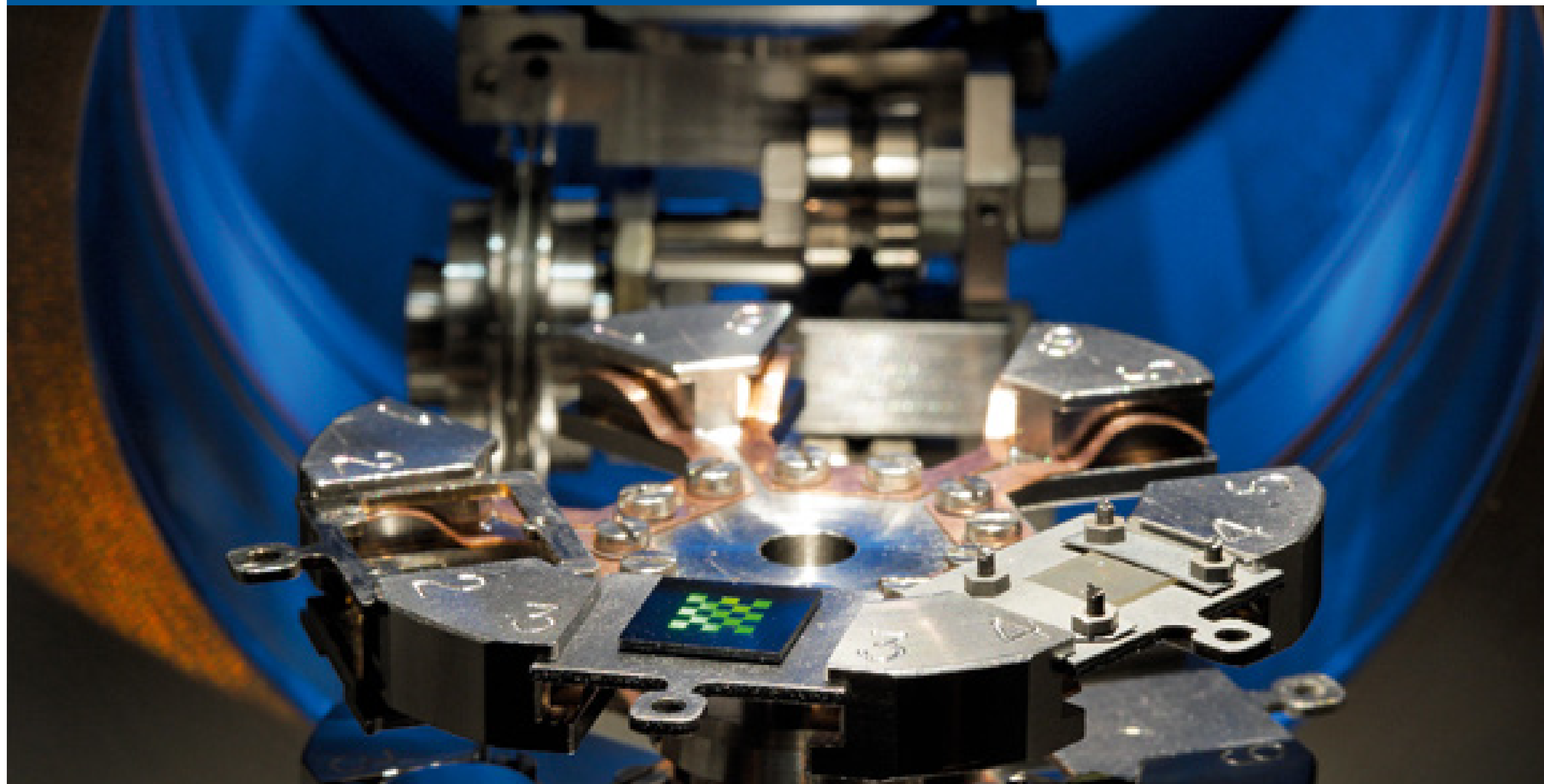

Image by Forschungszentrum Jülich

HRJRG-207

IDENTIFICATION OF LIQUIDS BY HILBERT SPECTROSCOPY FOR SECURITY SCREENING

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Among various ways of explosive detection under discussion, the techniques using electromagnetic radiation (i.e. microwave and terahertz imaging and spectroscopy) are considered as having great potential [1]. From the point of view of electromagnetic theory, the electric displacement-field response of a substance to a rapidly varying electrical field is defined by a complex dielectric function, which is determined by the internal dynamics of the substance's molecules [2]. Liquids, for example, can be reliably, with low rate of false alarms, identified by measuring their dielectric functions at the frequency range of their main dispersions and comparing them with reference data. However, the spectral range of dispersion for pure liquids is rather broad, from a few gigahertz (GHz) to a few terahertz (THz), and not covered by any single conventional spectroscopic technique.

New Hilbert-transform spectroscopy, which is based on high-Tc Josephson detectors, has a broad frequency range from a few GHz to 5 THz, large power dynamic range of 50–60 dB and can be used for a quick identification of liquids. To prove this idea, a concept of a liquid identifier based on a high-Tc Josephson detector has been suggested [3]. The liquid identifier consists of a broadband radiation source, a radiation coupling unit, the Josephson detector and a data acquisition system, controlled by a computer. Due to an extended frequency bandwidth required for the identification, all major parts of the liquid identifier such as the broadband radiation source, the radiation coupling unit and the Josephson detector could not be acquired on the market, but had to be developed from scratch.

Following the concept, two demonstrators of liquid identifier were developed. The first one had a quasioptical coupling unit. A photograph of the liquid identifier with quasioptical coupling is shown in fig. 1. In this demonstrator, radiation from a broadband polychromatic source was focused by a gold-plated elliptical mirror on a bottle with liquid, and the radiation reflected from the bottle was focused on the Josephson detector with the help of the second elliptical mirror. The broadband radiation source consisted of several frequency multipliers and could deliver polychromatic radiation in the frequency range of 30–500 GHz. A characterization of the frequency multipliers and the chains of frequency multipliers were done by a Hilbert-transform spectrum analyser [4]. The detailed description of the experimental setup can be found in [5].

The second liquid identifier had a radiation coupling unit based on a dielectric waveguide. The radiation coupling unit based on the dielectric waveguide was used to extend frequency range down to 1 GHz. In this demonstrator, the radiation of the broadband radiation source was directed to the liquid by a polyethylene waveguide, sandwiched between two metal plates, reflected from liquid and guided by another PE waveguide to the Josephson detector. In addition to the frequency multipliers, a frequency synthesizer was added to the radiation source. Such radiation source could deliver the radiation in the frequency range of 1–300 GHz. The detailed description of the experimental setup can be found in [6].

The reflected radiation was analyzed by the Josephson detector. The detector was based on a $YBa_2Cu_3O_7$-x bicrystal Josephson junction integrated in an electrically-driven, maintenance-free Stirling cooler. The junctions were optimized to ensure the required values of the frequency bandwidth, the power dynamic range and the detection accuracy. The scanning time of 0.2–5 sec and total measurement errors of 0.3% were achieved for our liquid identifiers.

The liquid identifiers were tested by liquids with various purities, including deionized distilled water (18.2 MOhm·cm), distilled water, tap water, acetone, alcohols, ethanol-water mixtures, two types of 30% H_2O_2/H_2O mixtures, NaCl and sugar aqueous solutions, various beverages and many other liquids. The deionized distilled water was used as a reference in all measurements.

Figure 1. Photograph of liquid identifier with quasioptical radiation coupling. Image by Forschungszentrum Jülich

At high frequencies (>30 GHz) the response of both liquid identifiers was proportional to the reflectance of liquid. At low frequencies (<20 GHz) the dielectric waveguide of the liquid identifier with waveguide coupling can be considered as a resonator with multiple resonance frequencies. The resonance frequencies and quality factors of the resonances were changed, when the bottle with liquid was attached to the waveguide. The response of the liquid identifier with waveguide coupling at low frequencies was proportional to the losses in liquid.

Both liquid identifiers demonstrated capability to distinguish water-based liquids from other liquids as well as similar water-based sugar-containing and sugar-free beverages, like Cola and Cola Zero [5,6]. The difference between the various types of water was more pronounced at low frequencies due to the losses related to an ionic conductivity.

The special attention was paid to the measurement of hydrogen peroxide, because hydrogen peroxide is a water-like liquid, a strong oxidizer, which can be used as an explosive or as a component for fabrication of explosives. We could detect the difference between water and 30% H_2O_2/H_2O mixture, which was not constant over the frequency range. The maximum difference of 6.5% was observed at 0.95 GHz, no difference was found at 32 and 95 GHz, but at 282 GHz the reflectance of 30% H_2O_2/H_2O was by 1.7% higher than the reflectance of water. At the frequency of 470 GHz, the difference between 30% H_2O_2/H_2O and water has increased up to 3.3% [7].

Due to a large difference in relaxation times $\tau 1$ for ethanol (163 ps) and water (8 ps), the reflectance measurements of the ethanol-water mixtures [8] can be used as an evaluation of the dynamic range and the sensitivity of the identifiers. The reflectance of the ethanol-water mixtures with varying ethanol content from 0% to 95%, measured by the developed liquid identifier with quasioptical coupling, is presented in fig. 2. The dynamic range of spectral reflectances of 200 has been demonstrated for the scanning times of a few seconds. The best selectivity to ethanol concentration has been achieved at the frequency range 100–300 GHz. This selectivity enhancement is related to the second relaxation time $\tau 2$ (3 ps) of ethanol [8]. Taking into account the experimental errors, the low concentrations of ethanol in water-ethanol mixtures can be detected with accuracy better than 0.1%.

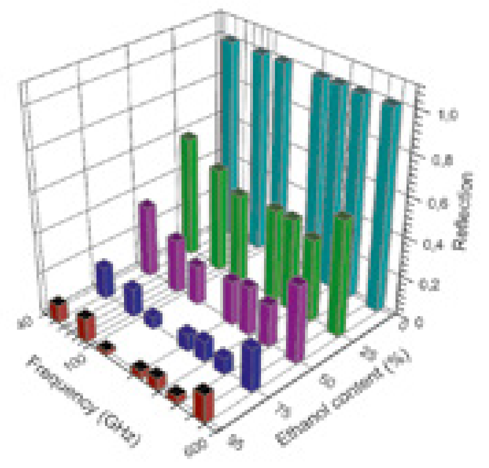

Figure 2. Response of liquid identifier to ethanol-water mixture.

In conclusion, we have suggested the concept of liquid identification based on Hilbert-transform spectroscopy and high-Tc Josephson detectors. Two demonstrators of liquid identifiers both based on this concept but with various, quasioptical and waveguide, coupling units have been developed. The frequency bandwidth of 1–500 GHz, scanning time of 0.2–5 sec and measurement error of 0.3% has been achieved. The demonstrators have been successfully tested by liquids with various purities. The possibility of identification of different types of water, acetone, alcohols, 30% H_2O_2/H_2O, beverages and many other liquids as well as the alcohol concentration in alcohol-water mixtures has been successfully demonstrated.

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HRJRG-314

DEFECTS IN MAGNETIC TiO_2 (DETI.2)

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Common ferromagnets such as iron or cobalt develop their magnetic order through exchange coupling of all of their delocalized, so called, 3d-electrons. The major goal of the DETI.2 is to investigate if a substitution of only a few % of magnetic 3d atoms into a non-magnetic oxide, i.e. titanium dioxide (TiO_2), can also lead to a ferromagnetic order, especially if the 3d electrons are influenced by structural defects. Such oxides are also considered as potential diluted magnetic semiconductors (DMS). An extensive study of this system during last decade was going either theoretically or experimentally; nevertheless, mechanisms of ferromagnetic order formation are still unclear.

Up to now it has been discovered that ferromagnetism in TiO_2 based DMS systems is strongly related to the structure of the film, the presence of different point defects (e.g. oxygen vacancies) and defect complexes, the positions of introduced 3d impurities in the matrix, etc., but there are several non-coherent attempts to explain experimental data (mainly high Curie temperatures and high magnetic moments per impurity atom) by theory (e.g., [1,2]). Moreover, films of the same composition but prepared via different methods like magnetron sputtering, MBE or PLD techniques, and ion implantation exhibit different magnetic properties [3]. In addition, it was discovered recently that even without any doping, oxygen deficient TiO_2 thin films and several other oxides like ZnO, In_2O_3 and HfO_2 with imperfect stoichiometry could be magnetic just due to different structural defects [4,5]. This so-called "defect-induced" magnetism represents a new kind of magnetic phenomena and could play an important role in the formation of ferromagnetic order in all oxide-based DMS systems. So, the main issues of interest in the field of DMS are the role of defects, the possibility of spin-polarization of free carriers and the presence of local magnetic polarizations on different sites inside the DMS systems.

To clarify the picture of electronic and magnetic interactions inside the doped DMS on the basis of TiO_2, the combined studies of magnetic, transport, structural, magneto-optic, magneto-transport, element-selective and defect studies are going within DETI.2 project. The equipment of project partners is allowing to perform standard XRD analysis; SQUID and VSM magnetometry; MO, MO spectroscopy, electronic transport and anomalous Hall Effect (AHE) measurements; SEM characterization, EDX analysis, Electronic Spin Resonance and Positron Annihilation Spectroscopy (PAS) experiments. Element-selective spectroscopies like XANES and XMCD with soft and hard X-Rays are going to be done at the external synchrotron radiation sources in Europe (BESSY, DESY, SOLEIL). Standard characterization techniques are necessary to rule out the presence of secondary phases or avoided cluster formation.

The particular interest of the project is focused on the origin of ferromagnetism in TiO_2 films doped by cobalt, vanadium or manganese. For these purposes the oxygen deficient and highly conductive TiO_2 films with thicknesses about 300÷600 nm have been prepared by sputter deposition and further the ion beam technology is used for introduction of local magnetic moments. Since the ion implantation a priori produces a lot of structural defects, the "reference" films are prepared also by doping during magnetron sputter deposition from alloy targets. A successful application of ion implantation for creation of other DMS materials is already confirmed [6] and this technique has a huge potential for the creation of different nanostructures by irradiation through lithographically defined masks.

Suspicious investigations of defect types and their concentrations on the local scale by non-conventional PAS technique should shed light on the role of negatively charged structural defects in formation of ferromagnetic order in studied DMS. So far only the influence of the crystal structure itself and the influence of positively charged oxygen vacancies (or their neutral complexes) have been considered. Our preliminary results (see Figure 1) demonstrate the correlation between the amount of negatively charged defects and the value of saturated magnetization in TiO_2-δ:V(1at.%) films with different conductivities prepared by sputtering. These "S-parameter" measurements being applied to undoped anatase TiO_2 films with amorphous, polycrystalline and epitaxial structures have shown the highest level of defects for amorphous film (As a rule of thumb: a larger "S-Parameter" reflects a higher amount of open volume defects and their larger sizes). The titanium atoms. These studies are planned for the second half of the project. The presence of magnetic polarization on oxygen atoms will directly confirm the assumption about involving of oxygen ions in a formation of ferromagnetic order in the films studied. The previous experience of project partners in this area of studies allows to expect the principal difference in results for DMS doped by different 3d atoms (Co, V and Mn).

The final step of the project is going to be dedicated to testing the possibility to create via ion implantation through lithographic masks DMS nano- and micro- structures with the same magnetic properties as observed for the "macroscopic" films.

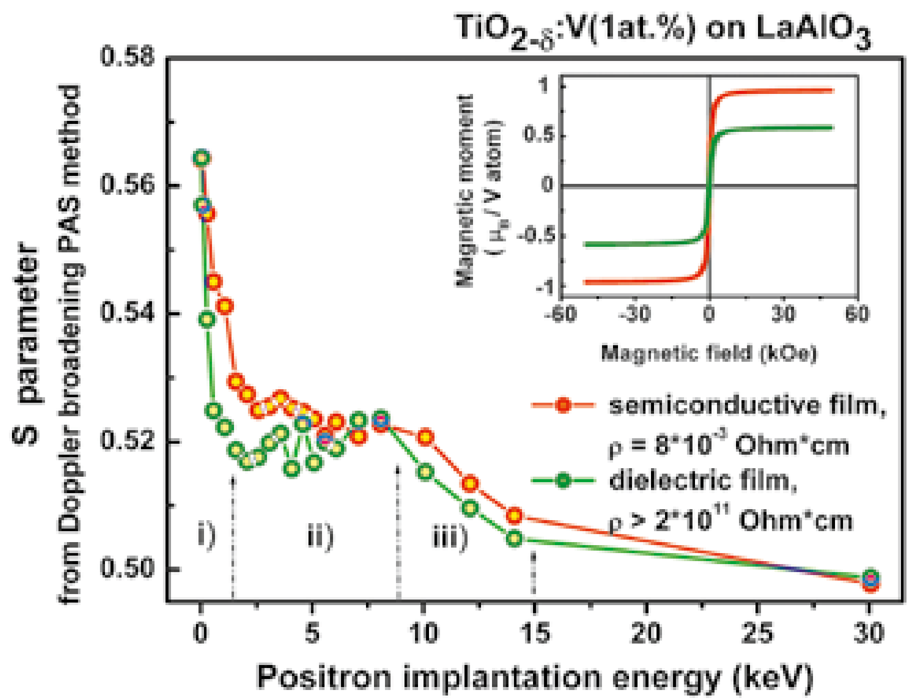

Figure 1. Energy dependence of the "S-parameter" from Positron Annihilation Spectroscopy (PAS) and corresponded SQUID magnetometry (see inset) for V-doped TiO_2-δ films with different conductivities at RT. There are three characteristic regions: i) represents the surface region of films, ii) relates to the "bulk" film and iii) corresponds to the interface with $LaAlO_3$ substrate.

ongoing measurements of positron lifetimes in the films through their energy would provide depth profiles of particular types of negatively charged defects in the studied films.

The answer about spin-polarisation of carriers, which is a main question from the point of view of spintronic applications can be provided by magneto-transport AHE measurements. The observed AHE is the direct evidence that the itinerant carriers and the ferromagnetic order are coupled together and the material could be considered for further technology. Within the project the tiny AHE was found for the anatase TiO_2-δ:Co(1at.%).

To go deeper inside the understanding of the magnetic properties, it is necessary to exploit the element- and shell-specific XANES, XMCD and XMLD techniques that will provide the information about valence states of introduced 3d impurities and their local magnetic polarisation, the presence of clusters and parasitic secondary phases as well as provide information about structure of TiO_2 matrix and possible magnetic polarisations of oxygen and

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HRJRG-316

HIGH-DENSITY PEPTIDE ARRAYS

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Today's analysis of blood samples is limited to a maximum of a hundred proteins. According to estimations, however, up to millions of different antibodies are contained in the circulating blood. These antibodies are formed as a reaction of our immune system to infections or metabolism disorders. The distribution of antibodies is like an open book of the disease history. One should only be able to read it.

The Helmholtz-Russia Joint Research Group (HRJRG) consisting of researchers from the Karlsruhe Institute of Technology (KIT), the University of Heidelberg (UH), and the Institute of Laser and Information Technologies of the Russian Academy of Sciences (ILIT RAS) is aimed at developing novel peptide arrays for antibody profiling. Peptides are short fragments of proteins which can specifically bind antibodies. Thus, they can be used for antibody detection (Figure 1). "Our goal is the fabrication of arrays with a density of a million different peptides per square centimeter. Only this high spot density, combined with the high quality of the peptides, will allow for an efficient read-out of information stored in the human immune system", says HRGRG spokesperson Dr. A. Nesterov-Müller from the Karlsruhe Institute of Technology.

The project focuses on the manipulation of special amino acid microparticles with laser radiation. Amino acid particles consist of a polymer matrix and amino acid derivatives inside the matrix. If the particle is deposited on an activated substrate and heated, the amino acid derivatives can diffuse inside the matrix and bind to the activated groups on the substrate surface. Thus, repeated selective deposition of all 20 biogenic amino acid particles in a combinatorial manner allows for the combinatorial synthesis of peptide arrays. Super-high resolution of the arrays is planned to be achieved by applying microstructured substrates, as shown in Figure 2, with different peptide spots being

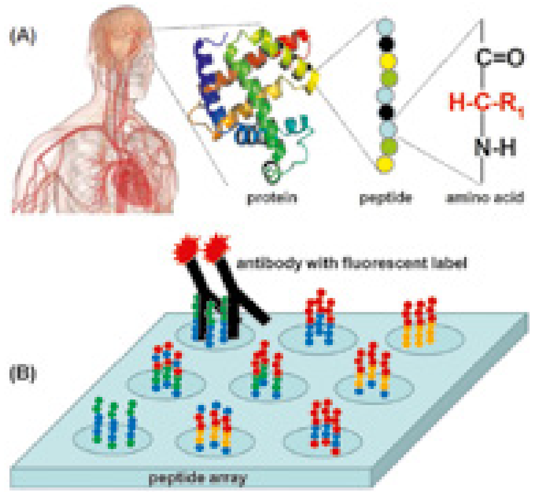

Figure 1; (A) Peptides are short protein fragments consisting of amino acids; (B) Selective binding of antibodies with peptide arrays.

synthesized in different cylindrical cavities. In this case, the pitch of the cavities will define the spot density of arrays to be produced.

The present project combines the expertise of Dr. Alexander Nesterov-Müller from KIT in particle-based array synthesis and microstructure technologies with the experience of Dr. Olga Baum from ILIT RAS in theoretical and experimental studies of physical effects by laser processing of organic materials. Prof. (apl.) Dr. Reiner Dahint from the University of Heidelberg focuses on the development of label-free detection methods in high-density array format with nanoparticle-based optically responsive layers.

From left to right: Alexey Yuzhakov, Evgeniy Shcherbakov, Olga Baum, Yulia Soshnikova, Emil Sobol. Image by ILIT RAS

While the German project partners develop the laser system for the combinatorial synthesis of peptide arrays and their analysis with label free detection methods, the Russian research group focuses on the theoretical description of the laser-assistance particle melting. The theoretical description of the melting process should allow understanding of the potential of the combinatorial laser methods in terms of spot density and peptide quality.

Dr. Alexander Nesterov-Müller (project spokesperson) studied physics at the Lomonosov Moscow State University from 1992 to 1998. He was conferred his PhD degrees in 2000 (laser physics, kand. nauk) and in 2006 (biotechnology, Dr.rer.nat.) and received the assistant professorship (2008, habilitation) at the University of Heidelberg. In 2011, he won the ERC starting grant and since that time he has been heading a working group focusing on the engineering of high-density molecular arrays at the KIT Institute of Microstructure Technology.

Dr. Olga Baum studied physics at Lomonosov Moscow State University from 1990 to 1996. After her PhD at Lomonosov Moscow State University, she started working at the theoretical department of ILIT RAS. Currently, Dr. Olga Baum is a senior researcher at the Biophotonics Laboratory of the Institute of Laser and Information Technologies of the Russian Academy of Sciences (lab head: Prof. E.N. Sobol).

Prof. (apl.) Dr. Reiner Dahint is head of the Biosensor and Biomaterial Research Group at the Institute for Applied Physical Chemistry, University of Heidelberg. Since 2008, he is adjunct professor at the chemical department of the University of Heidelberg. His areas of research are label-free optical sensors in nanoparticle technology, acoustic wave-based sensors for biomedical and environmental analysis, (bio)chemically micro- and nanostructured surfaces, interaction of proteins with artificial surfaces, protein-resistant surfaces, investigation of the formation, structure, and function of thin organic films as well as the design and construction of a new time-of-flight neutron reflectometer with combined infrared spectroscopic analysis for soft matter characterization.

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HRJRG-401

DEVELOPMENT OF METHODOLOGIES FOR STRUCTURAL STUDIES OF MEMBRANE PROTEINS VIA SMALL-ANGLE NEUTRON AND X-RAY SCATTERING

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Neutron scattering is a powerful tool to study condensed matter. However, the impact of this method on life science is less than those of X-ray scattering. Neutron scattering has important and unique advantages for life science and further developments of this method, and related experimental methodologies are required to realize this great potential. Our project aims to develop methodology for small-angle neutron scattering with membrane proteins. We believe that our approach would have a high impact on structural biology.

Membrane proteins are key functional components of cell membranes and participate in important cellular processes such as ion transport, catalysis, energy transformation, signal transduction, cellular sensing and communications. Dysfunction of these proteins leads to severe diseases. Almost 70% of therapeutic drugs currently available on the market are targeting membrane proteins. However, they have remained relatively poorly characterized compared to soluble proteins and comprise only 1% of proteins with known structure. X-ray crystallography has limited applications to membrane proteins, since their crystallization is still a great challenge. X-ray and neutron small-angle scattering (SAS) are powerful methods to investigate biological systems in a broad range of experimental conditions. Its efficiency increased remarkably due to developments of data treatment methodology and allowed to obtain low resolution structures of water soluble proteins (Svergun et al, 1987). This method belongs to very important tools of structural biology but not for the case of membrane proteins, where proteins are embedded into lipid membranes or surrounded by detergents. Protein environment contribute significantly to SAS-signal. It is still a challenge to separate contributions from membrane proteins and its surrounding and simultaneously avoid inter-protein interference. The contrast variation approach in neutron SAS gives a principal approach to the problem by matching protein environment by double simultaneous contrast variation of protein surrounding and water and choosing proper conditions to avoid inter-protein interference. The aim of the project is to develop the neutron SAS approach to obtain the structures of membrane proteins under physiological conditions.

Large-scale facilities of Joint Institute for Nuclear Research in Dubna and FRM-II in Garching are in use for neutron experiments. The study is focused on four membrane-mimetic systems (vesicles, bicelles, nanodiscs and amphipols) and four membrane proteins – bacteriorhodopsin, sensory rhodopsin II in complex with its cognate transducer, one of human G-protein coupled receptors and the complex of human membrane protein CD4 with HIV-1 viral protein U.

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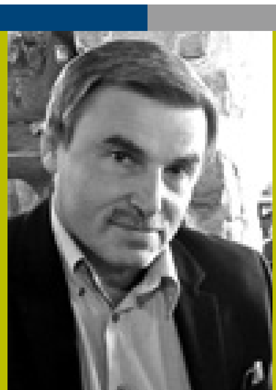

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HRJRG-402

SAPPHIRE ULTRA OPTICS FOR SYNCHROTRON RADIATION

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Project outline

The applicability of nuclear resonance scattering has until recently been limited to elements with a nuclear resonance below 30 keV, prominently iron, but also several rare-earth elements. In a joint effort of the partners at ESRF, Jülich and DESY, the method has been extended to antimony and tellurium, with nuclear resonances above 35 keV, where phonon spectroscopy with 1 meV resolution is now possible, but still not really accessible for general users. A major limiting factor for meV resolved nuclear resonance scattering and other high energy-resolution x-ray spectroscopy techniques is the availability of sapphires that are perfect from the x-ray optics point of view. Currently the only available sapphire that enables this extreme resolution in a backscattering monochromatization scheme has only a few spots with area ~300 x 300 μm^2 that are suitable and a thickness of 1 mm. This project aims at overcoming this limit by providing better sapphires that present both larger areas and most importantly a thickness of at least 3 mm, as required for reaching better resolution and sufficient reflectivity. Achieving this goal will require to explore various growth techniques and conditions, correlating the quality and defects as determined by topographic methods with these conditions, and finally, demonstrating the quality both by achieving sub-meV resolution above 30 keV, extending the inelastic nuclear resonance scattering method to elements with nuclear resonances above 40 keV, and opening this technique for general user operation.

Preliminary results

Crystal growth: improving the resolution of the sapphire backscattering monochromator requires in a first step to develop the methods of crystals growth. In order to investigate the reasons which limit the quality of sapphire crystals, a set of 15 crystals grown by different techniques was prepared. The used growth techniques include the Verneuil, Kyropoulos, Horizontally-directed solidification, and Heat-Exchanger methods.

Characterization: x-ray topography is the technique of choice for controlling the quality of crystals. Laboratory X-ray topography was performed in the A.V. Shubnikov Institute of Crystallography, Moscow, Russia. A layout of the laboratory setup is shown in Fig. 1. Further, white-beam topography was performed on the TOPO-TOMO beam line at the ANKA synchrotron radiation source, Karlsruhe, Germany.

Laboratory topography using Bragg reflection is more sensitive to the defects which lie near the surface, whereas using white-beam topography of higher energy synchrotron radiation defects in the volume of the crystals are more readily observed, such as oblique and helicoidal dislocations. The dislocation density is estimated to be of about 10^2 cm^{-2}. In order to reconstruct the 3D positions of dislocations the diffraction patterns were collected at different angles of the sample, the data analysis is ongoing. The comparison of laboratory and white-beam topograms are shown in Fig. 2. We found that with decreasing growth velocity a lower dislocations density is achieved. The presence of helicoidal dislocations indicates a high quantity of pinhole defects.

In a preliminary beam time at the nuclear resonance beam line P01, Petra III, DESY, Hamburg, the quality of one of the best sapphires was assessed by recording the spectral reflectivity in backscattering geometry with a ~1 meV channel cut monochromator at an energy of ~24 keV, as described in Ref. 1, see Fig. 3. These results are encouraging, as the intrinsic saphhire resolution function is <2 meV for this first batch of crystals, although only on a small area.

In parallel to the sapphire characterization, an experimental setup for future nuclear inelastic scattering measurements using a temperature controlled sapphire as backscattering monochromator was constructed for the P01 beam line at Petra III, DESY, see Fig. 4.

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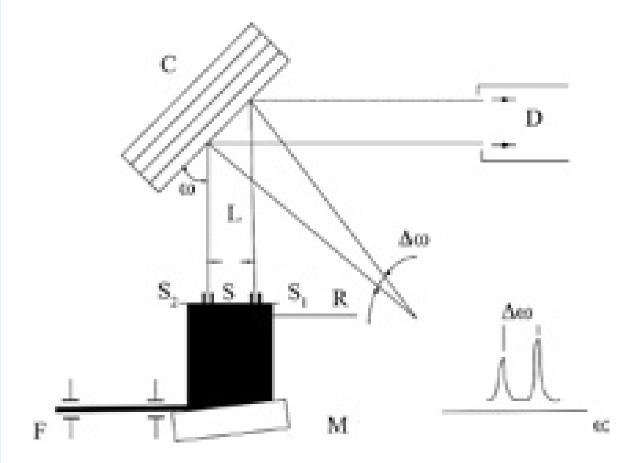

Fig.1. Laboratory setup for X-ray topography: F – X-ray source, M – monochromator crystal, S – slit, C – sample, D – detector. Double-slit mode provides measuring of the sample curvature.

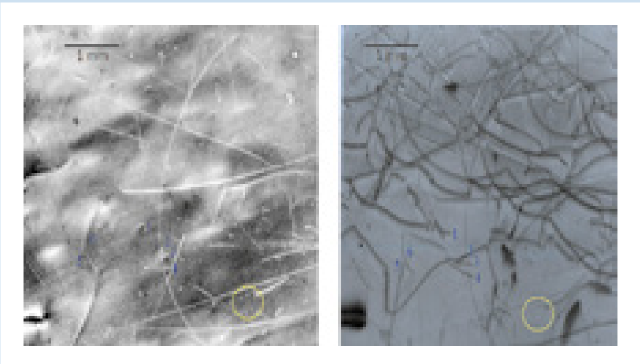

Fig. 2. Left: Laboratory topogram. Right: White-beam topogram. Identical dislocations are marked with blue numbers. Yellow circles also show the same defects.

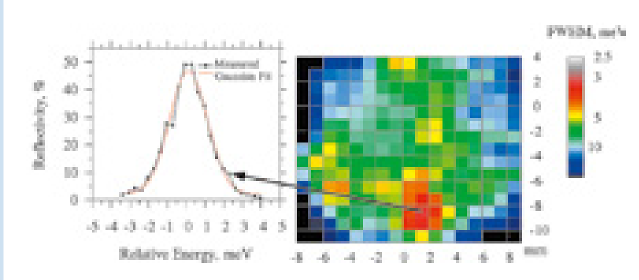

Fig. 3. Left: Backscattering spectral reflectivity measured at 24 keV at the best spot, and, left, map of the resolution function width of a sapphire grown by the Kyropoulos technique. Sapphire dimensions are in mm.

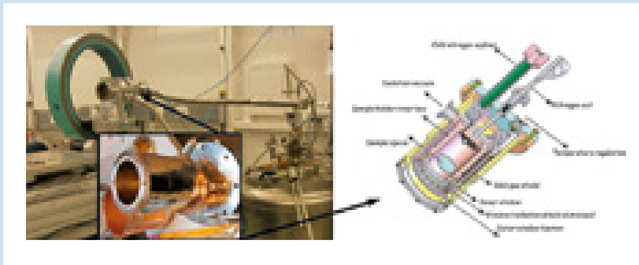

Fig. 4. Left: the housing for the sapphire, see inset, is mounted on a 2-circle Euler cradle and connected to a nitrogen cold gas generator. The sapphire is placed in the housing, see right, where the temperature is controlled with mK precision in order to carry nuclear resonance scattering measurements.

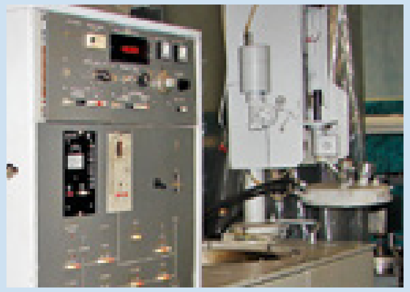

Fig. 5. New growth unit under construction.

Outlook

The immediate next steps in our project involve:

- systematic backscattering topography with meV resolution on the first batch of sapphires. These measurements will be carried out in February 2014 at the beam line ID18 of the European Synchrotron Radiation Facility.
- first tests of the backscattering monochromator at the P01 station of Petra III in January 2014.
- improvement of the growth technique for new batches of sapphires, which mainly involves a precise control of the requested very slow growth velocity that is required, see Fig. 5.

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Project partners

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STRUCTURE OF MATTER

The KArlsruhe TRItium Neutrino (KATRIN) experiment. Image by KATRIN/KIT

HRJRG-002

PHYSICS ANALYSIS AND CALORIMETRY AT THE TERASCALE

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The Helmholtz Russia Joint Research Group HRJRG-002 was approved in September 2007 to promote the scientific cooperation within particle physics and to provide attractive research conditions for young scientists. The program started on the 1st of November 2007 and ended on the 31st of October 2011. On average, the group consisted of 20 members from DESY and the three Russian Institutes.

Goals and achievements of the group

The Helmholtz-Russia Joint Research Group HRJRG-002 continued the long-lived and very fruitful cooperation between DESY and Russian Institutes beyond the common efforts for experiments at the electron-proton collider HERA at DESY, physics and detector R&D towards new activities at the proton-proton collider LHC at CERN in Geneva and for a future electron-positron linear collider (LC). Within the project excellent young scientists and students were supported and opened the possibility for a future career. All participating young PhD students achieved an attractive position in internationally recognized institutes. With the sound basis originating from the HRJRG the contributing PIs and group leaders were able to accomplish further career steps, for example, becoming deputy spokesperson of the international CMS Collaboration counting ~4.300 members.

The combination of physics and detector activities pursued in this Joint Research Group made the project extraordinary and exceptional. The basis of the project was provided by the profound experience in detector operation and physics analysis collected at HERA. The gained knowledge flowed directly into an imminent project at LHC and provided input to the projects for the future linear collider LC. For this healthy project future prospects were opened by closely relating physics, experiment and the development of novel technologies for the next generation of colliders.

HERA & Phenomenology:
The results of HERA on the structure of the proton, the underlying event, multi-parton interactions and dependencies of several QCD processes provide crucial input for discoveries as, for example, the Higgs-boson, for searches for new physics phenomena as well as precision studies at the LHC to achieve sufficient accuracy and significance. The understanding of the HERA results with their consequences for the LHC needed and still do need a strong effort in phenomenology. The studies for the physics analyses, requiring significant computing, were performed at the Tier 2 centers in Russia and at DESY as well as at the National Analysis Facility at DESY.

The analysis of HERA data progressed with a new ansatz for a fit of the proton parton density functions. These new, so-called un-integrated, parton density functions are now regularly employed for simulations of physics processes at the LHC. The novel CMS data have been compared with predictions of the production of forward jets using these parton densities and now open the possibility to determine the parton densities with much improved precision.

Phenomenological calculations and studies have been performed for various physics processes at HERA, the Tevatron and the LHC, for example the production of prompt photons and W- and Z-bosons. These processes are most important standard candles in particle physics and are employed to validate the detector performance and calibration and to prepare the basis for the discoveries. The strong activity within phenomenology is proven by the impressively large number of publications with the results produced during the time of this HRJRG-002.

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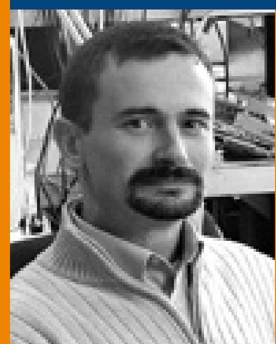

CASTOR & LHC:
The correct extrapolation of HERA results into the kinematic regime of the LHC needs input of initial data with a special hadron calorimeter in the forward region. Members of the project participated in the construction and operation of this calorimeter, named CASTOR, cultivated skills obtained at HERA and developed further knowledge in detector operation.

The efforts for the forward calorimeter in the CMS Experiment at LHC were pretty exciting and challenging. Only this Helmholtz-Russia Joint Research Group enabled the participation of DESY, MSU and ITEP in this project. The expertise flowing with these group members into the project was well appreciated by the CMS Collaboration, expedited the project considerably and in the end made it possible to be ready just in time albeit its start at a very late stage. First physics measurements of the energy flow in this novel kinematic regime as well as calibration and performance measurements with test beams at CERN have been published. During the time of the HRJRG-002 a new synergy with cosmic ray shower physics within the Helmholtz Young Investigator Group VH-NG-733 at KIT was developed and bears excellent fruits.

HCAL & LC:
One mainstream activity for a detector for a future linear collider involving both DESY and the participating Russian institutes is the development of a hadronic calorimeter. A novel technology was invented in Russia, for its readout based on solid state photo-sensors, the so-called SiPM. It is mandatory to strongly pursue its optimization to keep the leading position in this successful development. Beside this novel technology new reconstruction algorithms for hadronic energy deposition were developed and are still optimized employing the test beam data taken in different campaigns at CERN and FNAL.

Following the success of the first calorimeter prototype based on SiPMs, which was built by DESY and the Russian partners ITEP and MEPHI, the emphasis in the HRJRG-002 was on consolidating the technology, especially optimizing the layout of the scintillator tile read out, and exploiting the data collected at CERN and Fermilab test beams.

As a result, the calorimeter performance and simulation were validated, and a detector integration concept was developed, which represents a competitive option for a linear collider hadron calorimeter. It is thanks to this effort that the particle flow concept is now considered as being experimentally and technologically established. A proof of the successful work for the R&D is the fact, that also the experiments at LHC took note and employ the technologies for their upgrades. For example, in the CMS experiment the HCAL will be improved by changing the photon-detectors into SiPMs, the first part is already installed. For the future upgrade at even higher luminosities after ~2.022 calorimeters enabling the particle flow ansatz are the presently favoured option.

Conclusion

In summary, the activities of the group were centered around the development of experiments in high energy physics from HERA towards the LHC and the LC. The performed HRJRG-002 was tailored to allow efficient participation in this programme by selecting a few important key topics, where crucial expertise of participating Helmholtz and Russian institutes were brought in and further developed. Conducting the activities of the HRJRG as originally proposed strengthened the role of the participating Russian institutes and DESY in particle physics. The acquired experience provides the basis for a sustained, long-term participation in fore-front experiments of particle physics.

Acknowledgement

The members of the HRJRG-002 are very grateful to the Helmholtz Association and the Russian Foundation for Basic Research for providing such a successful funding support to intensify German-Russian collaborations and to foster excellent young scientists.

HRJRG-002 Participating Institutes:

- Deutsches Elektronen-Synchroton. DESY, Hamburg
- Institute for Theoretical and Experimental Physics, ITEP, Moscow
- Moscow State University, MSU, Moscow
- Moscow Engineering Physics Institute, MEPHI, Moscow

Group Members of the HRJRG-002:

- Principle Investigator (Germany): Dr. Kerstin Borras (DESY)
- Principle Investigator (Russia): Dr. Roman Mizuk (ITEP)
- Group Leaders: Dr. Felix Sefkow (DESY), Prof. Dr. Michael Danilov (ITEP), Dr. Michael Merkin (MSU), Prof. Dr. Boris Dolgoshein (MEPHI)
- 1 Key Researcher at DESY, 1 Key Researcher at ITEP
- 2 Post Doctoral Fellows at DESY, 2 Post Doctoral Fellows at MSU
- 3 Graduate Students at DESY, 3 at ITEP, 1 graduate student at MEPHI and 1 at MSU

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HRJRG-016

MAGNETIC NANOPARTICLES FOR BRAIN CANCER TREATMENT

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Cancer remains one of the most widespread diseases and leading cause of death worldwide, despite a certain progress in diagnosis and treatment methods in recent years. During last decade researchers have been investigating the applications of colloidal particles (or nanoparticles) that could act as delivery systems for targeted cancer drugs. The nanoparticles with radii between 1–10 nm provide large specific surface for functionalization (e.g. chemically active substances interacting with cancer cells). Along with it, if the magnetic nanoparticles are used, then, their transport and concentration in a given place can be additionally controlled by an external magnetic field, thus increasing the efficiency of the treatment and avoiding the spread of the nanoparticles in healthy tissues in the organism. Moreover, new possibilities for employing magnetic properties of the particles in medical diagnostics (magnetic resonance tomography) and therapy (magnetic hyperthermia) of cancer tumors appear.

The work of our Helmholtz-RFBR JRG (2007–2010) dealt with the study of magnetic nanoparticles with respect to their use in the treatment of brain cancer (glioblastoma). Biomedical applications require the magnetic nanoparticles to be placed in liquid conditions. The corresponding systems are known as magnetic fluids (or ferrofluids). For colloidal stabilization of magnetic fluids, the particles are coated with special shells of surfactants or polymers. The choice of the ferrofluids with the double sterical stabilization of nanomagnetite by short mono-carboxylic acids (lauric and myristic acids) as a source of magnetic nanoparticles for brain cancer therapy in humans was justified. The structure research and development of the synthesis resulted in record concentrations of magnetite in aqueous ferrofluids (up to 10 vol. %), which maintain their stability well in biological media. The presence of separate (non-aggregated) particles was shown for these systems. As a consequence, during in-vitro experiments a good penetration capability of magnetite nanoparticles with respect to cancer cells of glioblastoma has been revealed. The distribution of absorbed magnetite inside the cells was studied, which showed that nanoparticles are preferably adsorbed to karyons. It was proved that magnetic nanoparticles manifest low cyto-toxicity with respect to health brain cells (astrocytes) and moderate cyto-toxicity with respect to glioblastoma cells. With the help of a specialized magnetic unit the effect of an external magnetic field on the migration properties of the cells with incorporated magnetic nanoparticles in a physiological medium was studied. It was observed that the incorporated nanoparticles slow down the migration (increase in the tumor effective area) in the absence of the external magnetic field. When a static gradient magnetic field (strength of up to 170 mT, gradient of about 40 mT/cm) is on, a preferable migration towards the field increase takes place. A part of the cells migrating in this direction is at the level of 80–85%. The possibility for using gradient magnetic fields to control the cell migration in the case of glioblastoma cancer with incorporated magnetic nanoparticles was concluded.

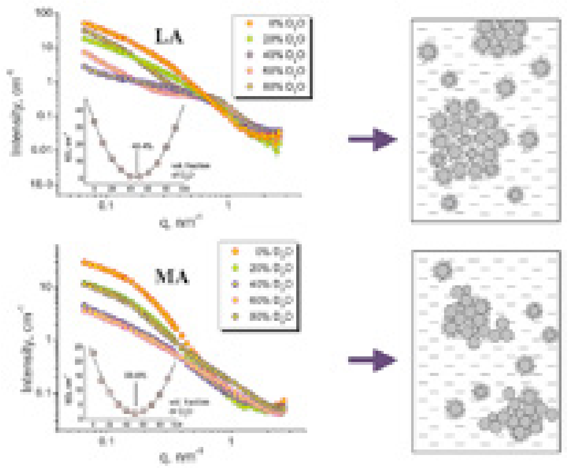

Figure 1. SANS contrast variation for 1% biocompatible aqueous magnetic fluids with magnetite coated by double layer of lauric (LA) or myristic (MA) acids. Changes in the scattering curves are followed when varying the content of heavy water (D2O) in the solvent. In insets the effective match points are found from the change in the forward scattering intensity. The revealed aggregation structures in the studied magnetic fluids are schematically shown to the right.

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Figure 2. Participants of BIOFC Workshop, HZG, January, 2010.

From the viewpoint of biomedicine, first of all, magnetic fluids should be considered as media for synthesis, storing and functionalization of magnetic nanoparticles. At the moment, there are several ways to stabilize water-based ferrofluids, but what concerns the biological media it is not possible to prevent aggregation completely. In biomedical context the formation of aggregates has side effects relating to the difficult elimination of nanoparticles from organisms, the possible appearance of blood clots, as well as the reduce in the therapeutic efficiency. Thus, the knowledge of aggregation regimes in magnetic fluids is a key point for their development in biomedical applications. In this connection, the important goal is a reliable diagnostics of aggregation and determination of the aggregation regimes and their control in biocompatible magnetic fluids.

For this purpose we developed the method of small-angle neutron scattering (SANS), which is quite sensitive to the aggregation processes in nanosystems. SANS is actively applied in structure research of magnetic fluids. The wide possibilities of the contrast variation (hydrogen/deuterium isotopic substitution) in neutron experiments allow us to 'look' inside the aggregates. Taking into account the complexity of magnetic fluids (which are mostly polydisperse), reasonable tasks for SANS in this case are to find out the type of aggregates formed in them under different conditions, conclude about their inner nuclear as well as magnetic structures, and obtain information about interaction between their different components.

Different aggregate classes depending on the stabilization mechanism (steric, electrostatic and steric/electrostatic stabilization) of magnetic particles (magnetite) in physiological conditions were studied. In Fig. 1 example of the SANS contrast variation application is given for water-based magnetic fluids used as a source of magnetic nanoparticles in the therapy of the brain cancer glioblastoma. These fluids are characterized by record achievable concentrations of magnetic material (up to 10 vol. %) with keeping high stability. The systems were synthesized basing on the coating of nanomagnetite with a double layer of fatty mono-carboxylic acids with short alkene chains, namely lauric (C12) and myristic (C14) acids. Despite the high concentration and long time stability, SANS shows the presence of aggregates in the systems. The contrast variation was achieved by diluting the initial samples to one concentration with different mixtures of heavy and light water. The found effective match points (see insets to Fig. 1) are shifted and show a difference in the composition of the aggregates. Schematic views of the fluid structures in Fig. 1 illustrate the main important conclusion of the analysis: there is a different rate in the surfactant coating of the particles in the aggregates, which is consistent with the longer chain of myristic acid. Among the studied systems in this way are water-based magnetic fluids with substitution of sodium oleate as surfactant by biocompatible polymer polyethyleneglycol at the magnetite surface, which aims at the increase in the life time of magnetic nanoparticles in living organisms by reducing the response of their immune systems. It was revealed that quite large amounts of polymer in the fluid structure results in a decrease in the aggregation stability, thus requiring an optimal polymer content to be chosen.

As a result of the project, the workshop on "Structural aspects of biocompatible ferrocolloids: stabilization, properties control and application" (BIOFC) was held in Geesthacht on January 28–29, 2010 (Fig. 2). It gathered together not only the participants of the Group but also a number of researchers on closed topics from various centers of Europe and Russia. It opened up a tradition of holding BIOFC workshops on a regular basis and was followed by the meetings in Dubna (Russia) on August 19–21, 2011, and Košice (Slovakia) on August 25–28, 2013.

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HRJRG-106

DEVELOPMENT OF A HIGH ENERGY ELECTRON COOLER FOR HADRON PHYSICS EXPERIMENTS AT COSY AND HESR

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Precision ion beams are the ultimate tool for gaining new insights into hadron physics in the multi-GeV range. For example, experiments on hadron-induced reactions close to the threshold energy require ion beams with the lowest possible transverse and longitudinal phase space. COSY was successful in these areas with its electron cooling in the low energy range and complementary stochastic cooling in the high energy range. For future experiments, however, decisive limitations of existing experimental possibilities will become clear. Investigations into rare reactions will require a significant increase in luminosity. This can only be realized with other target techniques, for example the use of pellet targets. Such high-density targets consist of small micro-spheres (pellets) of frozen hydrogen (diameter 20–40 micrometers), and allow COSY's luminosity for internal experiments to be increased by more than one order of magnitude. However, the existing stochastic cooling is not in a position to compensate for the expected increased heating of the circulating beam using such targets, which means that the use of new targets would be counteracted by faster beam losses.

That is why the completely new high-energy cooling system was developed for ion beams in the COSY ring. Together with the use of high-density targets, the method is intended to considerably increase the counting rate for studies on rare processes. Successfully implementing such a method is the only means of significantly reducing statistical errors in all experiments. At the same time, reducing the beam halo will considerably improve the data quality of future experiments.

The research and development projects connected with establishing this method of electron cooling and experience in using this type of cooled GeV proton beam represent a decisive milestone for the future utilization of cooled precision beams. Along with the expansion of the experimental possibilities at COSY, this step can also be taken as an essential preliminary stage in the implementation of high-energy electron cooling (8 MeV) at the HESR storage ring, at the future FAIR facility.

The idea of the electron cooler was proposed by the G.I.Budker in 1967 (Budker Institute of Nuclear Physics, Novosibirsk, Russia). The basis of the electron cooler process is the interaction of a "hot" ion beam circulated in the storage ring with a "cold" electron beam. The both beams move together along the special section of the storage ring. This method is widely used in the world for improving parameters of the ion beams. From 1988 the large number of the electron coolers was constructed in the different scientific centers LEAR, IUCF, TSR, CELSIUS, TARN-II, ESR, CRYRING, ASTRID, COSY, FNAL. The Budker Institute of Nuclear Physics produced 5 coolers for Germany (2), China (2) and LHC (1). Scientific collaboration with Germany on the electron cooling technology started from the first experiments with cooling at Novosibirsk. Later the electron cooler was made at Darmstadt laboratory GSI by German specialists. This cooler is in the operation up to now and is used for accumulation of rare ions at synchrotron ESR. In 1996 an additional new cooler was designed at BINP and installed at main synchrotron SIS-18. In 2013 the first cooling experiment was started on new 2 MeV cooler at synchrotron COSY.

The feature of the electron cooler for COSY is a combination of the wide energy range for operation and the high value of the maximum energy. After stopping FNAL electron cooler, the COSY cooler becomes the highest energy electron cooler. The production of the electron cooler for COSY requires solving many physics and technical tasks: high-voltage accelerator column with longitudinal magnetic field, the optics of the electron beam in the longitudinal magnetic field in wide energy range, the high-vacuum technology, the transportation of energy to devices located at high potential, the control system of large number of devices inside high voltage tank et al.

The schematic design of the setup is shown in Fig. 1. The electron beam is accelerated by an electrostatic generator that consists of 33 individual sections connected in series. Each section has two high-voltage power supplies with maximum voltage 30 kV and current 1 mA. The electron beam is generated in electron gun immersed into the longitudinal magnetic field. After that the electron beam is accelerated, it moves in the transport line to the cooling section where it will interact with protons of COSY storage ring. After interaction the electron beam returns to electrostatic generator where it is decelerated and absorbed in the collector.

During the COSY cooler project the following milestone was achieved. The manufacturing of the 2MeV cooler components was completed. The 2MeV electron cooler was assembled at BINP for electron beam commissioning. Required vacuum conditions in the cooler were achieved. High voltage and electron beam test was done. Electron gun perveance was measured and found in good agreement with computer simulations. Optical system of the scintillation profile monitor (SPM) at COSY was improved. Comparison measurements with SPM and IPM were performed, the results are in good agreement. The 2MeV electron cooler was assembled and commissioned at FZJ in COSY storage ring (see Fig. 1.). Figure 2 shows the participants of the celebration of the first cooling process in COSY ring.

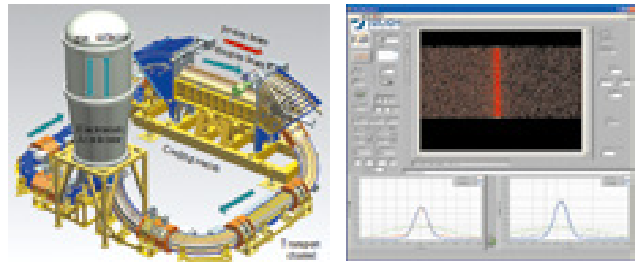

Figure 1: 3D design of 2 MeV COSY cooler. Shrinking of the proton beam profile at the electron cooling process.

Figure 2. Celebration of first cooling process in the COSY storage ring (Vsevolod Kamerdzhiev, Mao Lijun, Maxim Bryzgunov, Vladimir Reva, Dmitry Skorobogatov, Mikhail Kondaurov – stand from left to right, Juergen Dietrich, Vasily Parkhomchuk – sit from left to right).

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HRJRG-112

EXPERIMENTAL STUDY ON WARM DENSE MATTER BY INTENSE HEAVY ION BEAMS

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The Joint Research Group consisted of members from the Institute for Theoretical and Experimental Physics (ITEP, Moscow), Institute of Problems of Chemical Physics (IPCP, Chernogolovka), Joint Institute of High Temperatures (JIHT, Moscow), Technical University Darmstadt (TUD, Darmstadt) and GSI Helmholtzzentrum für Schwerionenforschung (GSI, Darmstadt).

The group aimed to study fundamental properties of high energy density (HED) matter using intese ion and proton beams available at two accelerator facilities – SIS-18 at GSI and TWAC at ITEP. Experimental investigations on the thermodynamic and transport properties of various materials in HED states were carried out. In particular, new experimental data has been obtained on thermophysical and transport properties such as heat capacity, thermal emission, optical reflectivity and electrical conductivity of refractory metals (tungsten and tantalum) during melting and in hot expanded liquid states as well as of other elements in the near and super-critical states, and spectroscopic studies on beam-induced light emission from dense gas targets relevant to the problem of transverse diagnostics of intense focused heavy ion beams have been performed. This data has been collected during a number of joint beam time experiments at GSI (over 700 hours of beam-on-target) as well as at ITEP.

HRJRG has developed, commissioned and applied sophisticated diagnostic instruments and methods for measuring basic physical parameters of warm dense matter (WDM) under the specific conditions of ion-beam heating. This includes fast radiation pyrometry with emissivity measurements, interferometric techniques for precision measurement of target velocity, volume and pressure, backlighting and schlieren methods using different photon sources for characterization of the hydrodynamic response of the on-beam heated matter and methods for transverse diagnostics of intense strongly focused heavy ion beams.

The group has also designed and constructed a worldwide unique facility for high energy proton microscopy (HEPM) experiments – PRIOR (Proton Microscope for FAIR). HEPM is a novel technique in HEDP and WDM research for probing the interior of dense objects by mono-energetic beams of GeV-energy protons. HEPM also has a great relevance for biophysics, medicine and industrial applications. Two international workshops on HEPM have been organized by the group in Germany and in Russia.

The activities of HRJRG have secured the essential basis for the future HED physics experiments that are planned at the future Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany. Several PhD students and young researchers both from Russia and Germany have been supported. Three PhD works have been completed within the framework of the project. The group has promoted frequent visits of young Russian researchers to GSI where they were gaining a unique experience of joint scientific work at a high international level.

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HRJRG-214

CONTROL OF NON-LINEAR PHASE SPACE DILUTION AND BEAM LOSS IN AN ENERGY RECOVERY LINAC: THE WAY TO SHORT HIGH INTENSITY AND LOW EMITTANCE ELECTRON BUNCHES

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The group uses synergies between the laboratories of the Budker Institute of Nuclear Physics (BINP), Novosibirsk, Russia and institutes of Helmholtz Zentrum Berlin (HZB) für Materialien und Energie, working in the field of Energy Recovery Linacs (ERL). The research topics include

- Operational issues of the Novosibirsk ERL and Free Electron Laser (FEL), including design and diagnostics of the 4-turn ERL
- Operation of high brilliance electron sources
- Design of the accelerator for the Berlin Energy Recovery Linac Project (BERLinPro)
- Design of the future ERL-based synchrotron light sources: Multiturn Accelerator-Recuperator Source (MARS) and Femto-Science Factory (FSF)

In the following a short summary of results achieved during 2011–2014 is given.

Radio-Frequency electron sources at BINP and HZB

Assembling and commissioning of the NovoFEL radio-frequency (RF) gun test facility was finished. The nominal accelerating voltage 300 kV at RF cavity of this gun and average electron beam current 40 mA were obtained. The diagnostics beam-line was developed and assembled, and the first experiments with electron beam have started.

Two prototypes of superconducting RF gun were commissioned at HZB [4,5,9,13,16]. The beam parameters were measured. To explain the obtained data, numerical modeling of the electron emission process from the cathode surface and from the micropoints located in the vicinity of the cathode was carried out. It was shown that the main reason for the emittance dilution is the roughness of the cathode surface [15]. The processes of the dark current formation and micropoints heating were also investigated. Based on this research the new method of superconducting RF cavities processing was proposed. Beam stability in the SRF gun cavity was studied [2].

Cathode insert design for a Superconducting Radio Frequency (SRF) gun cavity

Future light sources based on the energy recovery linac (ERL) require high brightness high current electron sources. A source meeting these requirements is the superconducting radio-frequency (SRF) photoinjector under development at Helmholtz Zentrum Berlin. The gun consists of a normal-conducting photocathode with high quantum efficiency grown on a cathode plug embedded inside a SRF gun cavity. The photocathode must be thermally and electrically insulated from the SRF cavity. A special photocathode insert was designed and built [14] to allow transfer of plugs into the gun cavity. Another task of the cathode insert is to carry away the heat power induced by RF fields and the drive laser on the cathode. Liquid nitrogen is used for cooling.

In order to test different contact and holding methods for the cathode plug on the cathode insert the thermocontact experiment was set up. Temperature and cooling performance measurements at heat loads of up to 10 W of power at significant points in the system were performed. The heating power can be introduced into the system either by Kapton foil heater glued to the cathode plug or with a high average power laser. The setup is now under commissioning.

Dark current measurements in the SRF guns

ERL projects rely on effective beam collimation to avoid dark current and beam tails losses in the accelerator. Collimator design for the injector of BERLinPro was proposed. The dark current measurements were done for BERLinPro prototype guns [11].

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Figure 1. Normal conducting RF gun at BINP. Image by BINP

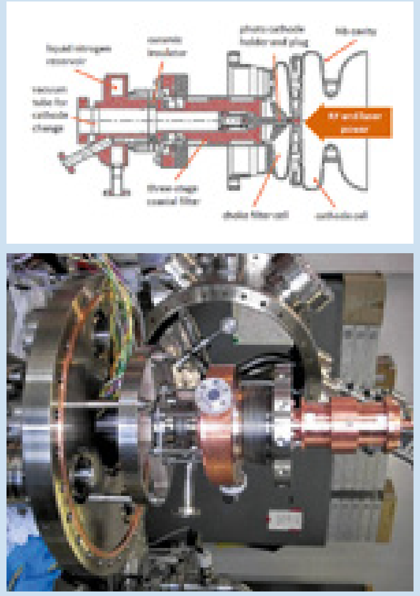

Figure 2. Insert design (above) and photo of the insert in the thermal test stand (below). Image by HZB

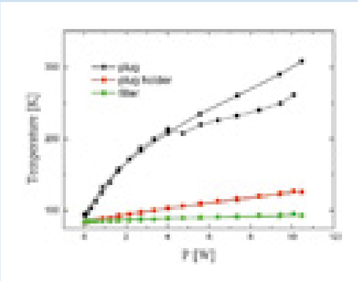

Figure 3. Results of temperature measurements of cathode plug with heater foil. Image by HZB

Magnetic optics design for short pulse ERL operation

Modelling and optimization of the optic for NovoFEL and BERLinPro with the focus on the short pulses was done. Beam dynamics simulations including space charge effects [3,7,10], coherent synchrotron radiation, and non-linear fields were carried out [6]. Beam parameters were measured at NovoFEL and compared with the simulation results. The lattice of the second order achromatic bend was calculated. For these calculations the measured magnetic field distribution was used. 5 mA average current in the 4-turn operation was achieved, that is the world record for multi-turn ERLs. Based on the simulation and measurements results BERLinPro magnets design was done [6].

Design of future ERL-based synchrotron light sources

Feasibility studies of the 4-th generation SR source based on the multiturn ERL with separate tracks for accelerating and decelerating beam were done by both teams at Novosibirsk and Berlin. The MARS [8] and FSF [12] projects are both in the phase of conceptual design preparation. Essential parts of the design were done in the framework of the joint research group.

The project of the compact ERL based free electron laser for the ultraviolet region was considered by the teams [1].

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HRJRG-303

MEASUREMENTS OF GAMMA RAYS AND CHARGED COSMIC RAYS IN THE TUNKA-VALLEY IN SIBERIA BY INNOVATIVE NEW TECHNOLOGIES

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The measurement of the high-energy particles arriving at earth from the cosmos provides a crucial observational window to the most energetic and violent processes in the Universe like Supernova explosions, Gamma Ray Bursts, or Merging of Galaxies. To considerably improve the accuracy of these measurements, two new technologies are presently developed within the project in the Tunka Valley located 50 km off Lake Baikal in Siberia. These two techniques are new generation wide-angle air Cherenkov detectors and recently developed radio antenna for measuring cosmic rays. Both detectors are deployed in the Tunka facility in Siberia and operate together with the established Tunka-133 air shower array. The development of these techniques extends the observational potential of high energy gamma ray and cosmic ray experiments and will allow to address the most intriguing problems of physics, including dark matter, quantum gravity and the evolution of our Galaxy.

Beyond its original objectives, this HRJRG already after its first year initiated a new quality of German-Russian collaboration in astroparticle physics: the HRJRG-driven prototype designs triggered the TAIGA-project at Tunka, that is based on a successfull Russian MEGA-Research Grant, awarded to a group headed by a leading scientist from the German Max-Planck-Institute.

Introduction

Gamma-ray astronomy is a rapidly developing area with many impressive results and a huge impact to fundamental physics. A number of high-performance instruments including satellites and Cherenkov Telescopes are operating today. While about 100 of sources are observed at energy higher than 1 TeV, no single photon has been detected above 100 TeV. The latter energy region is of primary interest for both astrophysics and fundamental physics. Uncovering this new energy window will enable us to:

- identify the most energetic cosmic objects;
- test physical processes at energies non-achievable in man-made laboratory experiments;
- study candidate particles for the mysterious dark-matter such as the axion-like particles;
- search for a decay of superheavy dark matter.

The goal of the project is to develop and test two new experimental techniques which will improve the sensitivity of cosmic-ray and gamma-ray observations: next-generation air-Cherenkov detectors and the radio technique. The Tunka facility in Siberia provides a world-wide unique environment for the deployment of these innovative detectors. It provides the required infrastructure and at the same time it is the location of the Tunka-133 array. The latter consists of state-of-art detectors which are used in the project as a well-established reference for tests of the new detectors.

Tunka-HiSCORE – the next-generation air-Cherenkov detector

The question of the origin of cosmic rays remains unsolved, even after a century of observations. If cosmic rays are indeed accelerated up to 10^{17} eV inside our Galaxy, there must exist Galactic "pevatrons" which emit gamma-rays and neutrinos at energies around 100 TeV and up to few PeV. The main motivation for HiSCORE is the search for the origin of cosmic rays and, more specifically, the search for cosmic ray pevatrons in the gamma-ray regime. At the same time, HiSCORE will be a valuable cosmic ray detector. Furthermore, HiSCORE will also provide the possibility to address fundamental questions of particle physics using air-shower data, like a search for axions in the Galactic magnetic field and for superheavy dark matter, and a search for Lorentz invariance violation.

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Figure 1: A Tunka-HiSCORE Cherenkov detector station, one of the nine stations operating since October, 2013 in Tunka. Design and construction were made in close collaboration between Russian and German groups.
Image by DESY

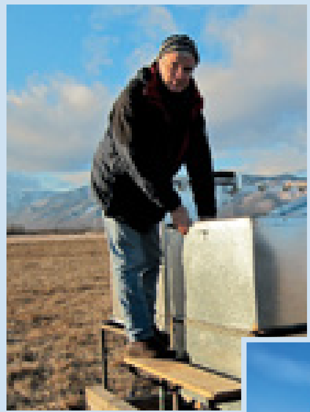

Figure 2: R.Wischnewski mounting electronics components for the HiSCORE prototype station.
Image by DESY

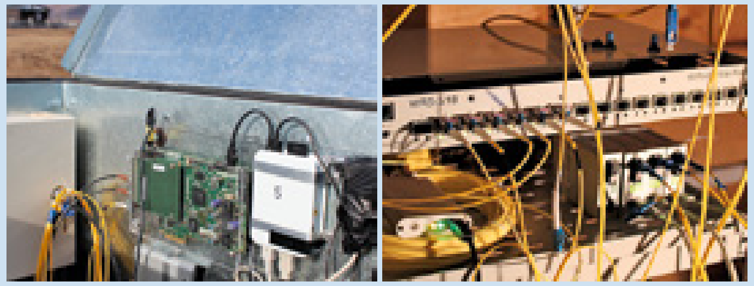

Figure 3: Nanosecond-Timing Units (White Rabbit) installed in HiSCORE stations (upper) and in the counting room (lower). Image by DESY

Figure 4: G. Rubtsov mounting antenna station, October 2012.
Image by INR

With HiSCORE, we are pursuing the concept of non-imaging air Cherenkov astronomy, based on the collection of Cherenkov photons from air showers on the observation level using wide-angle detector stations. The non-imaging technique allows to build a detector with a large field of view and to equip very large areas with a relatively small number of photosensors. In the case of HiSCORE as described here, only of the order of 200 sensors/km^2 are necessary. As opposed to that, a typical imaging air Cherenkov telescope array comes along with 10.000 data channels/km^2. Therefore, the non-imaging technique is well suited to detect ultra-high energy gamma-rays, for which huge detector areas are most important.

Design and construction of the wide-angle Cherenkov gamma-ray observatory Tunka-HiSCORE to study gamma-quanta fluxes from known galactic sources and unknown new sources is advancing well. The detector stations are placed at distances of 150 m from each other and are made of four photosensors (PMTs) with large area photocathodes (~20–30 cm in diameter), see fig. 1. The effective area of each PMT in the station is increased by four times by Winstone cones; this in turn decreases the energy threshold by a factor of 2. The observational solid angle is approximately 0.6 sr.

Within the project in 2012–2013 the first 0.1 km^2 area prototype array was built. This array consists of 9 optical stations with 4 PMTs each (see Fig.1), and is in routine operation since October 2013. The next development step is the installation of an 1 km^2 array and then its extension to 10 km^2.

For the Tunka-HiSCORE telescope, the biggest experimental challenge is the precision measurement of the light arrival times at all detector stations, distributed over many square-kilometers. A precision of 1 nanosecond (10^{-9} sec) is required for good angular resolution of gamma sources. For this purpose, typically a huge effort is undertaken by constructing application specific systems. The HRJRG has followed a less cost and labor intensive way – applying with minor modifications a state of art system, that has been developed at CERN for the usage at eg. LHC and is now in its test phase. This "White Rabbit" system (see fig. 3) is based on the well-established ethernet-technology. In collaboration with a young team from Humboldt University Berlin (joining the HRJRG effort in 2012) a full-scale prototype was built and installed within a few months. After a successful verification, White Rabbit is now at the heart of the 0.1 km^2 prototype array. This new technology can be applied also for other detector subsytems planned in the Tunka-array.

We note that the first large-scale installation of White Rabbit in Tunka-HiSCORE also triggered another synergy: DESY is considering to apply this technique also in the large CTA-project.

Tunka-REX radio array

Since the measurements of cosmic rays have reached the theoretical limit for energies, the main challenge for the physics of ultra-high cosmic rays is to increase the statistics and the measurement quality near the Greisen-Zatsepin-Kuzmin energy spectrum cut-off. To obtain a sufficiently large data sample from a detector on the surface of the Earth, we need to build economically reasonable large-area detectors with a high duty cycle. The radio detection method could be one of the perspective techniques for future investigations of ultra-high energy cosmic rays. Radio emission from extensive air showers was theoretically predicted and first detected about 50 years ago. The radio detection techniques became popular in the last decade again, because standard detection methods have reached technological and economical limits. Thus, a number of modern experiments aim at obtaining the main properties of extensive air showers, such as arrival direction, energy, shower maximum, and primary particle using the radio detection technique. These experiments proved that the radio emission can be detected from air showers with energies above 10^{17} eV, with an angular resolution for the arrival direction better than 1 degree. The open question is the precision of the reconstruction for primary energy and shower maximum. The current challenge is to reach a competitive precision with an economic radio array which can be scaled to very large areas.

The Tunka Radio Extension (Tunka-Rex) was deployed in the Tunka valley by this HRJRG. Tunka-Rex currently consists of 25 stations with a typical distance of 200 m, one next to each cluster center of Tunka-133. Each station consists of two crossed SALLA-type antennas to measure two components of the polarization. Tunka-REX is triggered externally by Tunka-133, and detects the radio emission of the same air showers. The combination of an air-Cherenkov and a radio detector provides a facility for hybrid measurements and cross-calibration between the two techniques. The main goal of Tunka-Rex is to determine the precision of the reconstruction of air-shower parameters using the radio detection technique, based on the cross-calibration with an air-Cherenkov detector. Data of both detectors are recorded by a shared data-acquisition system, and the radio antennas are triggered by the photomultiplier measurements.

Tunka-Rex started operation on 8 October 2012 (see Figure 4). Since then it operates within the Tunka-133 trigger, i.e. in dark moonless nights with good weather. As a result of the first year of operation, Tunka-Rex registered 131 events with a significant radio signal from extensive air showers with energies above 10^{17} eV in combination with the Tunka-133 air-Cherenkov array. This shows that the Tunka observatory is able to provide hybrid measurements which is the pre-requisite to perform a cross-calibration between the air-Cherenkov and the radio signal.

Conclusion

The project HRJRG-303 is an effort of young German and Russian researches under the guidance of experienced researchers in the field, started in spring, 2012. A group from Humboldt University Berlin (Informatics) has joined thereafter. Within 2 years, about 25 presentations on 18 national and international conferences were given. Two major results have been achieved so far:

1. A prototype of the new generation wide-angle air Cherenkov detector Tunka-HiSCORE was built and is in routine operation. With 0.1 km^2 instrumented detector area and 9 stations with 36 large area photosensors, the proof can be made that this technology allows to reach precision timing, a superior field of view and an extended energy range, compared to existing setups.
2. The Tunka-REX antenna array is operating since October 2012. The array registered 131 cosmic ray events for an effective measurement time of 392 hours.

The results will clarify the sensitivity and capability of the new detection methods and therefore might contribute to the design of large-scale projects like the next generation cosmic ray experiment AugerNext and the high energy gamma-ray project Cherenkov Telescope Array (CTA).

As next steps we plan the deployment of 1 km^2 and 10 km^2 Tunka-HiSCORE arrays which will allow for physics results and will target the fundamental puzzles of physics, including dark matter, quantum gravity and the origin of the cosmic rays. Moreover, the research may shed a light on the nature of the high energy neutrinos, recently discovered by IceCube detector.

With the specific aspect of this HRJRG group to execute the common research program at a Russian research facility, that had developed over the last 20 years, we are working successfully on optimal research, communication and organizational conditions and development of state of art technologies. HRJRG-303 activities already stimulated a successful application for a Russian MEGA-Research Grant, now linking, in addition to Helmholtz, also a Max-Planck Institute to the Russian research groups. This will help to establish high-energy Gamma-ray astronomy as an active research field in Russia, thus extending the spectrum of astroparticle-physics related research activities.

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HRJRG-400

DEVELOPMENT OF A PHOTO CATHODE LASER SYSTEM FOR QUASI ELLIPSOIDAL BUNCHES AT A HIGH BRIGHTNESS PHOTO INJECTOR

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Introduction

A high brightness electron source is one of the key issues for successful operation of linac-based Free-Electron Lasers (FELs) like the Free-electron LASer in Hamburg (FLASH), and the European X-ray Free-Electron Laser (European XFEL). The Self Amplified Spontaneous Emission (SASE) of the FEL process requires an extremely high space charge density of the radiating electron bunches implying high peak current, low energy spread and small transverse emittance of the electron beam. The latter property cannot be improved in a linac, and thus the emittance has to be minimized already in the injector. The Photo Injector Test facility at DESY, Zeuthen site (PITZ), aims to produce electron bunches with extremely small transverse emittance. Cathode laser pulse shaping is one of the key issues for high brightness photo injector optimization. A flat-top temporal profile of the cylindrical pulses reduces significantly the transverse emittance of space charge dominated beams. As a next step towards further improvement in photo injector performance 3D pulse shaping is considered. An ellipsoid with uniform photon density is the goal of the studies within the framework of a Joint German-Russian Research Group, including the Institute of Applied Physics (Nizhny Novgorod), Joint Institute of Nuclear Research (Dubna) and the Photo Injector Test facility at DESY, Zeuthen site (PITZ). The major purpose of the project is the development of a laser system capable of producing 3D quasi-ellipsoidal bunches and supporting a bunch train structure close to the European XFEL specifications. The laser pulse shaping is realized using the spatial light modulator technique. Laser pulse shape diagnostics based on a cross-correlator is under development as well. Experimental tests of the new laser system with electron beam production are planned at PITZ. First tests on the quasi-ellipsoidal laser pulse shaping are ongoing now.

Beam Dynamics Simulations

3D shaping of photocathode laser pulses is considered as a next step for further optimization of high-brightness photo injectors. Beam dynamics simulations have demonstrated a significant reduction of the transverse emittance of electron bunches produced by applying 3D ellipsoidal laser pulses to the RF photo gun. In order to illustrate the effect of 3D ellipsoidal pulses usage of the electron bunch properties simulated for such laser pulses were compared to results of simulations with cylindrical pulses with Gaussian and flattop temporal profiles. The European XFEL photo injector layout (1½-cell L-band RF gun and the first cryomodule with 8 superconducting TESLA cavities) was used as a benchmark for this comparison. The results of these simulations are shown in Fig. 1 for three above mentioned temporal pulse profiles. There is a clear advantage of the flattop laser pulse (which is currently the nominal pulse shape at PITZ) compared to the Gaussian temporal profile (which is a standard profile worldwide) in terms of projected (–40%), average slice emittance (–24%) and average slice brightness (+51%).

Further significant improvements on the electron beam brightness can be obtained by applying 3D ellipsoidal pulses of the cathode laser. So, the projected transverse emittance from the flattop pulse can be reduced by further ~32%, the average slice emittance by ~32%, the average beam brightness is 77% higher. These advantages of 3D ellipsoid laser pulses motivate experimental studies on such a cathode laser system in order to provide headspace on emittance/brightness required from the electron sources for a successful operation of modern FEL facilities.

Experimental developments on 3D ellipsoid laser pulses

A laser system capable of producing quasi 3D ellipsoidal UV pulses is under development at the Institute of Applied Physics (Nizhny

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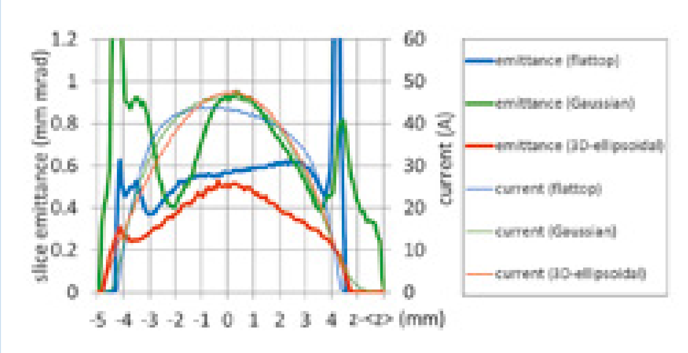


Parameter	Cath. Laser pulse profile		
	Flattop	Gaussian	3D ellipsoid
ε_{proj}, [mm mrad]	0.63	1.05	0.43
(ε_{slice}), [mm mrad]	0.55	0.72	0.40
(B_{slice}), [A ·(mm mrad)$^{-2}$]	135	90	240

Figure 1: Simulated properties of electron bunches in a photo injector for various temporal profiles of the cathode laser pulses applied: flattop, Gaussian and 3D ellipsoid. Left plot represents the normalized transverse slice emittance ε_{slice} distribution along the electron bunch (thick curves, left axis) and the corresponding beam current distributions Ib_{eam} (thin curves, right axis). The table represents the values of the normalized transverse projected emittance ε_{proj}, the normalized average slice emittance (ε_{slice}) and the average beam brightness $(B_{slice})=(I_{beam}/\varepsilon^2_{slice})$.

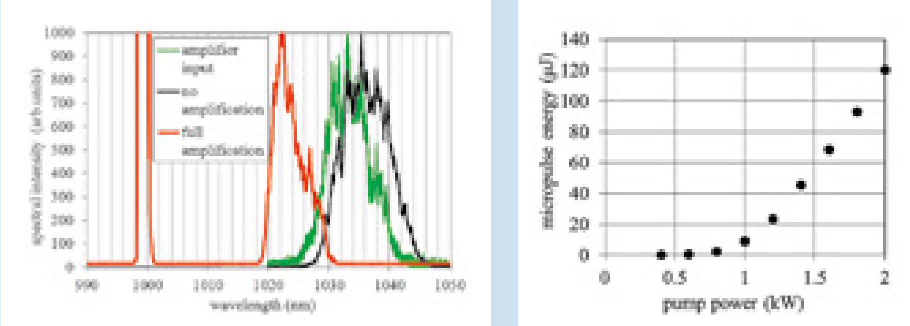
Novgorod, Russia) in collaboration with the Joint Institute of Nuclear Research (Dubna, Russia). PITZ at DESY (Zeuthen site, Germany) is the facility for experimental tests of this system with electron beam production. The laser system consists of a two-channel fiber laser, a diode pumped Yb:KGW disk amplifier, a 3D pulse shaper and frequency conversion crystals for second and fourth harmonics generation. A scanning cross-correlator system was developed and built to measure spatial and temporal distributions of the laser pulses.

The fiber laser oscillator generates 150 fs pulses at 45 MHz repetition rate. It includes a fiber pulse stretcher, a preamplifier and a system for pulse train (macropulse) formation. A piezoceramic cylinder inside the optical fiber coil of the oscillator is used for precise tuning of the pulse timing to the RF phase of the gun. The fiber laser output is splitted into two channels – working and diagnostics. Each channel is supplied with a powerful fiber amplifier. The spectra of both channels are centered at ~1.030 nm and have a width of 11 nm (FWHM). A typical spectrum measured at the fiber oscillator output is shown in Fig. 2a (green curve). The pulses from the working channel are amplified using a multipass Yb:KGW disk amplifier with a diode pump source LDM 2000-100, which was produced by Laserline GmbH. Due to the nonhomogeneous amplification spectrum, the center wavelength is shifted to 1.035 nm. However, in the case of strong amplification the crystal absorption spectrum is being strongly modified and the center line is strongly shifted to 1.022 nm (Fig. 2a). The dependence of micropulse energy after the amplification on the pump intensity is shown in Fig. 2b.

The working channel is used for further amplification, 3D pulse formation and frequency conversion. The pulse shaper is realized on a scheme based on Spatial Light Modulators (SLMs). The principle scheme of the 3D pulse shaper is shown in Fig. 3. The pulse shaper is based on a zero dispersion optical compressor. It consists of two diffraction gratings, two single Kepler telescopes with cylindrical and spherical lenses and two liquid crystal based SLMs. The modulators are located at the focal plane of the telescope made of cylindrical lenses which images one diffraction grating onto the other in the meridian plane (plane of the sketch in Fig. 3a). There is no such imaging in the sagittal plane which implies corresponding diffraction. However, these effects are not substantial for laser beams of 8 mm diameter focused by a cylindrical lens with a 405 mm focus. A telescope with spherical lenses images one SLM onto the other. The first SLM manipulates the phase of the laser pulse. A half-wave plate is installed before the second SLM. This introduces a 45 degree rotation of the laser pulse polarization and therefore the second SLM becomes an amplitude manipulator. The laser pulse is passing through the pulse shaper twice (Fig. 3a). The first pass forms the laser profile in the meridian plane and time, the second pass after a 90 degree rotation is responsible for the pulse shaper formation in the sagittal plane and time.

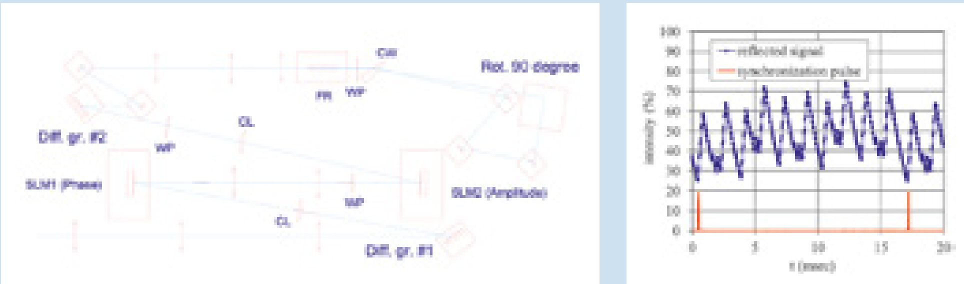
The HES 6010 NIR SLM produced by Holoeye Photonics AG (Germany) is used for the pulse shaper tests. According to the technical certificate, its reflection must not go below 60%. The measurements gave a value of 72% for horizontal polarization, required for the realized diffraction grating. But this value is a result of rather a long-term averaging. At the ms time scale (Fig. 3b) the signal after the SLM acquires a strong noise. This unexpected SLM property complicates the pulse shaping significantly. Different solutions with this SLM (including cooling of the SLM screens and tests with thicker liquid crystal matrix) did not bring significant reduction of the noise. Currently another type of SLM (Hamamatsu X10468-03 LCOS-SLM) with better stability control is under consideration.

The diagnostics channel is used to measure the spatial and temporal characteristics of the pulses generated in the working channel. A high-speed delay line is implemented in this channel in order to realize a high precision 3D pulse shape diagnostics realized in a scanning cross-correlator (SCC). A BBO crystal with 1 mm thickness is used for the nonlinear second harmonic generation from the non-collinear pulses overlap using varying time delays. Fig. 4a illustrates the working principles of the scanning cross-correlator. The major challenge for the SCC development was a high scanning speed determined by the macropulse duration (T=300 µs). A working laser pulse with t_m duration has to be scanned by a short diagnostic pulse of t_d length during the macropulse. Including margins to the working pulse duration implied a measurement window $t_w > t_m$ (Fig. 4a) within which the scanning has to be performed. The minimum time resolution of the SCC is determined by the number of pulses in a macropulse



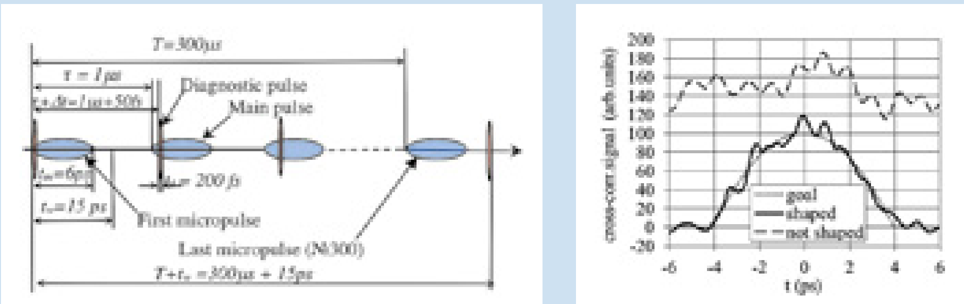
a. b.

Figure 2: a) Spectra of the fundamental harmonics: fiber oscillator output (green curve) and measured w/o (black curve) and with full (red curve) amplification. b) Dependence of micropulse energy (fundamental harmonics) after the amplification on the pump intensity.



a. b.

Figure 3: a) Setup of the 3D pulse shaper: Diff. gr. – diffraction gratings, SLM – spatial light modulator, WP – half-wave plates, CL – cylindrical lens, FR – Faraday rotator, CW – calcite wedge, Rot. 90 degree – rotator of the laser beam by 90 degree. b) Time evolution of the SLM reflectivity. Synchronization pulses from the SLM are shown on top of the horizontal axis.



a. b.

Figure 4: a) Time scheme of the scanning cross-correlator for 3D pulse diagnostics. b) Profiles of the measured cross-correlator function: upper dashed line – no pulse shaper applied, solid line corresponds to the amplitude mask applied to form the quasi-ellipsoidal pulse and additionally a theoretical profile of the ellipsoidal pulse (dotted curve).

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1. V V Zelenogorskii, A V Andrianov, E I Gacheva, G V Gelikonov, M Krasilnikov, M A Mart'yanov, S Yu Mironov, A K Potemkin, E M Syresin, F Stephan, E A Khazanov, "Scanning cross-correlator for monitoring uniform 3D ellipsoidal laser beams", QUANTUM ELECTRON, 2014, 44 (1), 76–82.

2. M. Krasilnikov, M. Khojoyan, F. Stephan, A. Andrianov, E. Gacheva, E. Khazanov, S. Mironov, A. Poteomkin, V. Zelenogorsky, E. Syresin, "DEVELOPMENT OF A PHOTO CATHODE LASER SYSTEM FOR QUASI ELLIPSOIDAL BUNCHES AT PITZ", Proceedings of FEL2013, New York, NY, USA.

3. E. Khazanov, A. Andrianov, E. Gacheva, G. Gelikonov, V. Zelenogorsky, S. Mironov, A. Poteomkin, M. Martyanov, E. Syresin, M. Krasilnikov, and F. Stephan, "Cross-Correlator for the Diagnostics of 3D Ellipsoidal Shaped UV Laser Pulses for XFEL Ultra Low-Emittance Photoinjector," in CLEO: 2013, OSA Technical Digest (online) (Optical Society of America, 2013), paper JTh2A.27.

N=300. A time step of the scanning procedure is $\Delta t=t_w/N=50$ fs. This is an estimation of the lower limit of the time resolution under the assumption of an infinitely short diagnostic pulse.

A simplified 3D pulse shaper setup for quasi ellipsoidal pulse generation was tested using the scanning cross-correlator. Linear chirped laser pulses with 40 ps length and 11 nm bandwidth were used for preliminary experiments. Only the amplitude mask was applied to form the pulse shape. The measured profile of the fundamental harmonic pulse is shown in Fig. 4b. The possibility to utilize a pulse train with 1 MHz pulse repetition frequency and 300 µs macropulse length to characterize picosecond pulses was successfully demonstrated. A time resolution of ~200 fs was achieved for the measurement window of 50 ps. First experiments to generate quasi-ellipsoidal laser pulses were performed.

HRJRG-408

TOPOLOGICAL SURFACE STATES UNDER THE INFLUENCE OF THE EXCHANGE INTERACTION

L. Yashina[1], A. Varykhalov[2], J. Sánchez-Barigga[2], A.A. Volykhov[1], A. Sirotina[1], D. Tsukanova[1], E. Gerber[1], V. Neudachina[1], M.E. Tamm[1], O. Rader[2]

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Topological surface states are a fascinating research subject. They require strong spin-orbit interaction, are highly spin polarized, enjoy protection of their existence by time-reversal symmetry and have promising implications for electrical transport and spin transport. Magnetism, here in the form of the exchange interaction, breaks time-reversal symmetry and therefore should strongly interact with topological surface states.

We have demonstrated that this interaction is not as strong as it was expected. Instead, the combination of magnetic material and topological material can lead to a number of new physical phenomena in addition to band-gap opening at the Dirac point, e. g., the quantum anomalous Hall effect. Since apparently little is known about the strength and spacial range of the interaction of topological surface states and magnetic materials, our concerted study of this subject in various classes of materials includes:

1. magnetic surface impurities and films deposited on topological insulators,
2. magnetic material in the bulk forming a dilute topological insulator,
3. magnetic films on a topological metal,
4. graphene turned magnetic topological insulator by intercalation.

The methods of investigation are ARPES, spin-ARPES and spin-PEEM as well as XMCD and the project integrates essential expertise by chemists (Prof. L.V. Yashina group) and surface scientists (Prof. A.M. Shikin group) and brings along multiple research opportunities for young scientists from Berlin, Moscow, and St. Petersburg.

We studied the effect of Fe impurities deposited on the surface of the topological insulator Bi_2Se_3 and Bi_2Te_3 by means of core-level and angle-resolved photoelectron spectroscopy. The topological surface state reveals surface electron doping when the Fe is deposited at room temperature and hole doping with increased linearity when the Fe is deposited at low temperature (8 K). We show that in both cases the surface state remains intact and gapless, in contradiction to current belief. The topological surface state of Bi_2Te_3 leads to high photoemisson intensity from its Dirac point. This allows us to investigate the effect of larger amounts of deposited Fe than previously achieved for Bi_2Se_3. The Dirac point is shown to stay intact up to at least a monolayer showing the robustness of the topological state towards disordered magnetic moments [1]. Our results suggest that the surface state can very well exist at functional interfaces with ferromagnets in future devices.

In collaboration with the Institute of Solid State Chemistry RAS (Prof. M. Kuznetsov) we studied the structure of Fe/Bi_2Te_3 interface from atomic level to submicron scale. At the atomic level interface reactions are observed. Adatoms relax strongly into the Bi_2Te_3 lattice and form chemical bonds both with Bi and to Te. Adatoms further react to substitute Bi, which is promoted by temperature. In addition to adatoms, iron clusters are formed, whose density increases drastically at higher coverage and/or deposition temperature. We found dominating clusters of 0.6–0.7 nm (i.e. ~3 atomic layers of Fe) high and ~2 nm wide and islands in their lateral dimensions. According to the DFT results for the system with three iron layers, the chemical interaction decreases compared to adatoms due to the Fe-Fe bonds formation. The clusters are randomly distributed over the surface. However, according to the X-ray photoelectron diffraction data, the ordered structure is formed at the interface, which includes interstitial and surface Fe atoms. Complete surface coverage is realized between 1 and 2 ML. Iron atoms react chemically with Bi_2Te_3 for all considered

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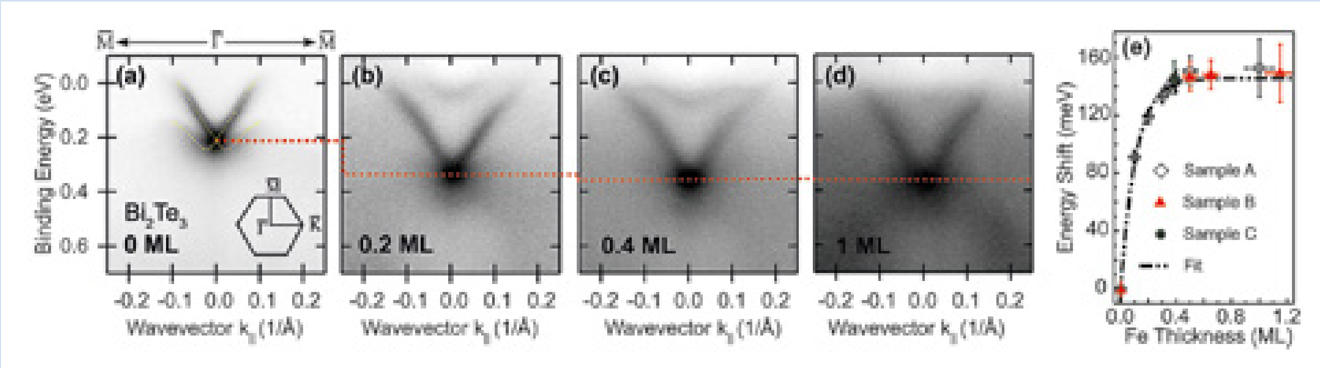

Figure 1. Behavior of the topological upon Fe deposition on Bi2Te3 surface. ARPES data (a-d) show the clean surface and increasing Fe coverage. At about 0.4 monolayer the doping reaches saturation (e).

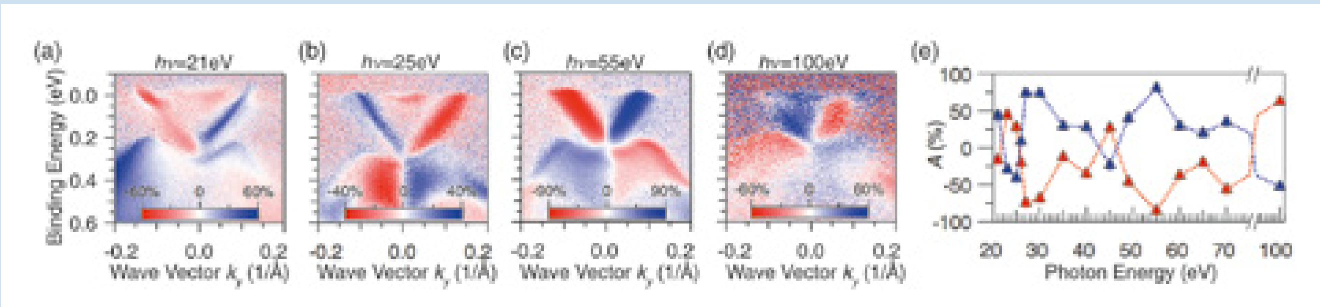

Figure 2. Change of the circular dichroism effect with photon energy – ARPES data

structure (with exception of thick surface layers), forming chemicals bonds to both Bi and Te.

The helical Dirac fermions at the surface of topological insulators show a strong circular dichroism which has been explained as being due to either the initial-state spin angular momentum, the initial-state orbital angular momentum, or the handedness of the experimental setup. All of these interpretations conflict with our data from Bi_2Te_3 which depend on the photon energy and show several sign changes. Our one-step photoemission calculations coupled to ab initio theory confirm the sign change and assign the dichroism to a final-state effect. Instead, the spin polarization of the photoelectrons excited with linearly polarized light remains a reliable probe for the spin in the initial state [2].

To perform further step to practical application the Bi_2Se_3 microflakes we studied in collaboration with Humboldt University of Berlin (Prof. S. Fischer). Temperature-dependent transport properties of high-quality exfoliated Bi_2Se_3 microflakes in the crossover regime from thin (>10 nm) to thick (>100 nm) are reported. High resolution transmission electron microscopy and combined energy-dispersive x-ray spectroscopy studies conforms the structure and stoichiometry of bulk and flakes. Angle-resolved photoemission spectroscopy proves single-Dirac-cone surface state and a well-defined bulk band gap in topological insulating state. Here, we demonstrate the usage of spatially resolved core-level photoelectron microscopy to investigate the surface stability of thin topological insulator films. Low temperature transport measurements from 4.2 K to 15 K conforms the high flake quality leading to metallic behavior and weak antilocalization (WAL), both signatures of the topological properties of surface states. Electron-electron scattering is negligible and electron-phonon scattering is the dominant mechanism in the temperature range from 30 K to 280 K. The temperature-dependent coherence length indicates that two-dimensional conduction is reached in Bi_2Se_3 flakes of 72 nm in thickness. Thickness-dependent measurements show that conductance is dominated by surface carriers at low temperatures.

The long-term stability of functional properties of topological insulator materials is crucial for the operation of future topological insulator based devices. Water and oxygen have been reported to be the main sources of surface deterioration by chemical reactions. In the present work, we investigate the behavior of the topological surface states

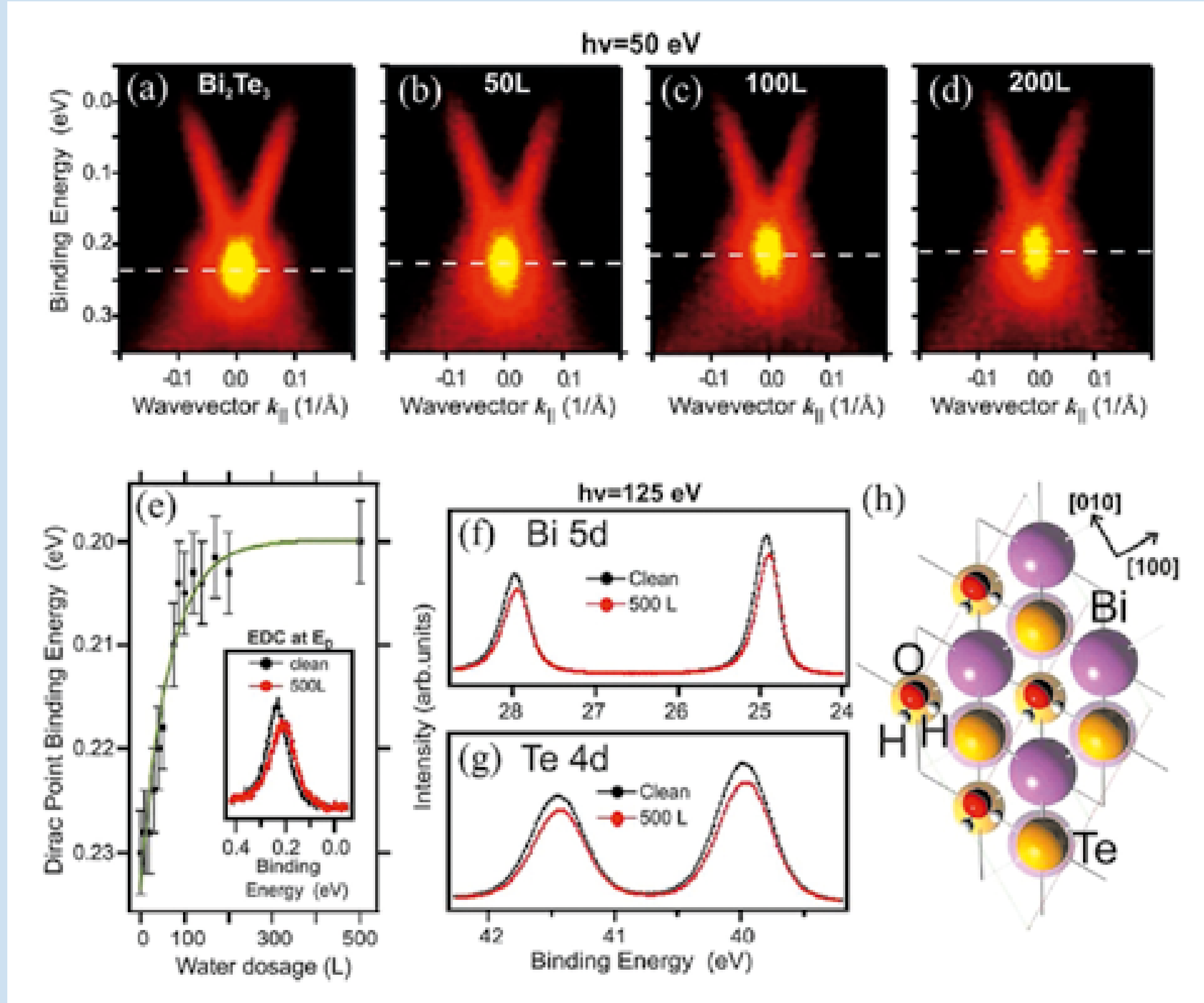

Figure 3. Water exposure of Bi_2Te_3% ARPES data (a-e), XPS data (f,g) and DFT model (h).

on Bi_2X_3 (X = Se, Te) by valence-band and core level photoemission in a wide range of water and oxygen pressures both in situ (from 10^{-8} to 0.1 mbar) and ex situ (at 1 bar). We find that no chemical reactions occur in pure oxygen and in pure water. Water itself does not chemically react with both Bi_2Se_3 and Bi_2Te_3 surfaces and only leads to slight p-doping. In dry air, the oxidation of the Bi_2Te_3 surface occurs on the time scale of months, in the case of Bi_2Se_3 surface of cleaved crystal, not even on the time scale of years. The presence of water, however, promotes the oxidation in air, and we suggest the underlying reactions supported by density functional calculations. All in all, the surface reactivity is found to be negligible, which allows expanding the acceptable ranges of conditions for preparation, handling and operation of future Bi_2X_3-based devices [3].

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1. Scholz M. R., Sánchez-Barriga J., Marchenko D., Varykhalov A., Volykhov A., Yashina L. V., Rader O. Intact Dirac cone of Bi_2Te_3 covered with a monolayer Fe Phys. Status Solidi RRL, 7 (2013) 139–141

2. Scholz M. R., Sánchez-Barriga J., Braun J., Marchenko D., Varykhalov A., Lindroos M., Yung Jui Wang, Hsin Lin, Bansil A., Min'ar J., Ebert H., Volykhov A., Yashina L.V., Rader O. Reversal of the circular dichroism in the angle-resolved photoemission from Bi_2Te_3 Physical Review Letters 110 (2013), 216801

3. Yashina, L.; Sánchez-Barriga, J.; Scholz, M.; Volykhov, A.; Sirotina, A.; Neudachina, V.; Tamm, M.; Varykhalov, A.; Marchenko, D; Springholz, G.; Bauer, G.; Knop-Gericke, A.; Rader, O. Negligible Surface Reactivity of Topological Insulators Bi_2Se_3 and Bi_2Te_3 Towards Oxygen and Water ASC nano 7 (2013) 5181–5191

HELMHOLTZ-RUSSIA JOINT RESEARCH GROUPS (TOTAL 32)

Grantees 2007	HRJRG Nr.	HRJRG Title	Helmholtz Research Centre	Russian Partners	Page Nr.
1	HRJRG-002	"Physics Analysis and Calorimetry at the Terascale"	Deutsches Elektronen-Synchrotron DESY	1. Institute For Theoretical And Experimental Physics (ITEP) (Moscow) 2. Skobeltsin Institute of Nuclear Physics, Lomonosov Moscow State University (SINP MSU) 3. Moscow Engineering and Physics Institute (MEPhI)	62
2	HRJRG-013	"High Dose Irradiation Damage of RAFM Steels"	Karlsruhe Institute of Technology (KIT)	1. Ulyanovsk State University 2. State Scientific Centre of Russia, Research Institute of Atomic Reactors (SSC RIAR) (Dmitrovgrad, Ulyanovsk Region)	10
3	HRJRG-022	"Hydrogen Isotopes Retention in First-Wall Materials for ITER and Fusion Power Reactors"	Max Planck Institute for Plasma Physics	1. Moscow Engineering and Physics Institute (MEPhI) 2. Russian Research Centre "Kurchatov Institute" (Moscow)	13
4	HRJRG-006	"Molecular Pathogenesis of Bilateral Breast Cancer"	German Cancer Research Centre	1. N.N. Petrov Institute of Oncology (St. Petersburg)	34
5	HRJRG-016	"Structural Aspects of Biocompatible Ferrofluids by Scattering Methods: Stabilization, Properties Control and Applications"	Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research	1. Joint Institute for Nuclear Research (JINR) (Dubna, Moscow Region) 2. Russian Research Centre "Kurchatov Institute" (Moscow)	64
6	HRJRG-025	"ECOLINK-Understanding Effects of Environmental Toxicants at Population and Community Levels: A Link Between Ecotoxicological Experiments and Field Observations within Eurasian Climate Scenarios"	Helmholtz Centre for Environmental Research – UFZ	1. Institute of Systematics and Ecology of Animals, Siberian Branch of Russian Academy of Sciences (Novosibirsk)	22
7	HRJRG-011	"Actinide Nano-Particles: Formation, Stability and Properties Relevant to the Safety of Nuclear Waste Disposal"	Karlsruhe Institute of Technology (KIT)	1. Chemistry Department of Lomonosov Moscow State University (MSU)	8
8	HRJRG-024	"Derivation of Germ Line Competent Rat ES Cells for Gene Targeting"	Max Delbrück Center for Molecular Medicine (MDC) Berlin-Buch	1. Institute of Cytology, Russian Academy of Sciences (St. Petersburg)	36
Grantees 2008	**HRJRG Nr.**	**HRJRG Title**	**Helmholtz Research Centre**	**Russian Partners**	**Page Nr.**
1	HRJRG-100	"Assessing the Sensitivity of Arctic Coastal Dynamics to Change"	Alfred Wegener Institute Helmholtz-Center for Polar and Marine Research	1. Geography Department of Lomonosov Moscow State University (MSU) 2. Melnikov Permafrost Institute, Siberian Branch of Russian Academy of Sciences (Yakutsk) 3. Nansen International Environmental and Remote Sensing Center (NIERSC) (St. Petersburg)	24
2	HRJRG-102	"Defining life/death decision in the crosstalk between DNA damage-induced apoptosis and DNA repair"	German Cancer Research Centre	1. Institute of Chemical Biology and Fundamental Medicine, Siberian Branch of Russian Academy of Sciences (Novosibirsk)	37
3	HRJRG-106	"Development of a High Energy Electron Cooler for Hadron Physics Experiments at COSY and HESR"	Forschungszentrum Jülich	1. Budker Institute of Nuclear Physics (BINP), Siberian Branch of Russian Academy of Sciences (Novosibirsk) 2. Joint Institute for Nuclear Research (JINR) (Dubna, Moscow Region)	66
4	HRJRG-110	"Seismic Tomography Algorithms for Fundamental and Applied Purposes"	Helmholtz Centre Potsdam – GFZ German Research Centre for Geosciences	1. A.A. Trofimuk Institute of Petroleum Geology and Geophysics, Siberian Branch of Russian Academy of Sciences (Novosibirsk)	26
5	HRJRG-112	"Experimental Study on Warm Dense Matter by Intense Heavy Ion Beams"	GSI Helmholtz Centre for Heavy Ion Research	1. State Scientific Center Institute for Theoretical and experimental Physics (ITEP) (Moscow) 2. Institute of Problems of Chemical Physics (Chernogolovka, Moscow Region) 3. Joint Institute for High Temperatures, Russian Academy of Sciences (Moscow)	68
6	HRJRG-116	"Genetic Susceptibility to Tuberculosis"	Helmholtz Centre for Infection Research	1. Central Institute for Tuberculosis (Moscow)	39
Grantees 2010	**HRJRG Nr.**	**HRJRG Title**	**Helmholtz Research Centre**	**Russian Partners**	**Page Nr.**
1	HRJRG-205	"Geodesy, Cartography and Exploration of Phobos and Deimos"	German Aerospace Center (DLR)	1. Moscow State University of Geodesy and Cartography (MIIGAIK) 2. Vernadsky Institute of Geochemistry and Analytical Chemistry (GEOKHI) (Moscow)	46
2	HRJRG-207	"Liquid Identification by Hilbert Spectroscopy for Security Screening"	Forschungszentrum Jülich	1. Kotel´nikov Institute of Radio Engineering (Moscow)	52
3	HRJRG-214	"Control of Non-linear Phase Space Dilution and Beam Loss in an Energy Recovery Linac: the Way to Short High Intensity and Low Emittance"	Helmholtz-Zentrum Berlin für Materialien und Energie	1. Budker Institute of Nuclear Physics (BINP), Siberian Branch of Russian Academy of Sciences (Novosibirsk)	69
4	HRJRG-216	"Hydrogen Behavior in Advanced and Radiation-damaged Materials for Fusion Applications"	Max Planck Institute for Plasma Physics	1. RRC "Kurchatov Institute" (Moscow) 2. National Research Nuclear University "MEPHI" (Moscow) 3. State Research Center of Russian Federation Troitsk Institute for Innovation and Fusion Research "TRINITI" (Troitsk, Moscow Region)	15
5	HRJRG-220	"Possible Beneficial Effects of TNF and/or Lymphotoxin Ablation in Carcinogen-induced and Sporadic Cancer, as Studies in Mice"	Max Delbrück Center for Molecular Medicine (MDC) Berlin-Buch	1. Engelhardt Institute of Molecular Biology (Moscow)	42
6	HRJRG-221	"Lake Baikal and Biological Effects of Global Change (LabEglo)"	Helmholtz Centre for Environmental Research – UFZ	1. Irkutsk State University, Institute of Biology	27
Grantees 2011	**HRJRG Nr.**	**HRJRG Title**	**Helmholtz Research Centre**	**Russian Partners**	**Page Nr.**
1	HRJRG-303	"Measurements of Gamma Rays and Charged Cosmic Rays in the Tunka-Valley in Siberia by Innovative New Technologies"	Deutsches Elektronen-Synchrotron DESY	1. Institute for Nuclear Research of the Russian Academy of Sciences (Moscow) 2. Irkutsk State University 3. Lomonosov Moscow State University (MSU)	71
2	HRJRG-304	"Communication Blackout Mitigation for Spacecrafts (COMBIT)"	German Aerospace Center (DLR)	1. Ioffe Physical-Technical Institute of the Russian Academy of Sciences (St. Petersburg) 2. Saint-Petersburg Branch of the Joint supercomputer Center of the Russian Academy of Sciences	49
3	HRJRG-308	"European and Russian Extreme events: Mechanisms, Variability and Future Climate Change (EUREX)"	GEOMAR Helmholtz Centre for Ocean Research Kiel	1. A.M. Obukhov Institute of Atmospheric Physics of the Russian Academy of Sciences (Moscow) 2. P.P. Shirshov Institute of Oceanology of the Russian Academy of Sciences (IORAS) (Moscow)	29
4	HRJRG-310	"The role of genetic interactions in the control of human metabolome"	Helmholtz Zentrum München – German Research Center for Environmental Health	1. Institute of Cytology & Genetics, Siberian Branch of the Russian Academy of Science (Novosibirsk)	43
5	HRJRG-314	"Defects in magnetic TiO_2 (DETI.2)"	Helmholtz-Zentrum Dresden-Rossendorf (HZDR)	1. Physics Department of Lomonosov Moscow State University (MSU) (Moscow) 2. National Research Centre "Kurchatov Institute" (Moscow) 3. Giredmet (Moscow)	54
6	HRJRG-316	"Very high-density peptide arrays by laser-induced particle melting in liquid phase"	Karlsruhe Institute of Technology (KIT)	1. Institute on Laser and Information Technologies of the Russian Academy of Science (ILIT RAS) (Moscow)	56
Grantees 2012	**HRJRG Nr.**	**HRJRG Title**	**Helmholtz Research Centre**	**Russian Partners**	**Page Nr.**
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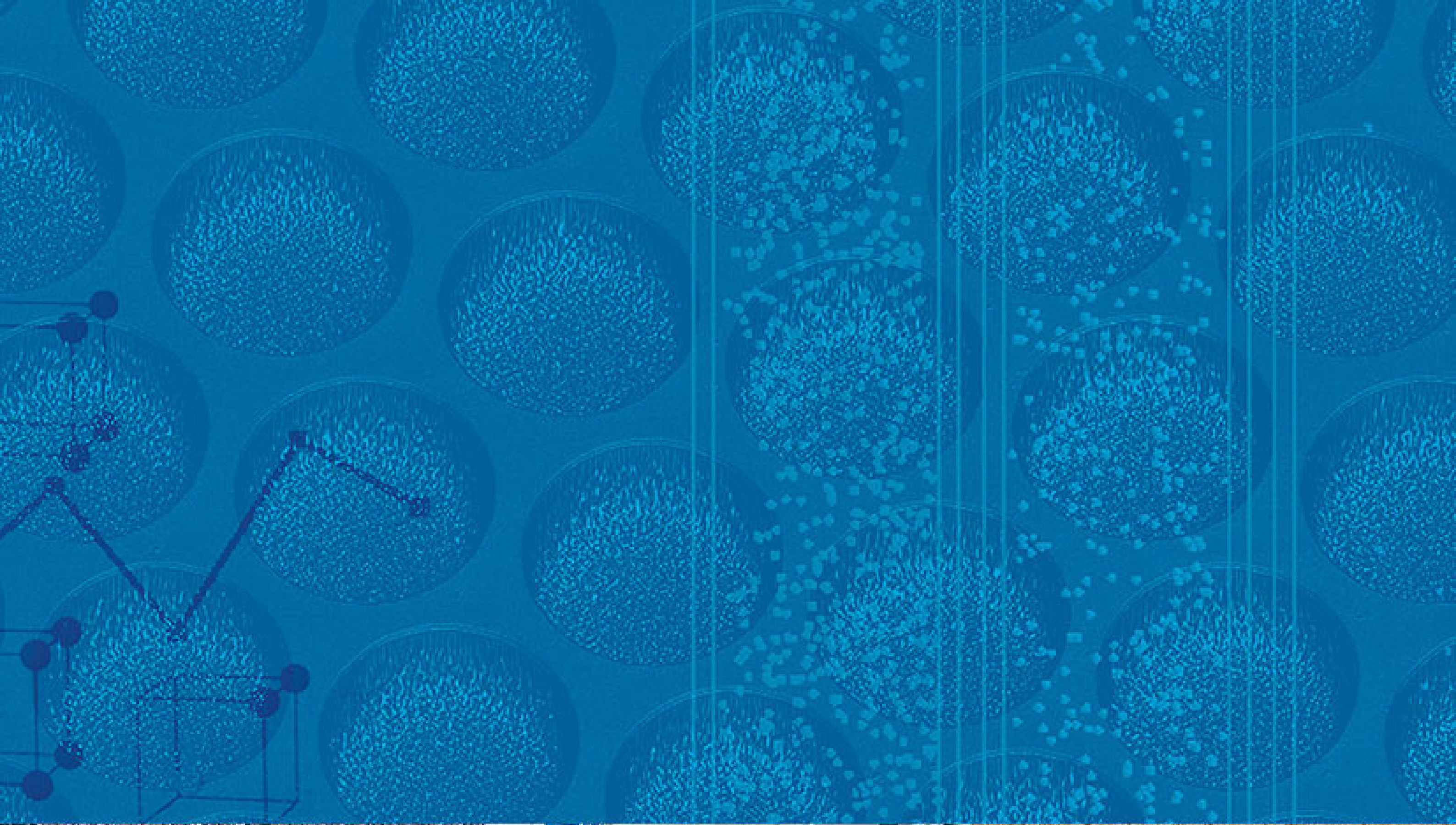
2	HRJRG-401	"Development of Methodologies for Structural Studies of Membrane Proteins via Small-Angle Neutron and X-ray Scattering"	Forschungszentrum Jülich	1. Moscow Institute of Physics and Technology, State University (Dolgoprudniy, Moscow Region) 2. Joint Institute for Nuclear Research (Dubna, Moscow Region)	58
3	HRJRG-402	"Sapphire ultra optics for synchrotron radiation"	Forschungszentrum Jülich	1. Shubnikov Institute for Cristallography of the Russian Academy of Sciences (Moscow)	59
4	HRJRG-404	"Structural properties of carbonate-silicate melts and their effect on fractionation processes in the deep Earth investigated by synchrotron radiation, spectroscopic and ion probe methods"	Helmholtz Centre Potsdam - GFZ German Research Centre for Geosciences	1. Institute for Physical Chemistry and Electrochemistry, Russian Academy of Sciences (Moscow) 2. National Research Nuclear University "MEPHI" (Moscow) 3. State Research Center of Russian Federation Troitsk Institute for Innovation and Fusion Research "TRINITI" (Troitsk, Moscow Region)	31
5	HRJRG-408	"Topological surface states under the influence of the exchange interaction"	Helmholtz-Zentrum Berlin für Materialien und Energie	1. Moscow State University, Department of Chemistry 2. St. Petersburg State University	77
6	HRJRG-411	"Tailoring nanoscaled features in novel steels for high-temperature applications using ion beam modification (ODS-HiTs)"	Karlsruhe Institute of Technology (KIT)	1. Institute of Theoretical and Experimental Physics ITEP (Moscow)	17



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