

## Characteristics of main research directions investigated at the institute and the achievements 2010–2014

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| Institute | Nuclear Physics Institute of the CAS, v. v. i. |
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*“The main mission of the NPI is to carry out scientific research in the fields of nuclear physics and related scientific disciplines, to contribute to the utilization of its research results, and to provide the research infrastructures. The principal activity of the NPI is scientific research in the field of nuclear physics and related scientific disciplines and the use of the nuclear physics methods and procedures in interdisciplinary fields of science and research, especially in biology, environmental science, medicine, radiopharmacy, and material science.”* **The Foundation Deed of the Nuclear Physics Institute of the CAS, v. v. i.**

Nuclear physics provides fundamental insights to the understanding the structure of the world. It has also important consequences for other natural sciences. Most principal projects of nuclear physics are so evolved that they are realisable only within wide international collaboration. NPI activities in the basic research are therefore oriented very much to the participation at topical international experiments. For these collaborations, however, the access to local small facilities and equipment is a prerequisite and of importance for supporting and testing concepts and instrumentation. Domestic equipment can also produce valuable basic results, attract international community, and is inevitable within the context of interdisciplinary and applied research. Generally, small facilities offer flexible procedures of access and research thus may also effectively react to and follow progress and needs of the fields. Theory studies form an integral part of NPI's activities.

The main research directions in NPI are thus based on three pillars (i) theoretical research and experimental research performed at (ii) large international collaborations and at (iii) home research facilities.

### **(i) THEORETICAL RESEARCH**

Main activities of the NPI theoretical research are naturally directed to studies of behaviour of general hadronic systems. Particularly, topics on hadron-hadron interactions, production of strangeness, structure of nuclei and hypernuclei, and weak and electromagnetic interactions in hadronic systems are pursued. Another branch of NPI theoretical research is focused on mathematical physics and its rigorous aspects in quantum theory. Here issues as quantum graphs and waveguides, spectral geometry and Schrödinger operators, theory with non-hermitian operators, and symmetries are studied. We consider the symbiosis of using the heuristic and rigorous methods of theoretical physics very fortunate, mutually influential, and fruitful. Theory team produces a lot of excellent results and its members are internationally recognized. There are many international collaborations of NPI theoretical physicists including experiment proposals and theoretical analyses for the experiments on advanced foreign facilities.

## **(ii) LARGE INTERNATIONAL COLLABORATIONS**

### **ALICE**

Experiment at CERN LHC is focused on the studies of hot and dense nuclear matter formed in ultrarelativistic heavy ion collisions at TeV energies. NPI members participated actively in experimental data taking and were involved in the offline monitoring of data quality. Their research activities have been oriented to studies of jet properties, members of the group are principal authors of 4 ALICE papers. As concern instrumentation and IT support, NPI group has been involved in upgrade studies of the Inner Tracker System and large scale computing activities.

### **STAR**

Experiment at RHIC BNL studies hot and dense nuclear matter formed in ultrarelativistic heavy ion collisions at 10's to 100's GeV energies. NPI members participated actively in experimental data taking, were involved in the offline monitoring of data quality and contributed to detector calibrations. Their research activities have been oriented to formulation of beam energy scan program, studies of correlation femtoscopy, jet properties, di-hadron correlations, and heavy flavor production. Members of the group are principal authors of 5 STAR papers. Concerning instrumentation and IT support, NPI group has been involved in preparation of Heavy Flavour Tracker and design of a new automated planning system.

### **HADES / CBM**

Experiment HADES at GSI is focused on investigation of hadron properties in medium formed in heavy ion collisions at GeV energies. NPI group participated actively in experimental data taking and operation of TOF and FW detectors. Its research activities concentrated on study of dilepton and strange particles yields in different combinations of projectile and target. Instrumentation activities concerned the upgrade of TOF detector and ECAL project as parts of the extensive HADES upgrade for the first phase of the FAIR project. Members of the group have been a corresponding author of 1 HADES paper and a technical coordinator of the ECAL project. NPI group is also involved in the development of PSD for the CBM experiment at FAIR.

### **KATRIN**

KATRIN project under construction at KIT aims at increasing sensitivity to the electron neutrino mass determination by one order of magnitude. NPI group is a founding member of the KATRIN collaboration with responsibility for the task Calibration and Monitoring. Its charge has been accomplished with parameters achieved that completely fulfil challenging requirements for successful KATRIN operation.

### **ESS**

ESS is a pan-European spallation neutron source under construction in Lund. NPI team is involved in design and construction of the instrument BEER - Beamline for European Materials Engineering Research - addressing the needs of the future

research of advanced materials for industrial applications. In 2014, our proposal of the BEER was labelled as ESS highest priority and selected among the suite of the first 7 instruments to be construct in 2015-2019.

## GANIL/SPIRAL2

At GANIL (Caen), NPI members participated in studies of nuclei far from the line of stability. For that, our senior scientist contributed originally to motivation and analysis of magic number systematics. Results have been published that complete the understanding of breaking  $N=28$  shell mechanism. NPI competencies and capacities in the field of fast neutron generators are strongly engaged in the preparation of the NFS (Neutrons For Science) facility at SPIRAL2. The calculations, design studies and also experiments connected to neutron targets development for NFS have been performed at NPI as well as the data for production reaction for the radioactive  $^{14}\text{O}$  and  $^{15}\text{O}$  ion beams at SPIRAL2 have been obtained.

## NUCLEAR ASTROPHYSICS

Our most important partners in the nuclear astrophysics field are from INFN-LNS (Italy) and Texas A&M University and lately GANIL. Experiments are arranged in collaborating laboratories but also on the NPI U120M cyclotron. Within the indirect ANC and THM methods, results have been got relevant to big-bang nucleosynthesis, CNO cycles as well as to future fusion reactors.

## (iii) RESEARCH AT HOME FACILITIES

### Center of Accelerators and Nuclear Analytical Methods (CANAM)

The basic research infrastructure of the NPI has been concentrated in the center CANAM – for brief description, support and administration see Appendix 3.3.

Within CANAM, analytical, characterization, modification and production methods based on the charged nuclear particles (light and heavy ions) and thermal and fast neutrons are offered. The methods give unique opportunities and provide detailed information that cannot be obtained in other ways. The broad arsenal of experimental methods is employed for basic and applied studies in various research fields (such as in physics, materials science, chemistry, biology, biomedicine, energetics, engineering, electronics, environmental science, archaeology, cultural heritage, etc.).

Support of the CANAM from MEYS and consequent implementation of the open access regime in 2012 has significantly contributed to the extension of the user community and higher efficiency of exploitation of NPI infrastructure capacity.

### U-120M cyclotron

U-120M is an isochronous  $K=40$  cyclotron with negative and positive modes of acceleration of ion beams up to  $^4\text{He}$ . In the positive acceleration mode it provides beams of very good quality ( $\Delta E/E$  better than  $1/1000$ ) that have been utilized in astrophysical experiments as mentioned above. NPI cyclotron has also been employed by NPI teams and their collaborators in measurements of excitation functions for production of medical radionuclides, extensive measurements of thick target yields of

various Tc radioisotopes related to the cyclotron production of Tc-99m, production of the monitoring isotopes for KATRIN, study of data for radioactive ion beams production for SPIRAL2, testing detectors and electronics for CERN LHC and FAIR, measurements of the deuteron induced activation data of high-power accelerator components, irradiation of biological samples for estimating DNA radiation damage, and research on fluorescent nanodiamonds production methods.

### Fast Neutron Generators

High-power broad-spectrum and variable-energy quasi-monoenergetic fast neutron generators based on proton and deuteron beams from the negative-ion acceleration mode of U-120M have been developed. They are mainly utilized in research concerning neutron data for research and technology. Data with relevance for accelerator-driven neutron sources and activation of materials for fusion technology have been acquired. Neutron hardness test of microelectronics for ATLAS@LHC upgrade has also been an important application.

### Tandetron laboratory

NPI activities employing a wide portfolio of nuclear analytical and modification methods installed at the Tandetron accelerator (terminal voltage from 200 kV to 3 MV) are focused, in collaboration with domestic and foreign institutions, to investigation of nanostructures in crystalline materials for photonics and spintronics, metal/polymer nano-composites and nano-structures, and graphene based structures. Fabrication and characterization of novel materials with a high application potential, such as materials for biosensors, and the potentiality of microbeam writing in producing diffractive optical elements has been prospected. Study of energetic losses in different materials is important for various nuclear applications.

### Facilities at the neutron channels of the LVR-15 reactor

NPI groups employ neutron channels hired at LVR-15 research reactor operated by the Research Center Řež. The neutron diffraction team is oriented to material research with topics including deformation mechanisms of metals under thermo-mechanical loading, microstructure of novel materials, high-temperature materials, and nanostructures made from metallic materials. Crystallography investigation concerned monitoring of the structural changes in the Li battery material during its live cycle, magneto-caloric materials and techniques for determination of graphen structural properties. Studies on Bragg diffraction optics and development of the simulation software for modelling neutron scattering instruments form a prerequisite for the successful participation of the team in the ESS project.

The neutron activation analysis team has established cooperation with leading domestic and foreign institutions on topics of environmental research, agriculture and nutrition, nuclear technology, material research, and reference materials. Geo- and cosmochemical research is mainly focused on isotopic composition of tektites within context of their source materials. Studies in geomycology look at trace element accumulation in mushrooms. Study hair samples of Tycho Brahe besides attracted greatest attention of the general public. Important methodological development concerning improvement of standardization procedures in INAA has been achieved.

## TR24

Within the evaluated period, a significant upgrade of the CANAM instrumental base has started. The project comprises the rebuilding of the tower of the former Van de Graaff accelerator and purchasing of the new cyclotron TR24 of the Canadian provenance. This project with the total budget of about 230 mil CZK represent the biggest investment upgrade since the NPI foundation.

### **Other NPI experimental facilities**

#### Laboratories of the Department of Radiopharmaceuticals

In laboratories, studies of labelling of potential therapeutic radiopharmaceuticals based on monoclonal antibodies and puromycin modified and labelled with Y-86, Ga-68 and Sc-44 have been done. Much attention was paid to separation and quality control techniques for the cyclotron-produced Tc-99m. Automation systems and new systems for radiopharmacy and nuclear chemistry technologies have been developed.

#### Laboratories of the Department of Radiation Dosimetry

The team Dosimetry of Ionizing Radiation has established cooperation with leading domestic and foreign institutions and uses the department's as well as outside laboratories. DRD instrumentation serves as a basis for dosimetry and microdosimetry studies of complex radiation fields concerning e.g. quality and out-of-field doses of therapeutic ion beams. In the field of radiation biophysics and radiobiology, investigation both on the subcellular and cellular level has been performed. In radiocarbon laboratory, based on liquid scintillator spectrometry, a study of the impact of fossil fuel combustion on increasing atmospheric CO<sub>2</sub> concentration has been performed. Radiocarbon dating method has been also applied in analyses for archaeology or paleoenvironmental research. Environmental research concerning tritium and <sup>14</sup>C activities in the surroundings of nuclear power plants has been conducted.

## Research Report of the team in the period 2010–2014

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| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Theoretical Physics                            |

*Main activity of the team (covering the NPI Department of Theoretical Physics) is naturally directed to theoretical studies of behavior of general hadronic systems. In principle properties of such systems are governed by the laws of quantum chromodynamics (QCD). In practice our understanding of the properties of the hadron spectrum and of the hadron interactions is limited: The lightest hadrons, the pseudoscalar pions, kaons and eta are the only hadrons well understood at low energies in model-independent way within the context of the chiral perturbation theory (ChPT). All other hadrons and complex hadronic systems must necessarily be described in terms of more or less QCD-motivated models. Theoretical understanding of hadronic systems would not be complete without taking into account also their electromagnetic and weak interactions. Recent remarkable experimental progress in this field motivates our activity also in this direction.*

*The true understanding of real physical systems requires analyzing them from the first principles using proper mathematical tools. This is the basic motivation of mathematical physics, the field which forms a strong part of the Department. We find the symbiosis of using the heuristic and rigorous methods of theoretical physics very fortunate, mutually influential, and fruitful.*

### HADRON-HADRON INTERACTIONS

*While the effective field theory defines interactions of pseudo-Goldstone bosons near threshold, its form is still not fully fixed, especially in less precise strange sector. Thus, QCD or ChPT inspired modelling, complemented by precision studies based on general analytic properties are still hot topics. Such models are tested in few-hadron systems and their response to external fields or by submerging interacting hadrons into larger systems up to infinite nuclear medium.*

Together with our former student J. Smejkal we developed a model that successfully describes the s-wave interactions of the pseudoscalar pseudo-NG meson octet with the ground state baryon octet. The meson-baryon effective potentials are constructed to match pertinent scattering amplitudes derived from the underlying chiral Lagrangian. Recently, the data fitted in the antiKN sector were supplemented by a very precise measurement of the characteristics of the 1s level in the kaonic hydrogen atom. We applied this model to antiKN and  $\eta$ N interactions ([Eur.Phys.J.A43\(2010\)191](#); [Nucl.Phys.A881\(2012\)115](#); [Nucl.Phys.A919\(2013\)46](#)). In both sectors the low energy meson-baryon interactions are strongly affected by baryon resonances  $\Lambda(1405)$  and  $N^*(1535)$  residing close to the respective thresholds, which are generated dynamically. The  $\Lambda(1405)$  resonance results from a superposition of two nearby poles, coupled with a different strength to the antiKN and  $\pi\Sigma$  channels.

With our frequent collaborators Yu.S. Surovtsev of JINR Dubna and R. Kaminski from INP Krakow we pursued the multi-channel description of the s-wave pion-pion scattering, based on analyticity and unitarity of the S matrix and using the uniformizing procedure. We demonstrated importance of the multi-channel approach by comparing the one- and two-channel analyses of the  $\pi\pi$  scattering data ([Phys.Rev.D86\(2012\)116002](#)). In the former case, the  $f_0(500)$  resonance (the  $\sigma$  meson) is relatively narrow, which is consistent with most of the other approaches (based on the Roy-like equations) - however, the description of the coupled KK

channel is not satisfactory. In the latter analysis, the  $\sigma$  meson gains significantly larger width, the pole is located further from the real axis, and the description of the KK channel is much improved. We used our multi-channel amplitude for the s-wave  $\pi\pi$  scattering to account for the interaction of mesons in the final state in decays of  $J/\psi$  and  $Y$  mesons ([Phys.Rev.D89\(2014\)036010](#); [Phys.Rev.D91\(2015\)037901](#)). Our analysis showed that the data on the  $J/\psi$  decay from BES Collaboration are better described using a broad  $f_0(500)$  resonance. We modified the multi-channel s- and p-wave  $\pi\pi$  amplitude using the Roy-like equations to include the crossing symmetry requirement. Then, the  $\sigma$  pole is shifted closer to the origin, consistently with the values reported by the PDG ([Phys.Rev.D90\(2014\)116005](#)).

With our long-term collaborator J. Revai from RMI Budapest we explored different properties of the  $\bar{K}NN-\pi\Sigma N$  system using Faddeev-type Alt-Grassberger-Sandhas equations. We calculated near-threshold Kd scattering amplitudes, including the scattering length, and fitted to them parameters of an effective optical Kd potential. Using this potential together with Coulomb interaction we calculated the 1s level shift and width of kaonic deuterium ([Nucl.Phys.A890-891\(2012\)50](#); [Phys.Rev.C90\(2014\)034003](#)). We also performed calculations of the quasi-bound state in the Kpp system and predicted its binding energy and width. A new method of calculating a subthreshold resonance position and width in a three-body system was proposed and used together with the direct search of the resonance pole ([Phys.Rev.C90\(2014\)034004](#)).

Interesting results on hadron-hadron interactions in the nuclear medium were obtained in close collaboration with A. Gal and E. Friedman from the Hebrew Uni Jerusalem: The effects of the nuclear medium on the branching ratios of the elementary  $\bar{K}N$  reactions were calculated ([Phys.Rev.C82\(2010\)024609](#), [Phys.Lett.B698\(2011\)226](#)): The energy and density dependence of the  $Kn \rightarrow \pi\Lambda$  rate enabled us to reproduce the A-dependence of the  $\Lambda$ -hypernuclear production rates measured in processes induced by stopped kaons at FINUDA (Frascati).

We studied the in-medium  $\bar{K}N$  and  $\eta N$  interactions near and below threshold. We explored the role played by subthreshold meson-baryon dynamics in K-atom, K-nuclear and  $\eta$ -nuclear bound-state calculations within various in-medium models of  $\bar{K}N$  and  $\eta N$  interactions. New analyses of kaonic atom data revealed appreciable multi-nucleon contributions. Strong energy and density dependencies of scattering amplitudes at and near threshold were taken into account in self-consistent calculations of K-nuclear quasi-bound states ([Phys.Lett.B702\(2011\)402](#); [Phys.Rev.C84\(2011\)045206](#); [Nucl.Phys.A881\(2012\)159](#)). The calculated K absorption widths are comparable or larger than the corresponding K binding energies for all K-nuclear quasi-bound states, exceeding considerably the level spacing. In view of the sizable widths predicted by our calculations, an unambiguous identification of K-nuclear quasi-bound states in ongoing experimental searches would be difficult. The strong energy dependence of the s-wave  $\eta N$  scattering amplitude at and below threshold was included self-consistently in  $\eta$ -nuclear bound state calculations ([Phys.Lett.B725\(2013\)334](#); [Nucl.Phys.A925\(2014\)126](#)). This approach was found to impose stronger constraints than ever on the onset of  $\eta$ -nuclear binding. We calculated binding energies and widths of  $\eta$ -nuclear states in selected nuclei across the periodic table within several underlying  $\eta N$  models.

The PANDA experiment at FAIR is going to explore the interaction of antiprotons with nucleons and nuclei. These measurements will provide us with new information on the anti-pN and anti-p-nucleus potential, and anti-p annihilation in the nuclear medium. We performed first fully self-consistent calculations of anti-p-nuclear bound states using complex potentials consistent with anti-p-atom data ([arXiv:1502.05523 \[nucl-th\]](#)). The corresponding anti-p width in the medium significantly decreases; however, it still remains considerable for the anti-p potentials consistent with experimental data.

## PRODUCTION OF STRANGENESS

*Our activities in this direction naturally complement those described above. Moreover, we provide theoretical analysis for several international experimental collaborations.*

The strangeness photo- and electroproduction on nucleons provides complementary information on the structure and interactions of baryons in the SU(3)-flavor sector. Apart from the study of the reaction mechanism, a correct description of the elementary production is very important for precise predictions of the cross sections for electroproduction of hypernuclei. For the Uni Mainz-A1 Collaboration we analyzed the transition region between photoproduction and electroproduction (very small values of the virtual-photon mass) ([Nucl.Phys.A881\(2012\)187](#); [Eur.Phys.J.A48 \(2012\)14](#)). Using the isobar model, we showed that the longitudinal couplings of virtual photons with baryons in the effective Lagrangian are not as important as it was considered in some isobar models. We also predicted the polarized-interference structure function which was compared to results from the MAMI experiment.

In collaboration with Tohoku Uni-NKS2 Collaboration we calculated the cross sections for the inclusive  $\Lambda$  production on the deuteron in PWIA and compared them with the data from Tohoku, which provided a very strict test of the isobar models ([Nucl.Phys.A914\(2013\)69](#)).

For the INFN Rome-Hall A Collaboration we provided physical motivation, predictions of the cross sections and proposed suitable kinematics for the experiment on electroproduction of kaons off the proton planned in Jefferson Lab ([Phys.Rev.C81\(2010\)052201\(R\)](#); [Nucl.Phys.A914\(2013\)34](#); [Phys.Rev.C91\(2015\) 034308](#)).

Motivated by the Gent Regge-plus-resonance (RPR) model and using new experimental data we constructed our version of the model for kaon photoproduction on the proton. The RPR model was also used in the study of photo- and electro-production of kaons off nucleons in specific kinematical regions: the small-kaon-angle region and the production with very small virtual-photon mass. These results are important for the analysis and interpretation of experimental data and for proposing new experiments at JLab.

We constructed also an isobar model for photoproduction of kaons on the proton ([Nucl.Phys.A914\(2013\)14](#)). In the model we included contributions from the exchanges of nucleon resonances with spin 3/2 and 5/2 and hyperon resonances with spin 3/2. Significant improvement of the description of the process is observed in the small kaon-angle region, which is crucial for calculations of the cross sections for electroproduction of hypernuclei.

## STRUCTURE OF NUCLEI AND HYPERNUCLEI

*Because the world is made of nuclei the detailed understanding of their structure is condemned to be the condition necessary both for the basic research and for applications.*

Together with collaborators we have developed the Equation of Motion Phonon Model (EMPM) ([Phys.Rev.C90\(2014\)014310](#)). The total Hamiltonian is diagonalized within the Hilbert space comprising particle-hole and the multi-particle-hole excitations. The resulting eigenstates are in general highly correlated states which go beyond the Mean-Field description. The transition probabilities were calculated to get the photoabsorption excitation spectra. This model is successful mainly in the description of such phenomena as Pygmy Dipole Resonance (PDR) and fragmentation of the Giant Dipole Resonance (GDR), where the multi-particle-hole type of excitations plays an important role. Further applications include the dipole response in  $^{132}\text{Sd}$  within a self-consistent multiphonon approach, and calculations of the nuclear response using a realistic nucleon-nucleon interaction with a density-dependent corrective term.

We explored strong decay of  $\Lambda$  hypernuclei to hyperfragments ([PoS\(Baldin ISHEPP XXI\)\(2012\)101](#); [PoS\(Baldin ISHEPP XXII\)\(2015\)129](#)). This study was motivated by planned experiments at JLab and Mainz aiming at systematic study of the fragments from the primary p-shell hypernuclei. For modeling the hyperfragment production we used the Translation



Invariant Shell Model and we focused on  $s^{-1}s_{\Lambda}$  components of strangeness analogue states for simplicity. The studied problem is linked to more general issues, such as the cluster structure of ordinary p-shell nuclei.

In order to study cluster formation inside hypernuclei and changes in the structure of the nuclear core caused by the hyperon, we extended the approach of Fermionic Molecular Dynamics to the case of nuclear systems with non-zero strangeness. In collaboration with T. Neff and H. Feldmeier from GSI Darmstadt we formulated a relevant model, developed a corresponding code and performed first calculations of s-shell hypernuclei.

In collaboration with A. Nogga from FZ Juelich we calculated the two main weak decay modes of the hypertriton: the non-mesonic decay,  $\Lambda N \rightarrow NN$ , and the mesonic one  $\Lambda \rightarrow \pi N$ . The two-body potential involving the non-mesonic mode was calculated in the previous years in momentum space within an effective field theory framework up to NLO. The implementation of this decay in a hypernuclear code, where the particles are constrained by the initial and final nuclear wave functions has been done during 2014. Both the mesonic and non-mesonic decays of the hypertriton have been implemented in a hypernuclear code recently.

With our former student and colleague P. Navratil, now at TRIUMPH, and R. Roth from Uni Darmstadt we have used hypernuclei as a testing ground for YN ( $Y = \text{hyperon}$ ) and YY interactions. Again, the ChPT provides a bridge that connects QCD in the strangeness sector with the low-energy hypernuclear physics. Building on the no-core shell model (NCSM) we developed a reliable *ab initio* method for nuclear systems with strangeness capable of employing realistic interactions. We formulated NCSM methodology to accommodate different species of fermions and to incorporate the coupled-channel nature of hypernuclear systems ([Few Body Syst.55\(2014\)745](#)). To obtain satisfactory convergence of the calculations, the similarity renormalization group effective interaction was implemented optionally accompanied by the importance truncation of the model space basis. We demonstrated that the NCSM is a powerful method and performed *ab initio* calculations of  $\Lambda$ -hypernuclear systems up to the p-shell ([Phys.Rev.Lett.113\(2014\)192502](#)).

In collaboration with FMP Charles University, some aspects of the dynamics of quantum many-body systems have been studied within the context of the interacting boson model of nuclear structure (IBM). We propose that the adiabatic separation of collective and intrinsic motions in many-body systems is related to increased regularity of the intrinsic dynamics. The surmise is verified on the separation of rotations from intrinsic vibrations in the IBM ([Phys.Rev.C82\(2010\)014308](#); [Phys.Rev.Lett.105\(2010\)072503](#)).

## WEAK AND ELECTROMAGNETIC INTERACTIONS

*Building a ChPT description of the hadronic electroweak interaction is still not entirely completed. The Standard model of the electroweak interactions, even after the discovery of the Higgs boson, is not able to describe all experimental data. In any case, the new data in the neutrino sector open the door to New Physics.*

In collaboration with E. Epelbaum of Uni of Bochum, R. Machleidt of Uni of Idaho and P. Ricci of INFN of Florence we performed consistent calculations of weak processes of light nuclei within the ChPT. Our approach differs from alternative ones in that our axial currents respect the nuclear version of the PCAC relation (analog of the vector continuity equation for vector currents). The results published so far ([Phys.Lett.B709\(2012\)93](#)) concern a muon capture on deuterium. Main physical outputs of this calculation are bounds on poorly known value of the ChPT low-energy constant  $d^R$ , which enters also into calculations of important astrophysical processes, such as proton–proton fusion and solar neutrino scattering on deuterons.

In collaboration with V.B. Belyaev and F. Šimkovic of JINR Dubna and P. Ricci we have completed the study ([AIP Conf.Proc.1572\(2013\)106](#)) of the influence of the double charge

exchange reaction on cooling of strongly magnetized white dwarfs, making use of a simple basic model of the structure of their magnetic field. Our calculations however show that the influence of the considered exotic reaction on the luminosity of white dwarfs would be rather difficult to confirm experimentally.

Together with former students P. Benes and A. Smetana we have analyzed the consequences of fermion masses spontaneously generated by a new strong dynamics ([arXiv:1101.3456 \[hep-ph\]](#)). First, one consequence is universal: There is no generic electroweak mass scale. In contrast with the canonical Higgs mechanism the masses of the intermediate W and Z bosons result from the composite 'would-be' NG bosons, and are expressed in terms of masses of the electroweakly interacting fermions by sum rules. Second, if the new dynamics is defined as a completely broken gauge flavor dynamics, the consequences are numerous. In particular: (1) There is a *composite* Higgs particle with calculable properties ([Eur.Phys.J.C73 \(2013\)2513](#)). (2) There are the massive pseudo NG bosons, the composite axions. (3) There are superheavy Majorana neutrinos ([JHEP 1304\(2013\)139](#)). Although the implications of the dynamical fermion mass generation, based on the Goldstone theorem and the Ward-Takahashi identities are safe, the very calculations of the fermion masses are not. We have to refer so far to rather schematic models.

## QCD

*Understanding the structure of hadrons directly from its colored constituents is hard. Some methods can, however, be borrowed from attempts at understanding the nonperturbative hadron dynamics.*

In collaboration with P. Bicudo of Technical Uni of Lisbon we developed systematic methods for solving the Bethe-Salpeter equation accompanied by the solution of the Schwinger-Dyson equation for a confined quark propagator in Minkowski space. We provide a description of the spectra of the pseudoscalar ([Phys.Rev.D90\(2014\)016005](#)) and vector ([Phys.Rev.D86\(2012\)096004](#)) charmonia together with a comparison of the conventional approaches in Euclidean space. The efficiency and reliability of numerical methods in both frameworks are discussed.

The important challenge to understand the QCD matter at high temperatures is tested experimentally in ultrarelativistic heavy-ion and proton-ion collisions at present. The observed phenomena were analyzed in terms of the Z-scaling suggested at our Department in international collaboration with M. Tokarev, A. Aparin and T.G. Dedovich of JINR Dubna. Z scaling manifests itself in the fact that the inclusive spectra of various types of constituents can be described by a universal scaling function ([J.Phys.G40\(2013\)055005](#)).

## QUANTUM THEORY ON GRAPHS AND WAVEGUIDES

*A quantum particle confined to a configuration space of nontrivial geometry and/or topology experiences an effective interaction coming from the confinement. The team members played a leading role in formulating this idea and deriving its numerous consequences.*

First, it was a longstanding open problem whether any coupling, consistent with the probability current conservation requirement, can be approximated by a family of "fat graphs", i.e. whether its Hamiltonian is a limit of Laplacians on a shrinking system of thin tubes. In collaboration with T. Cheon of Kochi Uni and O. Post of Durham Uni ([Ann.Phys.325\(2010\)548](#), [Commun.Math.Phys.322\(2013\)207](#)) we provided an affirmative answer for networks having either a Neumann type boundary, or no boundary at all, showing that this can be achieved by adding properly scaled potentials and magnetic fields in combination with a suitable local modification of the graph topology.

Second, the corresponding problem with the hard-wall, or Dirichlet, boundary exhibits a completely different behavior. Squeezing limits in this case were obtained earlier for bent

smooth tubes; in the considered period the limit was extended to situations with weak regularity assumptions, also in presence of a magnetic field ([Ann.H.Poincaré 15\(2014\)1993](#), [Rev.Math.Phys.24\(2012\)1250018](#)). The limits for sharply broken or branching tubes were proved to be nontrivial if the system exhibits threshold resonances; a full solution to this problem is still missing.

Third, the problem of the high-energy asymptotics of the resonance number in quantum graphs was inspired by a recent surprising observation that graphs with “balanced” vertices in which the wave functions are coupled by the simplest, so-called Kirchhoff, matching conditions may exhibit a smaller number of resonances than Weyl’s law would predict. In collaboration with E.B. Davies of King’s College, London, ([J.Phys.A: Math.Theor.43\(2010\)474013](#)) we were able to find necessary and sufficient conditions under which such an effect occurs. We have also shown that application of a magnetic field cannot change a “Weyl” graph into a “non-Weyl” one; however, it can change the effective size of a non-Weyl graph ([Phys.Lett.A375\(2011\)805](#)).

Fourth, a related topic belonging to the above category concerns quantum waveguides, i.e. the dynamics of a particle confined to tubes or layers. It is known that a nontrivial confinement geometry has spectral consequences; these are the results to which members of the group contributed significantly in the past. A new important contribution in the period in question obtained in collaboration with E. Zuazua of Uni of Bilbao ([J.Diff.Eqs 250\(2011\)2334](#)) is the proof of a Hardy-type inequality for Laplacian in twisted tubes of a non-circular cross section. This result is not only relevant to quantum physics which motivated it, but has also consequences for the heat equation (governing the heat flow, Brownian motion, etc.); it turns out that twisting leads to a faster cool-down/death of the Brownian particle.

Fifth, another quantum graph result concerns periodic quantum systems. It is often assumed that spectral-band edges correspond to quasimomentum values from the edge of the Brillouin zone. However, it was observed in a quantum graph context that this may be false. The mentioned result obtained in collaboration with P. Kuchment of Texas A&M Uni and B. Winn of Loughborough Uni ([J.Phys.A: Math.Theor.43\(2010\)474022](#)) shows that this remain to be the case, i.e. that the band edges may correspond to points in the interior of the Brillouin zone, even if the graphs are periodic in one dimension only provided the graphs cells are connected by more than a single edge.

## SCHRÖDINGER OPERATORS AND SPECTRAL GEOMETRY

*Properties of quantum mechanical system pose numerous mathematical questions concerning the corresponding Hamiltonians concerning, in particular, relations between their spectra, the involved potentials, and geometry of the configuration space.*

In collaboration with A. Laptev of Imperial College ([Commun.Math.Phys.326 \(2014\) 531](#)) we derived, using a Prüfer-type transformation, new inequalities of Lieb-Thirring type for one-dimensional Schrödinger operators with matrix potentials. This result can be used, in particular, for estimation of eigenvalue moments for Hamiltonians of star-shaped quantum graphs. It is worth mentioning that the result includes not only an estimate of the moments from above but also a tight lower bound.

A large group of our results concerns systems the Hamiltonians of which are strongly singular Schrödinger operators with  $\delta$ - and  $\delta'$ -type potentials. Physically they are usually referred to as “leaky” graphs because they describe quantum motion confined to the graph “skeleton” which, however, does not exclude a tunneling between the graph edges. In collaboration with K. Pankrashkin of Orsay ([Commun.PDE 39\(2014\)193](#)) we derived strong-coupling asymptotic expansions for eigenvalues in the situation when the interaction support is a smooth manifold.

We have also analyzed some interesting particular cases; for instance, together with J. Behrndt of Uni of Graz and V. Lotoreichik ([J.Phys.A:Math.Theor.47\(2014\) 355202](#)) we found the

spectrum of a Schrödinger operator with a  $\delta$ -interaction supported by a conical surface and analyzed its properties.

The last named topic has also connections to spectral geometry. As another item in this category, in collaboration with L. Parnowski of Uni College London ([Portugal.Math. 71\(2014\)141](#)) we analyzed strong coupling in Robin billiards which became an object of interest recently. We were able to contribute to this effort: we derived a two-term strong-coupling asymptotic eigenvalue expansion in such systems.

Furthermore, together with P. Freitas of Uni of Lisbon ([arXiv:1403.6666 \[math-SPI\]](#)) we obtained several non-asymptotic results concerning this spectral problem, the prominent among them is a counterexample to Bareket's conjecture stating that the lowest eigenvalue of the Laplacian, subject to attractive Robin boundary conditions, is maximized by the ball. We demonstrated that this need not be true if the region is not simply connected, the counterexample being a circular annulus.

Other spectral-geometry results obtained concern the so-called Payne's nodal-line conjecture stating that the nodal set of a second eigenfunction of the Dirichlet Laplacian for any planar region cannot consist of a closed curve. In other words, the second fundamental frequency of any drum corresponds to vibrations of a membrane with stationary points hitting the boundary. Following our earlier result obtained in collaboration with P. Freitas that the conjecture does not hold for unbounded regions but it holds for thin curved tubes we have been able to extend this claim to thin curved layers ([J.Diff.Eqs 258 \(2015\) 281](#)).

## QUANTUM THEORY USING NON-HERMITIAN OPERATORS OF OBSERVABLES

*In a way inspired by the Dyson mapping in nuclear physics and PT-symmetry project in field theory, we joined the trend of a deeply innovative theoretical synthesis of these two complementary approaches to the foundations of quantum theory.*

A particular attention has been paid to non-selfadjoint Hamiltonian operators with real spectra. In literature it was often argued that by a similarity transformation such operators can be made self-adjoint, and thus legitimate, generators of quantum evolution. One of our most influential and mathematically rigorous results ([Phys.Rev. D86\(2012\)121702](#)) shows that such a belief may be ill-founded since no such similarity transformation exists for the paradigmatic example of imaginary cubic oscillator. This led us to recommend a replacement of the popular differential-operator toy models by their mathematically less complicated difference-operator analogues and more-parametric generalizations ([Ann.Phys.327\(2012\)893](#)). The new models were shown not to suffer of mathematical inconsistencies and they proved to provide a truly rich menu of alternative dynamical scenarios of the fall of quantum system into an instability.

In parallel we worked on a highly desirable return of attention to the properly treated differential-operator models. In a way motivated by their natural emergence in physics-oriented applications we revealed an interesting relationship between the spectrum (mainly, its anomalies and, in particular, the localization of the "exceptional" points of the loss of its reality) and the topology encoded in a quantum system, be it a "kinematical smearing" of the coordinates or the conventional graph structure of their support ([Can.J.Phys.90\(2012\)1287](#), [J.Phys. A43\(2010\)335303](#)).

Using the large-momentum techniques, the model-building role of branch-point encircling topology has been clarified for the complex-path-supported pseudo-Hermitian "tobogganic" quantum systems ([SIGMA.7\(2011\)018](#)), revealing also the existence of a connection between the supersymmetry and the planarizability and observability aspects of quantum toboggans.

An incessant mathematics-oriented analysis helped us to find connections between special chain-interaction models and the properties of classical orthogonal polynomials, with special emphasis upon their Gegenbauer-polynomial subfamily ([Phys.Rev.A82\(2010\)052113](#)), with an



immediate applicability in anomalous scattering and in the non-numerical analysis of certain sufficiently elementary gain-and-loss media in classical optics.

One of the key theoretical puzzles opened by our recent three-Hilbert-space representation of quantum theory appeared to be the manifest loss of the locality of interaction due to the Dyson's mappings. In a toy model making the degree of this nonlocality tunable we were able to present a set of new constructive resolutions of the puzzle ([J. Phys.A44\(2011\)075302](#)).

Subsequently, great emphasis was put on the analyses of the mechanisms of the loss of stability of toy-model quantum systems in general and on certain specific coupled-cluster many-body systems in particular ([Acta Polytech.54\(2014\)85](#)). A partial classification has been obtained of phenomena of spontaneous symmetry breakdown and of a generic "quantum catastrophe" form including also specific forms of the phase transitions of two complementary kinds. A one-to-one correspondence was identified between the phase transition (alias quantum catastrophe) and the occurrence of the Kato's exceptional point which is real. Special emphasis was put upon the detailed dynamical picture of the unfolding of the degenerate exceptional-point singularities ([Ann.Phys.336\(2013\)98](#)).

Finally, using an analogy between non-Hermitian quantum Hamiltonians and certain pseudo-bosonic number-like operators, a mathematical completion of the formalism of unitary quantum mechanics using Dyson mappings was achieved to cover the systems in which certain operators in Hilbert space were found unbounded ([J.Phys.A 45\(2012\)115311](#)).

## CONSEQUENCES OF SYMMETRIES IN QUANTUM SYSTEMS

*Symmetries play a key role in physics, and their consequences are far from exhausted. We have mentioned already some of their uses in problems listed above. Here we add their more general attributes.*

Local (and nonlocal) symmetries of a quantum system can provide insight into its physical properties by reflecting its spectral characteristics. Together with M. Plyushchay of Santiago Uni and A. F. Correa of Valdivia Institute we analyzed one-dimensional quantum models of spin-less and spinning particles in the field of the magnetic vortex and revealed a rich structure of nonlocal integrals of motion ([Ann.Phys.325\(2010\)2653](#)). The existence and properties of these hidden symmetries were explained in alternative way with the use of a special nonlocal unitary transformation of Foldy-Wouthuysen type ([Phys.Lett.B692 \(2010\)51](#)).

Low dimensional Dirac operators appear frequently in description of quantum systems, e.g. in graphene or topological insulators. In collaboration with M. Plyushchay, F. Correa, A. L.M. Nieto and J. Negro of Valladolid Uni and S. Kuru of Ankara Uni we focused on the analysis of exactly solvable models. In their construction, we employed algebraic techniques like potential algebras ([Ann.Phys.331\(2013\)216](#)) or factorization known in supersymmetric quantum mechanics ([Phys.Rev.D83\(2011\)047702](#), [Phys.Rev.D90\(2014\)125003](#), [Phys.Rev.D 85\(2012\)045035](#), [J.Phys.A47\(2014\)115307](#)). Besides providing information about spectral properties, a rich background of symmetries allowed us to consider other interesting concepts, e.g. shape-invariance of one-dimensional Dirac operators. These results were complemented by a qualitative analysis of the spectral properties; we looked for generic conditions that lead to confinement of Dirac fermions in graphene in the settings where translational symmetry is present ([Ann.Phys.349\(2014\)268](#)).

Our former student T. Brauner, working in the considered period abroad, together with his new collaborators, obtained a number of valuable model-independent results, some on the existence and properties of the excitations of the NG type in systems without Lorentz invariance: (1) The number of NG bosons equals the number of broken generators minus the number of pairs of broken generators whose commutator has a nonzero vacuum expectation value ([Phys.Rev.D84\(2011\)125013](#)). (2) The most general effective Lagrangian for the NG

bosons of spontaneously broken global internal symmetry up to fourth order in derivatives was constructed ([JHEP 1408\(2014\)088](#)). (3) The massive NG bosons were defined and their properties clarified ([Phys.Rev.Lett.111\(2013\)021601](#)). (4) The notion of general coordinate invariance was extended to many-body, not necessarily relativistic, systems ([Phys.Rev.D90\(2014\)105016](#)).

## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Ultrarelativistic Heavy Ions                   |

The team is actively involved in research in two large international collaborations, STAR at RHIC BNL and ALICE at the CERN LHC, where it focuses on studies of hot and dense nuclear matter, cold nuclear matter as well as proton-proton collisions. In addition, the team also participates in studies of structure of weak interactions at ISOLDE at CERN. At the end of 2014 the team consisted of 3 senior research scientists (J. Bielčíková, M. Šumbera, J. Ferencei), 4 research scientists (D. Adamová, S. Kushpil, D. Zákoucký, J. Bielčík-25% FTE), 4 postdocs (P. Federič, F. Křížek, R. Vertési, P. Chaloupka - 10% FTE), 7 Ph.D. (V. Kučera, D. Makatun, J. Pospíšil, J. Rusňák, D. Tlustý, M. Vajzer, T. Vaňát), 2 MSc. (V. Pacík, K. Vysoká) and 2 Bc. students (M. Adam, M. Kocmánek). In 2010-2014 there were 4 Ph.D. (P. Chaloupka, J. Kapitán, M. Zerola, D. Tlustý) and 3 MSc. theses (J. Rusňák, M. Sloboda, Z. Barnovská) defended in STAR and 2 MSc. theses in ALICE (V. Kučera, Č. Zach). Until 2012 the team had 2 additional scientists, P. Chung and V. Kushpil.

In 2010-2014, the team members participated actively in experimental data taking both at RHIC and CERN and fulfilled successfully their obligations given by collaboration rules. They were also actively involved in the offline monitoring of data quality (ALICE and STAR) and contributed to detector calibrations (e.g. P. Federič, calibration of the STAR Time Projection Chamber in 2014). The team members were also actively participating in detector upgrades for ALICE, STAR and ISOLDE and large scale computing for ALICE and STAR as outlined below.

In the evaluated period, the research activities related to physics observables in ALICE and STAR covered studies of jet-like correlations and jets, production of quarkonia and open charm mesons, correlation femtoscopy as well as formulating ideas for the Beam Energy Scan programme at RHIC. Two team members served also as conveners of the Physics Working Groups (STAR: J. Bielčík, Heavy-Flavor PWG, 2009-12, ALICE: J. Bielčíková, PWG-Jets, from 2013). The research results achieved by team members were presented at international conferences, workshops, symposia and schools (STAR: 65, ALICE: 30, ISOLDE: 3, phenomenology of heavy-ions 3, 3 seminars abroad) including Quark Matter, Hard Probes, SQM, ICHEP and EPS-HEP. The team members are also principal authors of STAR and ALICE collaboration papers published in 2010-14 or papers in various stages of internal review process at the end of 2014. Below an overview of the main research results grouped topically is given.

### BEAM ENERGY SCAN PROGRAMME IN STAR

The discovery of perfect quark-gluon liquid (sQGP) in 2005 made with active participation of the team members provides an important milestone in the long-term goal of condensed matter physics of QCD - to map out as much of the QCD phase diagram as possible, trying to understand various ways in which the hadron-to-sQGP transition may occur. Highlights of this part of soft physics programme at RHIC were presented by M. Šumbera at Hadron Collider Physics Symposium 2011 in Paris. The goal of the ongoing Beam Energy Scan (BES) programme is to search for the turn-off of sQGP signatures, signals of QCD phase boundary and existence of a critical point in the QCD phase diagram. M. Šumbera was involved in

formulating goals of this programme and reported first results from the BES programme at the International Symposium on Multiparticle Dynamics (ISMD) 2012 and EPS HEP 2013.

## CORRELATION FEMTOSCOPY

Bose–Einstein correlations of bosons emitted from a thermalized source carry important information about the space-time extent of the particle emitting source. Previous three-dimensional analyses of the pion source revealed a heavy, non-Gaussian tail in the direction of the pair transverse momentum. Its interpretation in terms of pure hydrodynamical evolution is, however, complicated by the strong contribution of feed-down from longlived resonances to the pion source. On the other hand, kaons provide a much cleaner probe of the expanding fireball. The team members recently carried out the first three-dimensional (3D) kaon correlation analysis, using Cartesian harmonics decomposition technique. In contrary to pions, the 3D kaon source function is largely Gaussian. Comparison with thermal and a hydrokinetic model simulations show that resonance decays, as well as non-zero emission duration and/or rescattering in the hadronic phase play an important role. The results of the 3D extent of the kaon source with respect to the pair transverse momentum favour the hydrokinetic model over the exact  $m_T$ -scaling featured by perfect hydrodynamical models. This complex physics analysis was performed solely by the team members P. Chung, R. Vertési, P. Chaloupka and M. Šumbera. The physics results are published on behalf of the STAR Collaboration in *L. Adamczyk et al. (STAR), Phys. Rev. C 88 (2013) 034906*. The results were also presented at several major international conferences, such as EPS HEP 2011, PANIC 2011 and ISMD 2013 (M. Šumbera), Strangeness in Quark Matter 2013 (R. Vertési).

Motivated by previous  $\pi$ – $\Xi$  correlation analysis in Au+Au collisions at 200 GeV (Ph.D. thesis of P. Chaloupka, Chales Univ., 2010) where  $\Xi^*(1530)$  resonance was observed for the first time in heavy-ion collisions, R. Lednický (JINR Dubna and IoP Prague), P. Chaloupka and M. Šumbera formulated correlation femtoscopy–based approach to narrow resonance formation via final state interaction. Since in this case relative momenta of the particles forming the pair are not negligible when compared to the widths of single particle spectra usual form of the smoothness approximation has to be generalized. Results were presented by M. Šumbera at ISMD 2011.

## STUDIES OF JET PRODUCTION AND ITS MEDIUM MODIFICATION

Jets are collimated sprays of particles created by hadronization and fragmentation of hard scattered partons. In p+p collisions, measurements of jet properties allow to test pQCD predictions and in parallel serve as a reference for jet measurements in heavy-ion collisions. In heavy-ion collisions jets serve as a probe of hot and dense matter formed. Studies of their in-medium modification are expected to provide a higher sensitivity to the medium properties than measurement of inclusive particle production or di-hadron correlations at large transverse momentum, which suffer from number of limitations. The leading hadrons are a mixture of parent quarks and gluons and in addition as a fragmentation product, they carry only a fraction of parton's energy and ultimately sample a wide range of partonic energies. The jet reconstruction in large and fluctuating background present in heavy-ion collisions is however very challenging and first results were reported by STAR only in 2008.

The team members under lead of J. Bielčíková, who currently serves as a convener of the Physics Working Group of Jets in ALICE and in past served in this position in STAR, significantly contribute to studies of jets both in ALICE and STAR.



## ***Studies of jet properties in ALICE***

Ph.D. student M. Vajzer under supervision of J. Bielčík and J. Bielčíková, performed an analysis of inclusive charged jet spectra in p+p collisions at 7 TeV. The main physics results are fully corrected cross sections of charged jets for several resolution parameters  $R=0.2-0.6$  and their relative ratios as a measure of jet collimation. These results were submitted together with other jet shape properties in p+p collisions at 7 TeV to *Phys. Rev. D* (arXiv:1411.4969) on behalf of ALICE. M. Vajzer and J. Bielčíková are principal authors of this ALICE paper together with O. Busch (Univ. of Heidelberg), S. Prasad (Bose Institute Kolkata/Wayne State Univ.) and C. Pruneau (Wayne State Univ.), who performed jet shape studies. The results were presented by M. Vajzer at several international conferences (EPS HEP 2013, Hot Quarks 2012 and posters at Quark Matter 2012 and Hard Probes 2012).

M. Vajzer worked in 2013 closely with colleagues from ALICE at University in Muenster (J. Wessels, C. Klein-Boesing). During his 3-month DAAD research visit in Muenster, fruitful collaboration on POWHEG simulations among the two teams was established. The results of this scientific stay and following studies performed already at NPI are various jet properties in p+p and p+Pb collisions analyzed in POWHEG. These results are now widely used in ALICE for comparisons with data. M. Vajzer presented his results at the Quark Matter 2014 conference (poster) and they will be a part of the ALICE paper on full jet production in p+Pb collisions under preparation.

Ph.D. student V. Kučera focused under supervision of J. Bielčíková on studies of strange particle production in jets and underlying event in p+Pb and Pb+Pb collisions at the LHC. This study, which employs excellent particle identification capabilities of ALICE, is expected to bring important insights into baryon and meson production mechanisms in heavy-ion collisions. Already at RHIC energy it was observed that baryon/meson ratios are enhanced relative to those in p+p collisions. In order to quantify whether this is due to radial flow, parton coalescence and recombination in medium or some other effects, it is necessary to establish whether these enhanced ratios are also present in jets produced in p+Pb/Pb+Pb collisions. J. Bielčíková and V. Kučera together with X. Zhang and M. Ploskon (LBNL, USA), initiated studies of strange particles,  $\Lambda$  and  $K^0_S$  produced in jets in p+Pb collisions at 5.02 TeV energy. The results were presented at several conferences, including the presentation of V. Kučera at Hot Quarks 2014. A paper proposal was approved by ALICE in November 2014. V. Kučera and J. Bielčíková are principal authors of this manuscript under preparation together with X. Zhang and M. Ploskon.

The analysis of strange particle production in Pb+Pb collisions is performed by V. Kučera and J. Bielčíková together with the Ph.D. student A. Zimmermann (Univ. of Heidelberg). Particle identification techniques were consulted with the ALICE group at IPHC Strasbourg (France), where V. Kučera has his co-supervising institution in a framework of Czech-French double-doctorate studies. V. Kučera presented the preliminary results at Hot Quarks 2014. The investigation of systematic uncertainties began at the end of 2014 and a paper for ALICE, where V. Kučera and J. Bielčíková will be principal authors together with A. Zimmermann, is expected in 2015.

The last jet analysis in ALICE carried by our team was related to hadron-jet correlations. This novel technique introduced by ALICE enables the collinear-safe measurement of reconstructed jets in heavy-ion collisions with a low infrared cutoff, over a wide range of jet energy and resolution parameters. F. Křížek, who joined the team in 2013, analysed the spectra of charged jets recoiling from a hadron with large transverse momentum in p+p collisions at 7 TeV and their correlations. The obtained results serve as a constraint of pQCD calculations. While the data are surprisingly in a good agreement with PYTHIA, the NLO pQCD calculations overshoot the measured data largely, which points to a necessity to perform NNLO calculations.

The measurement in p+p collisions established also the crucial baseline for the measurement of recoil jet spectra in Pb+Pb collisions in order to quantify medium modification of recoiling

jets. The analysis was finalized in 2014 and F. Křížek is a principal author of a related ALICE paper draft on h+jet production together with L. Cunqueiro (CERN), P. Jacobs (LBNL, USA) and R. Ma (Yale/BNL), who performed the analysis in Pb+Pb collisions. The paper proposal was approved in 2014 and is in a final round of internal collaboration review and will be submitted to Phys. Rev. C in spring 2015. The results were presented by F. Křížek at 10<sup>th</sup> High- $p_T$  Physics at RHIC/LHC era workshop in 2014 and the related proceedings.

### ***Studies of jet properties in STAR***

At RHIC energy in addition to large and fluctuating background in heavy-ion collisions, jet analyses are challenged by relatively small production rate of jets relative to the LHC, where jet production is copious. Ph.D. student J. Kapitán and MSc. student J. Rusňák under supervision of M. Šumbera and J. Bielčíková, performed analysis of full jet spectra in d+Au collisions at 200 GeV. The results were presented at several conferences including talks at Hard Probes 2010 and Hot Quarks 2010 and a poster at Quark Matter 2011. The results are a part of J. Kapitán's Ph.D. thesis defended at Charles University in 2012.

In 2012, the team members (J. Rusňák – already a Ph.D. student) then significantly extended the pioneering STAR measurements in Au+Au collisions from Run7 data (2007) data using a moderate low-momentum cut-off on leading hadron in a jet while keeping a low-momentum constituent cut of 200 MeV/c and analysed high statistics Au+Au data set from Run11 (2011). The preliminary results on nuclear modification factor of charged jets in Au+Au collisions revealed a large suppression of jet production (jet quenching) in central Au+Au collisions and were presented by J. Rusňák on behalf of the STAR Collaboration in the invited plenary talk at the Hard Probes Conference 2013. In 2014 J. Rusňák focused on detailed evaluation of various systematic uncertainty sources and refinement of the p+p reference.

The publication of final results on behalf of STAR is expected in 2015. J. Rusňák, J. Bielčíková, P. Jacobs (LBNL) and M. Lamont (BNL), with whom the team members closely work, will be the principal authors of this STAR collaboration paper.

### **DI-HADRON CORRELATION STUDIES IN STAR**

Di-hadron correlations are commonly used to study jet properties on a statistical basis and these studies have a long-standing tradition in research carried by the team members. Earlier studies of associated particle distributions on the opposite side of the trigger particle, the so called away-side peak, revealed their significant modification in Au+Au relative to p+p and d+Au collisions at the top RHIC energy of 200 GeV (e.g. *Adams et al. (STAR), PRL 91 (2003) 072304*). J. Bielčíková in collaboration with O. Catu, H. Caines (Yale) and M. van Leeuwen (LBNL) performed systematic investigation of system size dependence of associated jet-like yields in hadron-triggered jets in d+Au, Cu+Cu and Au+Au collisions at 200 GeV in STAR, which were finalized shortly prior to this review (2009) and published in their final form in *Abelev et al. (STAR) Phys.Lett. B683 (2010) 123*. J. Bielčíková was a principal author of this paper together with O. Catu, H. Caines and M. van Leeuwen.

In the evaluated period the research focus of J. Bielčíková moved toward the systematic analysis of associated particle distribution on the near side of the trigger particle, which is also significantly modified in central Au+Au collisions. In contrast to p+p and d+Au collisions, where a jet-like peak narrow in azimuth and pseudorapidity is present, in central Au+Au collisions at 200 GeV an additional structure narrow in azimuth ( $\phi$ ) but broad in pseudorapidity ( $\eta$ ) was observed by STAR and later confirmed by the PHOBOS experiment. This structure, commonly referred to as the ridge, is found to be independent of  $\Delta\eta$  and extends at least over 4 units of  $\Delta\eta$ . The systematic study of energy and system size dependence of near-side di-hadron correlations enables determination of the jet-like correlations and the ridge properties at fixed

densities with different geometry. The study was performed in d+Au, Cu+Cu and Au+Au collisions at 62 and 200 GeV measured by STAR. The properties of jet-like correlation were found to be in a reasonable agreement with PYTHIA predictions, which is surprising considering that PYTHIA is a p+p event generator. There is also a remarkably little dependence of jet-like yields on the collision system at both 62 and 200 GeV except for central Au+Au collisions at 200 GeV. In central Au+Au collisions at 200 GeV the jet-like correlation is substantially broader and the spectrum of associated hadrons softer than in peripheral collisions than those in collisions of other systems in this kinematic regime. This may indicate that fragmentation is modified in the most central Au+Au collisions at 200 GeV and the parton fragments softer, perhaps due to a mechanism such as gluon bremsstrahlung.

Our studies revealed presence of the ridge not only in Au+Au collisions at 200 GeV as we reported earlier, but also in Cu+Cu collisions and also at a lower energy of 62 GeV. This demonstrates that the ridge is not a unique feature of large collision systems at the top RHIC energy. The fact that we found the measured ridge/jet ratio is within errors equal for both studied RHIC energies sets significant limits to models in which the ridge origin is not caused by hard parton scattering. First, when the ridge is measured using the standard ZYAM model, the ridge is comparable in Cu+Cu and Au+Au collisions and its energy dependence is the same as the energy dependence of the jet-like correlation. Second, when the jet-like contribution was subtracted and the 3<sup>rd</sup> component of the Fourier decomposition ( $v_3$ ), related to triangular flow and initial state fluctuations, calculated, different trends for Cu+Cu and Au+Au collisions were observed but no difference between the two energies was observed. J. Bielčiková worked on this study in collaboration with C. Nattrass (Yale/UTK) and H. Caines (Yale) and is together with them a principal author of the related STAR publication *B. Abelev et al. (STAR), Phys.Rev. C85 (2012) 014903*.

We note in context with studies at the LHC that recently the ridge-like structures were also reported at an order of higher collision energies in Pb+Pb collisions but surprisingly also in small systems such as high-multiplicity p+p collisions and p+Pb collisions. Combination of our data including their future extension to lower RHIC energies at 7-39 GeV in BES programme with those from the LHC will be a powerful tool to distinguish between various theoretical interpretations of the ridge in small and large collision systems.

## HEAVY-FLAVOUR PRODUCTION AT RHIC ENERGY

The measurements of production of hadrons containing a charm or a beauty quark play a key role in the STAR experimental programme. Heavy quarks are produced in the initial stage of a nucleus-nucleus collision and traverse through the dense nuclear medium and interact with the surrounding matter before they hadronize to particles measured in detectors. Production of heavy flavour hadrons can be influenced by two types of nuclear effects: cold nuclear matter effects and final state effects due to parton interactions with the produced nuclear matter. The properties of the nuclear matter could be studied by systematic investigation of these effects on open heavy flavor (D and B mesons) and quarkonia ( $J/\psi$  and  $\Upsilon$ ) production. The respective analyses were carried out by D. Tlusty, R. Vertési and P. Federič and were supervised by J. Bielčik.

### *Open heavy flavour studies*

The measurement of open heavy flavour mesons gives the most direct access to heavy quark kinematics. The HFT detector, completed and installed in 2014, will enable a precise displaced vertex determination and start a new era of open charm studies in STAR. However, the data collected in Run14 will become available for physics analyses only in 2015. Thanks to the large coverage of the STAR experiment also before the installation of the HFT it was possible to reconstruct D mesons in their hadronic decay channel ( $K+\pi$ ) without topological analysis, but with limited precision.

Ph.D. student D. Tlustý focused on the measurement of  $D^0$  and  $D^*$  meson production in hadronic channel in p+p collisions at 200 GeV. This analysis was completed and published on behalf of the STAR Collaboration in *Phys. Rev. D* 86 (2012) 72013 and also presented by D. Tlustý at several international conferences. D. Tlustý and J. Bielčik are principal authors of the mentioned publication together with X. Dong (LBNL), M. Mustafa (Purdue Univ.), K. Oh (Pusan Nat. Univ.), W. Xie (Purdue Univ.), Y. Zhang (USTC). The main results are differential and integrated cross sections of  $D^0$  and  $D^*$  production. The data are also used as a reference for the extraction of the nuclear modification factor of D mesons in Au+Au collisions but also constitute a crucial test of pQCD calculations. The data are consistent with an upper limit of FONLL calculations. In 2013 D. Tlustý extended his analysis to the data from p+p collisions at 500 GeV in order to extract the c-cbar production cross section for this highest available p+p collision energy at RHIC. In 2014, D. Tlustý with the help of a new team member, postdoc P. Federič, extended the  $p_T$  reach of D meson spectra up to 18 GeV/c exploiting the data triggered by the STAR Barrel Electromagnetic Calorimeter. The analysis of the D meson production in p+p collisions at 500 GeV was completed in 2014 and publication of the results is expected in 2015. D. Tlustý, P. Federič and J. Bielčik will be its principal authors.

The results on open charm production described above were presented by the team members also in talks on major international conferences (Strangeness in Quark Matter 2013, EPS HEP 2013, Quark Matter 2012, Hard Probes 2012, ICPAQGP 2010 etc. and related proceedings). The results are also a part of D. Tlustý's Ph.D. thesis defended at CTU in Prague in December 2014.

### **Quarkonia production**

Quarkonium yields have been predicted to be sensitive to the color deconfinement and therefore were expected to be a key signature of the Quark Gluon Plasma. Earlier research mainly concentrated on the charmonium states, such as the  $J/\psi$  meson. However, charmonium production is sensitive to recombination and therefore the signal is less easy to interpret. Bottomonium states, in contrast, are considered to be less sensitive to the latter effect. Since the different states are expected to dissociate at different temperatures, the bottomonium states, Upsilon 1S, 2S and 3S may serve as a thermometer of the strongly interacting QGP.

STAR has recently published measurements of the Upsilon ( $Y$ ) states in p+p, d+Au and Au+Au collisions at 200 GeV and found that the suppression of the  $Y(1S)$  state in the plasma is stronger than in cold nuclear matter, while the excited states are even more strongly suppressed (*L. Adamczyk et al. (STAR), Phys.Lett. B735 (2014) 127*). R. Vertési, started to work in 2013 in parallel on the determination of the  $Y$  yields in a unique data set of U+U collisions, where even higher energy density can be reached than in Au+Au collisions at the same collision energy. This study is expected to provide further insights to the mechanism of deconfinement in heavy-ion collisions and help to understand nature of the strong interaction. The measured  $Y(1S)$  suppression in central U+U collisions is found to be within errors consistent with measurements of  $Y$  suppression at the LHC reported by CMS. R. Vertési presented his results at several international conferences (ICHEP 2014, PANIC 2014 (talks), Quark Matter 2014 (poster) and related proceedings). The paper based on his analysis is in preparation in STAR and R. Vertési will be its exclusive principal author.

### **INNER TRACKER SYSTEM OF THE ALICE EXPERIMENT**

Since its beginning in 1993 the team is involved the ALICE Inner Tracker System. During the LHC RUN1 (2010-13), S. Kushpil provided an important support for operation of 2 ITS middle layers consisting of Silicon Drift Detectors (SDD). Strong sensitivity of SDD's drift velocity on ambient air temperature demands its permanent

calibration using charge injectors. S. Kushpil reported results of her activity at 2nd international conference TIPP 2011 and Nuclear Science Symposium and Medical Imaging Conference (NSS/MIC), 2012, IEEE.

A new MAPS-based ITS detector is expected to be ready before LHC RUN3 which will start in 2020. The team members (F. Křížek, S. Kushpil, T. Vaňát, J. Pospíšil, K. Vysoká, P. Příbeli) under leadership of J. Ferencei play an active role in several R&D activities for the ITS upgrade project. Until 2012, the research scientist V. Kushpil also participated in these efforts before he moved to another team at NPI.

This new silicon tracker will allow ALICE to measure charm and beauty production in Pb+Pb collisions with sufficient statistical accuracy down to very low transverse momentum, measure charm baryons and perform exclusive measurements of beauty production. These measurements are essential in order to understand the energy loss mechanism and thermalization of heavy quarks in QGP.

As a part of the R&D activities, the team conducted series of measurements to determine Single Event Upset (SEU) probability for SRAM memories in 180 nm technology from TowerJazz foundry foreseen for mass production of the ITS silicon pixel chips. The results confirmed the SEU rate at the acceptable level of  $10^{-13} \text{ cm}^2 \text{ bit}^{-1}$  causing rather tolerable data corruption ( $\sim 10^{-9} \text{ bit}^{-1}$  for the central, most affected chip) with no necessity for a special protection. This was an important verification of technology suitability for production of monolithic active pixel sensors (MAPS) with on-chip integrated electronics. Measurements performed at U-120M cyclotron in NPI together with those carried by our team members at higher energies in Paul Scherer Inst. in Villigen are a part of the published *“Technical Design Report for the Upgrade of the ALICE Tracking System”*, *Journal of Physics G, Nuclear and Particle Physics* 41 (2014) 087002, p. 38-39. The investigations will continue for higher currents to study functional failures (Single Event Latch-ups).

For the ITS readout modules located approximately 1m from the LHC beam pipe in radiation environment with expected lifetime total ionization dose of 10 krad, the use of a large number of field programmable arrays (FPGA) with 4896 input/output high speed (1.2 Gbit/s) channels is planned. Due to limited financial resources only commercial grade FPGA, i.e. with no expensive radiation hardness certification, can be considered to be used in such large quantities. With this goal in mind the team performed series of detailed measurements at the NPI cyclotron and tested the radiation hardness of selected FLASH type of FPGA's from Microsemi, the only company producing this type of FPGAs. Up to now 2 types of FLASH FPGA from Microsemi were tested, namely SmartFusion2 and IGLOO2. As expected the radiation hardness of the configuration memory was confirmed to be excellent with no SEU observed up to the values of 100 krad. However, failure of the reprogramming circuitry already at low values of ionization doses of just few krad was determined. The team is cooperating with the experts from Microsemi to seek the suitable solution. The results were reported by T. Vaňát at the *Space FPGA Users Workshop, 2014, European Space Research and Technology Centre, Netherlands*.

Next, in collaboration with IEP SAS Košice in Slovakia, two high-speed cable candidates for data transfer from ITS silicon chips with suitable electrical parameters were tested for radiation resistance (total ionizing dose of 1 Mrad) at the NPI cyclotron. The cables, produced by Samtec (USA), 100  $\Omega$ , 30 AWG Micro Twinax and Accelerate Twinax Ribbon unfortunately during neutron activation analysis, which was also performed, revealed high chlorine, resp. high bromine contents and thus did not meet CERN safety criteria. Dedicated ALICE ITS halogen-free cable is under production by Samtec and will be subsequently analyzed for the presence of halogen elements at NPI and then irradiated at the cyclotron in 2015.

Considerable effort in the R&D activities was invested into automation of irradiating procedure at the cyclotron based on the predefined radiation doses. Computer and manually operated "beam stopper"/"energy degrader" was designed and constructed by F. Křížek and J. Ferencei. It allows a quick decrease of the proton beam energy at the expense of beam width increase

(in the ultimate case even absorbs the proton beam completely). Detailed simulations, performed using GEANT4 and SRIM programmes, were found in a good agreement with experimental measurements performed using the ionization chamber and the TimePix detector.

## **HEAVY FLAVOR TRACKER FOR THE STAR EXPERIMENT**

The team has been actively and continuously participating in preparation of a new Heavy Flavor Tracker (HFT) for STAR ever since 2007. The HFT was completed and installed in spring of 2014 and took successfully data in Run14. Ph.D. student J. Rusňák took over the responsibilities initiated by the Ph.D. student J. Kapitán back in 2007, which resulted in extensive simulations of the HFT performance for reconstruction of D and  $\Lambda_c$  charmed hadrons and which were a part of the Technical Design Report. These studies are documented in J. Kapitán's Ph.D. thesis defended at Charles University in 2012. J. Rusňák contributed to development of tracking software based on Kalman filter as well as performing sensor alignment surveys at LBNL, USA in summer 2013, where the HFT detector was assembled before its shipping to BNL.

## **LARGE SCALE COMPUTING ACTIVITIES FOR STAR**

The team carries continuous computing research for STAR since 2007. In the evaluated period, 2 Ph.D. students were active in this area. M. Zerola, who defended his Ph.D. thesis at CTU in Prague (2012), and D. Makatun, who joined the team in 2011. Scientific work of both students, supervised by M. Šumbera and co-supervised by J. Lauret (STAR computing coordinator, BNL), deals with and attacks the complex problem of efficient data movements on the network within a distributed environment.

Research of M. Zerola focused on real life data transfer and placement needs for large experiments such as STAR and its peta-scale requirements for data storage and computational power. He designed a new automated planning system and evaluated its performance. It was the first time in large experiments when an automated planning approach was used for reasoning about data transfers and CPU allocations. M. Zerola showed that computational complexity of the transfer problem is strongly NP-hard and proposed a 2 stage constraint model, coupling path planning and transfer scheduling phase for data transfers to a single destination. Several techniques for pruning the search space were explored and implemented. Next, an extension using the Mixed Integer Programming methods and several simplifications in scheduling phase were proposed and resulted in faster solving times while losing only a negligible fraction of the makespan quality. Simplistic yet robust architecture allows convenient job submission via web-interface while the back-end planner and the set of data movers take care of the work on behalf of users. With upcoming requirements for more frequent cloud computing, where data storage is constrained and the needs for prompt feeding CPUs by data is important, the automated data transfers and job allocation can greatly simplify user's task. This was addressed and an extension of the model for reasoning about computational power was proposed.

D. Makatun, who continues in this research, accomplished in 2014 studies of cache performance based on simulation using real-access pattern both from STAR and ALICE. D. Makatun also worked on development of RIFT (Reasoner For Intelligent File Transfer) and deployed it to the STAR computational farms RCF at BNL and NERSC at LBNL as well as to a local computational site at NPI.

The results were presented at international workshops ACAT 2010 and 2011 (M. Zerola) and ACAT 2013 and 2014 (D. Makatun).

## LARGE SCALE COMPUTING ACTIVITIES FOR ALICE

In 2010-2014, the research activity of our team included also computing for ALICE. We have been active in the ALICE Offline project ever since 2000 and have 1 representative in the ALICE Computing Board (D. Adamová). In particular the team is responsible for data processing and simulations in the Czech Republic. These activities take place in the computing center prague1cg2, involved in the Worldwide LHC Computing Grid (WLCG) and located in the Institute of Physics CAS (IoP) in Prague. Prague1cg2 provides currently up to 3 thousands computer cores (CPU) and over 1.1 PB of disk space for ALICE. A part of the disk capacity is located directly at NPI. It is interesting to note that at the end of 2009 we had about 400 CPU and 60 TB of disk space. The available computing and storage infrastructure has been built and gradually extended during last 10 years. The capacity is continuously being fully exploited. Since 2012, the ALICE Constitution introduced compulsory provision of computing and storage capacities for individual member institutions corresponding to their participation in the experiment. Therefore correct supply of resources is necessary and is continuously monitored. The resources delivered by our team on behalf of the Czech Republic are above 100% of the initial ALICE requirements.

Our job is to monitor progress of the production and in case of a problem find its cause and eliminate it. This requires daily checking of monitoring portals, knowledge of production software, which includes both ALICE software and the WLCG tools, and continuous communication with the ALICE Offline team at CERN. Our next task is to perform the installation and ongoing software upgrades required for the proper operation of data and simulation production at the computing centre. Furthermore, we have to ensure a regular supply of new hardware to meet increasing ALICE requirements. During 2010-2014, over 12 million of jobs were processed in the Czech Republic and over 17 PB of data was read from the Prague/Rez storage cluster for further processing. In connection with the coordination of production of ALICE in CR we are working together with colleagues from IoP and CERN on the development, testing and debugging of ALICE and WLCG software tools. A very interesting work was done by the MSc. student Č. Zach, who performed simulations of the ALICE computing model evaluating effects of various requirements on data location and the percentage of analysis jobs on the duration of these jobs and their efficiency. He also extended the simulation package MONARC2 used for the simulations. The work was presented at the CHEP conference in 2010 and was highly rated in the track wrap-up plenary talk (Č. Zach, CHEP 2010).

The results of our work, as well as reports on the results of the ALICE production and so called status reports have been regularly presented at large international conferences and workshops (D. Adamová: CHEP 2010 and 2012, Winter Meeting on Nuclear Physics, Italy 2010-2013 and 2014, ACAT 2014; Č. Zach CHEP 2010). The team members co-organized the international workshop ACAT2014 in Prague (D. Adamová, M. Šumbera). D. Adamová wrote together with P. Saiz Chapter 9 in the book *Grid Computing, Technology and Applications, Widespread Coverage and New Horizons*, ISBN: 978-953-51-0604-3, 2012. In the last 2 years, we were also involved in the Online-Offline (O2) Upgrade, specifically in the working group CWG10 (Control, Configuration & Monitoring).

## STUDY OF WEAK INTERACTIONS AT ISOLDE CERN

Experiments at the isotope separator ISOLDE at CERN study structure of weak interactions. The Standard Model (SM) is based on the pure vector-axial vector character of the electroweak interaction nevertheless experimental data allow existence of other types of weak interactions (e.g. scalar interactions are ruled out at the 7% level). D. Zákoucký is involved in experiments studying at ISOLDE specific low energy  $\beta$ -decays in order to search for possible scalar or tensor components or at least significantly improve the current experimental limits on their

existence. Two experimental facilities with very different experimental methods are employed. The Low Temperature Nuclear Orientation (LTNO) facility NICOLE (Nuclear Implantation into the Cold Online Equipment) is used to cool and orient radioactive isotopes produced at ISOLDE and the angular distributions of  $\beta$ -particles emitted in the decay of the oriented sample are measured. Specific  $\beta$ -decays sensitive to the possible admixture of tensor interaction (forbidden by the SM) are chosen. For that purpose, special HPGe detectors able to work at liquid He temperature were developed and produced at NPI. The results were published in *Phys.Rev. C90 (2014) 035502*.

The WITCH (Weak Interaction Trap for CHarged particles) facility consisting of a world-unique combination of 2 Penning traps and a retardation spectrometer allows to trap the radioactive nuclei and to form a cooled and scattering-free radioactive source, where nuclei decay at rest. Precise measurements of the shape of energy spectrum of recoiling nuclei, which is very sensitive to the character of the weak interaction, enable to search for a possible admixture of a scalar/tensor component. First results with  $^{35}\text{Ar}$  isotope, sensitive to a possible admixture of a scalar interaction, were published in *Phys.Rev.C90 (2014) 025502*. In 2014, work on a new method to study the same effect started and will be implemented after the ISOLDE beam-line will be rebuilt to enable polarization of the incoming beam of radioactive ions (using lasers). The results were published in total 9 papers (NIM, Phys.Rev.C) and out of 51 contributions at conferences and workshops, D. Žákoucký had 3 presentations (Bormio 2010 and 2014, ARIS2014). To the mentioned papers D. Žákoucký contributed at the level of about 15%.



## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Relativistic Heavy Ions, Neutrino Properties   |

Activities of the scientific team are developed in the three directions: experimental study of hadron's properties in medium, accelerator driven transmutation technologies, and neutrino mass measurement in tritium decay.

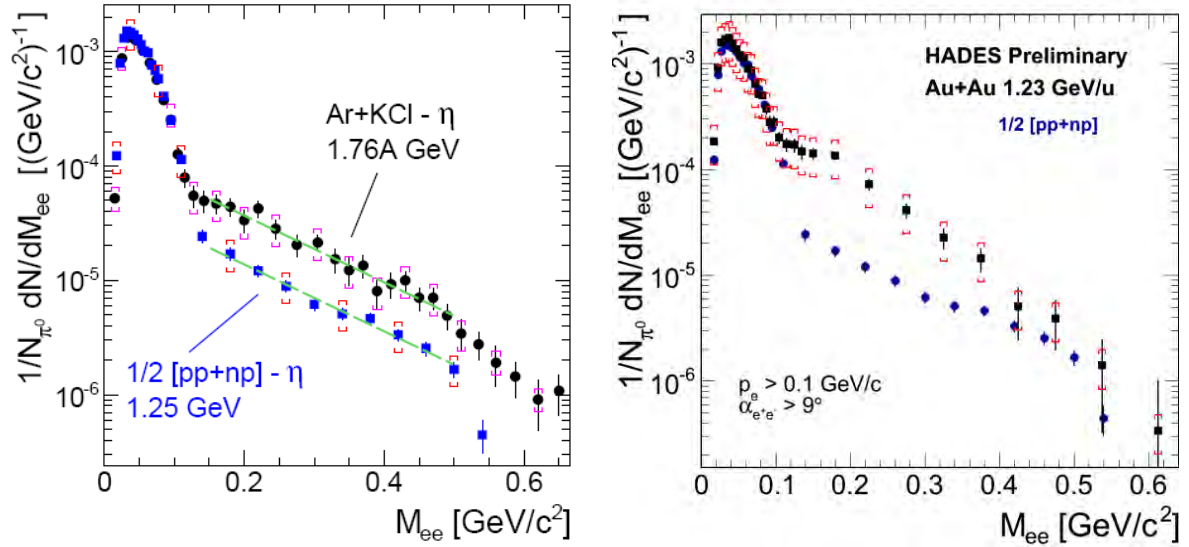
### EXPERIMENTAL STUDY OF HADRON'S PROPERTIES IN MEDIUM

Part of the team studying compressed and hot nuclear (hadronic) matter in relativistic heavy-ion collision (RHIC group) participates in the HADES collaboration. The collaboration operates the **H**igh **A**cceptance **D**i-**E**lectron **S**pectrometer (HADES), which is a dedicated facility for studies of the di-lepton decay of the vector mesons (i.e.  $\rho$  and  $\omega$ ). Vector mesons have a short life time and, for example, most of the  $\rho$  mesons decay already inside the nuclear matter. One of the branches of their decay leads to electron-positron pairs, which do not interact with the surrounding hadronic medium and hence provide undisturbed information about the properties of the original vector mesons inside the hot and dense nuclear medium. Also hyperon embedded in the nuclear medium presents a unique probe of the deep nuclear interior, which makes it possible to study a variety of otherwise inaccessible nuclear phenomena. Therefore experimental program of HADES and in particular of our group concentrates on the measurement of dilepton and strange particles yields in different combinations of projectile and target.

HADES was built with a significant contribution of the Czech Republic and it is installed on the SIS18 accelerator beam at Helmholtzzentrum für Schwerionenforschung ([GSI](#)) Darmstadt, Germany. The Czech team developed, built and operates large scintillation detectors, i.e. Time Of Flight wall (TOF) and Forward Hodoscope. These detectors are important part of particle identification chain in HADES as well as they are used to determine reaction centrality.

#### ***Hot and compressed nuclear matter (Ar+KCl and Au+Au experiments)***

Our group participated during the evaluation period on the analysis of previous experiments, interpretation of measured data and paper writing. Particularly analysis and interpretation of dilepton data from Ar+KCl experiment was done by F.Krizek in his PhD thesis, which he successfully defended in 2008. Results of his analysis were presented in international conferences, like QM2009, and final results were published in overview paper *Dielectron production in Ar+KCl collisions at 1.76 A GeV.*, Phys. Rev. C84(2011)014902. The strong enhancement  $\sim 3x$  over properly scaled superposition of the dielectron sources measured in elementary pp and quasi-free np reactions, see HADES previous papers, is visible in the "excess region". It suggests indeed that additional contributions from secondary processes in the dense phase of the collision are needed, leading to a non-linear scaling of the pair yield with  $A_{\text{part}}$ . In fact, at a given bombarding energy the excess scales  $Y_{\text{excess}} \propto A_{\text{part}}^{1.4}$ , i.e. much more strongly than pion production does. It is also interesting to note that the DLS result obtained in the Ca + Ca system also follows this trend. This might be interpreted, in analogy to sub threshold ( $K^-$ ,  $K^+$ , or  $\eta$ ) meson production at SIS18, as a fingerprint of in-medium effects related to multi-step processes, with baryonic resonances probably playing an important role.

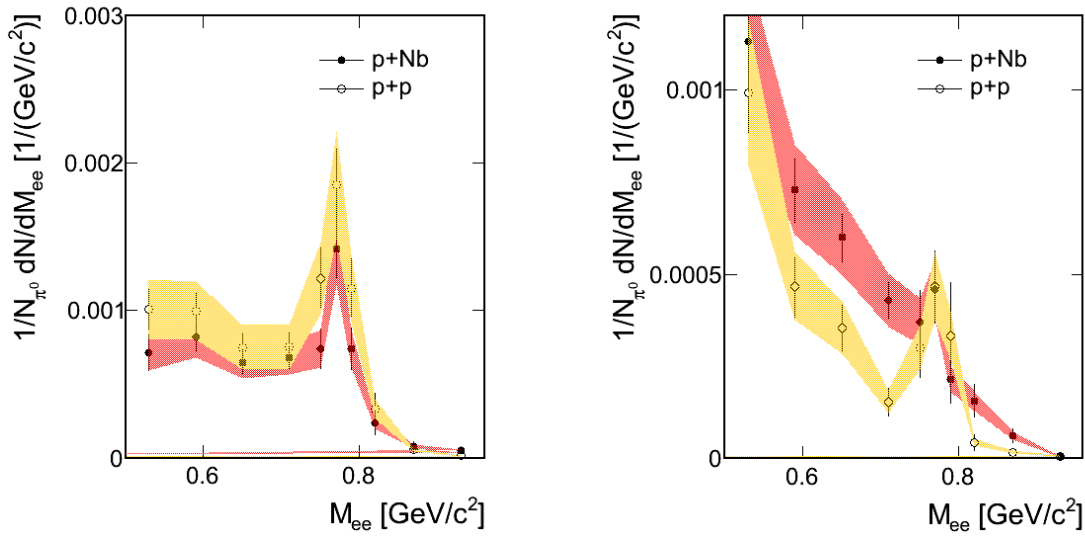


To further clarify these findings, about seven billion Au+Au collisions at 1.23A GeV have been recorded in April/May 2012 with an event rate of 10 kHz. First conclusion from the experiment analysis is an 8x higher dilepton yield in comparison to the factor 3x obtained in the previous Ar+KCl experiment, see for example A.Kugler talk at PANIC14 conference in Hamburg or T.Galatyuk (TU Darmstadt) talk at QM2014 conference in Darmstadt. As the analysis of the AuAu experiment is almost closed, series of publications on dilepton and strangeness production, neutral mesons, particle spectra etc. can be expected soon. To summarize, results indicated that medium effects are important both in the case of vector mesons and in the strangeness production inside a collision zone.

Members of the Czech team have been present during the six week beam time of Au+Au experiment and served as detectors (TOF, FW) experts, shift leaders (seniors) and DAQ experts. We prepared the calibration of the TOF detector including time-walk correction, performed analysis of embedded simulation data into experimental one with the aim to deduce on efficiency corrections. We also deduced the size of the collision zone (centrality of collision) and orientation of the reaction plane per event from the data. Particularly, data from the Forward Wall detector were studied in order to understand stability of the detector during the beam time and to determine the reaction plane. Satisfactory agreement between observed multiplicity of charged particles and prediction of transport model for different centralities was obtained. These analysis tasks were coordinated by member of our team P. Tlustý. He also was and still is active in the pion analysis group.

### **Cold nuclear matter (pp and pNb at 3.5GeV, pion induced collisions)**

We also found, see paper *First measurement of low momentum dielectrons radiated off cold nuclear matter. Phys.Lett. B715 (2012) 304-309*, similar effect comparing dilepton yields at p+p and p+Nb collisions at 3.5 GeV. The figures below show comparison of dilepton yields between p+Nb collisions and properly scaled p+p collisions. While for fast pairs with  $p_t > 800$  MeV/c there is no difference seen in left figure, for slow pairs with  $p_t < 800$  MeV/c the enhancement below rho-mass is clearly seen in right figure. Let us mention that the enhancement observed in Ar+KCl is also concentrated at small  $p_t$  of dilepton pairs.



To continue in the study of cold nuclear matter and also due to the limitations of available beam time at SIS18@GSI in 2013-2014 years, HADES collaboration decided to concentrate on pion induced reaction on heavy target after heavy ion campaign. During two experiments in 2014, secondary pion beam with rather broad distribution of momenta allowed excellent scanning of corresponding excitation functions exploiting dedicated pion beam line with active magnetic elements and pion tracker system. Achieved intensity of secondary pion beam was about 300 000/spill, extraction time about 2 seconds, full spill duration was about 4 seconds. Czech group repaired, tested and operated besides TOF and FW also small Hodoscope detector. This detector was used to control focusing of secondary pion beam and it was placed behind the target. Data from the Hodoscope detector together with the diamond START detector were analysed by L. Chlad (our diploma student). The pion tracker brought the possibility to determine with high precision momenta of each pion interacting with the target.

During the first period of pion beam time, i.e. in July 2014, most attention was put on the study of strange mesons and dilepton production in W and C targets exploiting secondary pion beam with momenta 1.7 GeV/c. It was collected enough statistics which allowed to clearly identify  $\phi$ ,  $K^0$ s,  $K^+$ ,  $K^-$ , mesons and  $\Lambda$  hyperon already on-line. For example obtained statistics will allow to study absorption of kaons in cold nuclear matter and to derive corresponding kaon potential. The second period in August - September 2014 was devoted to the study of the excitation function of one- and two-pion and dilepton production in pion-nucleon reactions in the so-called second resonance region. Particularly pion beam at momentum 0.656, 0.690, 0.748, and 0.800 GeV/c was exploited. Both the polyethylene target and carbon target were used and allowed thus to extract pion-proton interaction in polyethylene target by subtracting carbon contribution. Kinematical constrains for two-pion output channel were used to achieve the same goal. Data analysis on pion elastic scattering were independently analysed by L. Chlad (our diploma student) and P. Ramos (our PhD student). They both will continue in the analysis of the data during their PhD studies.

### **Upgrade of HADES experimental setup**

In the past five years the HADES spectrometer has undergone an extensive upgrade to be used at the first phase of the FAIR project for experiments at energies up to 10 GeV per nucleon. NPI scientists significantly contributed to this upgrade by changing the readout of TOF detector to a new faster TRB2+Shower addons. TRB based readout was intensively tested and tuned during the test beam times in 2011 and later used in AuAu@1.23 AGeV experiment in 2012 and pion beam times in 2014. Particularly it allowed increase of counting

rate in 2012 Au+Au experiment to 10 kHz from 2 kHz maximum rate available before the upgrade.

Another upgrade project is the Electromagnetic Calorimeter (ECAL) project for the HADES headed by the NPI group. The ECAL will allow measuring the direct decay of the eta and pi mesons by means of detection of photon pairs from their decay. Such data are very important mainly for experiments, where production of these particles is not well known, which is the case of reactions at energies 10 GeV per nucleon expected at FAIR. This will enable precise determination of meson production cross-sections. The knowledge of these cross-sections will allow us to properly account for corresponding dilepton yield from Dalitz decay of neutral mesons in the energy regime of the SIS100 beam, revealing other possible non-trivial sources of dileptons. Moreover, the investigation of  $\omega$  production via the decay channels  $\pi^0\pi^+\pi^-$  and  $\pi^0e^+e^-$  can be done combining the two photon detection in the ECAL calorimeter with a charged particle detection in the rest of the HADES spectrometer. Last but not least, great interest in the photon measurements is coming from the HADES strangeness program studying mainly neutral  $\Lambda(1405)$  and  $\Sigma(1385)$  resonances in elementary and heavy ion reactions.

Member of our group P. Tlustý is a technical coordinator of the ECAL project since its beginning before 2010. In the period 2010 – 2014 all crucial parts of the calorimeter were developed and tested. Lead glass modules as the active part of the detector were loaned from OPAL collaboration, disassembled, cleaned and prepared for the new photomultipliers. Two types of photomultipliers were selected as the suitable ones (1.5" EMI9903KB photomultipliers from former MIRAC experiment and new 3" photomultipliers Hamamatsu R6091). A 600 pieces of 1.5" photomultipliers were tested on gain and dark current and only perfect pieces were selected to be built in ECAL. The ECAL stability monitoring and calibration will be based on LED light pulses and optical distribution system with multimode optical fibres. These were developed in cooperation with the Optical laboratories of Faculty of Mathematics and Physics, Charles University in Prague. Remote controlled short pulse source for LED is being developed as well. A novel readout based on PaDiWa and TRB3 boards was developed for the calorimeter in GSI Darmstadt, and intensively tested by the Czech group with pulser and real signals from ECAL modules induced by cosmic muons and monitoring LED pulses.

Three test beam times on secondary quasi mono energetic photon beam at MAMI Mainz and electron/pion beam at CERN were organized by us in order to measure relative energy resolution and time resolution of the modules, electron/pion separation power and to test the read-out chain. The ECAL Technical Design Report (TDR) was approved by the FAIR council in 2014.

### ***Miscellaneous***

Czech scientific team around HADES organized one HADES collaboration meeting in Prague (5/2013) with about 75 international participants and co-organized a summer school for HADES students in Řež (10/2011). Members of the team actively participated in regular HADES collaboration meetings, which occurred twice a year. A. Kugler chaired HADES Collaboration board and was member of HADES executive board up to the end of 2014.

### ***R&D for future CBM@FAIR***

Scientists from the RHIC group are also members of the Compressed Baryonic Matter (CBM) experiment as a successor project to the HADES. The CBM experiment is under preparation to study the nuclear matter at extreme conditions with aim to detect hadrons, leptons and photons originating in the nucleus-nucleus collisions at energies up to 35 GeV per nucleon. The detailed study of rare phenomena as e.g. "open charm" production or di-lepton decay of vector mesons – thus the probes which bring the most valuable information on the state of matter in extreme conditions – will be possible thanks to high FAIR beam intensities.

The NPI group participated in the development of the Projectile Spectator Detector (PSD) for measuring the projectile fragments which will provide information on the reactions centrality and the reaction plane. Reaction plane reconstruction and particle flow were studied by simulations using various reaction models. These simulations were carried out by our PhD student V.Mikhaylov in 2014. The results show that the PSD can be used as standalone detector for the centrality determination and, depending on the collision energy, has a comparable impact parameter resolution to that of the silicon tracking system. This provides an independent method in the CBM experiment for the centrality determination based on spectator fragments. Regarding the flow, it was found out that the DCM-QGSM model is the most suitable for the collision fragment generation in the spectator region and energy region desired at CBM, and that the qualitative agreement with the experiment data for directed flow is acceptable for the PSD case.

An important characteristic of the avalanche photodiodes (APD) planned for the detector readout is the radiation hardness to the neutron fluxes of  $10^{13}$  n/cm<sup>2</sup> which corresponds to two months of CBM experiment operation. APDs from Hamamatsu, Zekotek and Ketek were irradiated using quasi-monoenergetic and white-spectrum neutron sources at Řež cyclotron. A dedicated setup was developed to measure Capacitance-Voltage (C-V), Current-Voltage (I-V), and Capacitance-Frequency (C-F) characteristics of ADP before, during and after the irradiation. After the irradiation, the C-V technique showed significant decrease of hysteresis and fast but not complete self-annealing. The I-V curve revealed about 1000 times increase of dark current after irradiation. The C-F study showed significant increase of short-living traps in Silicon. These results were presented on several conferences and CBM meetings and published in conference proceedings. Based also on the results of the Czech group, the PSD Technical Design Report was approved at the end of 2014.

## ACCELERATOR DRIVEN TRANSMUTATION TECHNOLOGIES

Spallation reactions as a perspective source of neutrons has been studied with an increased interest in the last decades. These studies are motivated by the need of high neutron fluxes for material research, transmutation of nuclear waste or production of nuclear fuel from thorium. Accelerator driven systems producing high fluxes of neutrons, due to their high safety and unique properties, seem to be both perspective energy source and nuclear waste transmutation facility.

The main activity of the group concerns study of prototypes of such a system, i.e. of setups consisted of heavy metal target and uranium blanket, irradiated by relativistic proton and deuteron beams at JINR Dubna. Within the international research project “Energy and Transmutation of Radioactive Waste” our group study various aspects of spallation reaction, neutron production, transport and usage of spallation neutrons for transmutation of nuclear waste. Last years it took part in several experiments with the spallation target “Kvinta” irradiated by deuteron beams of various energies, where a high energy neutron production and transmutation of radioactive samples were studied. We concentrate on study of neutron field spatial and energy distributions as well as on detailed study of neutron induced reactions. Activation detectors from Au, Al, Bi, In, Ta, and Y have been used to measure high energy neutron spectrum in dedicated places of the setup. Analysis and simulation of these and also previous experiments was mostly finished, discussed on international conferences and published. Cross-sections of ( $n,xn$ ) activation reactions were measured using quasi mono energetic neutron source at Řež and Uppsala cyclotrons in the framework of ERINDA (European Research Infrastructures for Nuclear Data Applications) project. Data were published in series of papers (most recent is *Studies of ( $n,xn$ ) cross-sections in Al, Au, Bi, Cu, Fe, I, In, Mg, Ni, Ta, Y, and Zn by the activation method, NIM A726 (2013) 84-89*) and included in the EXFOR database. Cross-sections of relativistic deuterons on natural copper were measured as well. The data for 38 different reactions and eight deuteron energies were discussed on many conferences and finally published in paper *Cross-section studies of relativistic deuteron reactions on copper by activation method, NIM B344 (2015) 63-69*.

Members of the group organized two international meetings, namely 1st ERINDA Progress Meeting and Scientific Workshop, January 16-18, 2012, Vila Lanna, Prague, and fourteenth session of the AER Working Group F - "Spent Fuel Transmutations" and meeting of INPRO IAEA Collaborative Project SYNERGIES "Synergetic Nuclear Energy Regional Group Interactions Evaluated for Sustainability", April 10 – 13, 2012, Liblice. Both meetings served as a place for intensive discussions on spallation data measured by the group.

## **NEUTRINO MASS MEASUREMENT IN TRITIUM DECAY**

"Electron spectroscopy group" is fully engaged in the international project KATRIN (Karlsruhe TRItium Neutrino experiment) the aim of which is to increase sensitivity to the electron neutrino mass ( $m_\nu$ ) determination by one order of magnitude up to 200 meV within 3 years of the measurement time. The experimental method consists in the measurement with unprecedented precision of the end point beta spectrum shape observed in the tritium decay. Our group belongs to the founders of the project together with the physicists from Germany, Great Britain, Russia and USA.

Our team participates in the KATRIN task Calibration and Monitoring, one of us is a co-leader of the task (D. Venos). Two of us are the members of the KATRIN collaboration board (O. Dragoun, D. Venos).

### ***KATRIN and our role in it***

The KATRIN complex with length of 70 m consists of rear section, windowless gaseous tritium source (WGTS), differential pumping section, cryogenic pumping section, electron pre-spectrometer (PS), electron main spectrometer (MS), monitoring spectrometer (MoS) and focal plane detector (FPD). Both pumping sections prevent the tritium molecules to reach the PS, MS and FPD and to cause additional background. The beta electrons guided by magnetic field from the WGTS into non-tritiated part will be electrostatically analysed in the MS and afterwards detected in the FPD.

There exist five systematic effects which uncertainties have the direct influence on the  $m_\nu^2$  value to be determined in the KATRIN experiment. The knowledge and stabilization of the experimental parameters related to these effects is crucial for the sensitivity on neutrino mass of 200 meV. Our activity in the KATRIN project is related to two systematic effects and to the calibration of the energy scale.

The first systematic effect is represented by an unrecognized instability of the analyzing 20 kV high voltage (HV) at the MS which causes a negative shift of the fitted  $m_\nu^2$ . Additionally to the measurement of the HV by means of the two precision high voltage dividers and two voltmeters, the HV stability will be monitored with the MoS. Any change of electron line position in the spectrum measured at MoS with suitable source of mono energetic electrons of stable energy can indicate the instability of the HV. The second systematic effect is connected with the plasma charge and its fluctuation expected in the WGTS due to the huge amount of the tritium decays. It was suggested to apply the gaseous source of the mono energetic electrons into WGTS without and with the tritium inside. From the comparison of the measured spectra of mono energetic electrons the information about the plasma behaviour will be obtained.

The calibration of the KATRIN energy scale will allow determining the energy of the tritium spectrum end point. Including relevant atomic and molecular binding energies and atomic constants the value of the endpoint energy can be directly compared with a mass difference of the tritium and helium atoms which is available from the independent Penning trap measurement. This comparison represents important cross-check of the analysis procedure. In this case the gaseous source emitting the electrons with known energies applied into WGTS will be used for the energy calibration.

Our team suggested using in the MoS the solid  $^{83}\text{Rb}$  ( $T_{1/2}=86.2$  d) source prepared by the vacuum evaporation or by the implantation of the  $^{83}\text{Rb}$  on a suitable substrate. The daughter isotope  $^{83\text{m}}\text{Kr}$  ( $T_{1/2}=1.8$  h) possesses K shell conversion electrons of the 32.2 keV transition, K-32, with energy of 17824 eV that is close to the tritium endpoint energy of about 18575 eV. The reliable production of the vacuum evaporation and/or implanted sources and the stability of the K-32 electron energy at level of 3 ppm/month was our task. Evidently, a similar  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  generator, on the contrary capable to emanate the  $^{83\text{m}}\text{Kr}$ , is suitable for application into the WGTS. Such a gaseous source of mono energetic electrons will provide information about plasma charge value (from shift of the conversion line) and its fluctuation (from broadening of the conversion line). The calibration of the energy scale can be determined with up to 4 electron lines observed in the  $^{83\text{m}}\text{Kr}$  decay. Moreover, the check of the KATRIN spectrometer response function will be accomplished. For this purpose we suggested and developed the source based on deposition of the  $^{83}\text{Rb}$  into the zeolite beads. The reliable production of such a source, large emanation of  $^{83\text{m}}\text{Kr}$  from the zeolite and strong binding of the  $^{83}\text{Rb}$  in the beads (the contamination with rubidium would increase the background in KATRIN complex for a long time) were the main aims in this work.

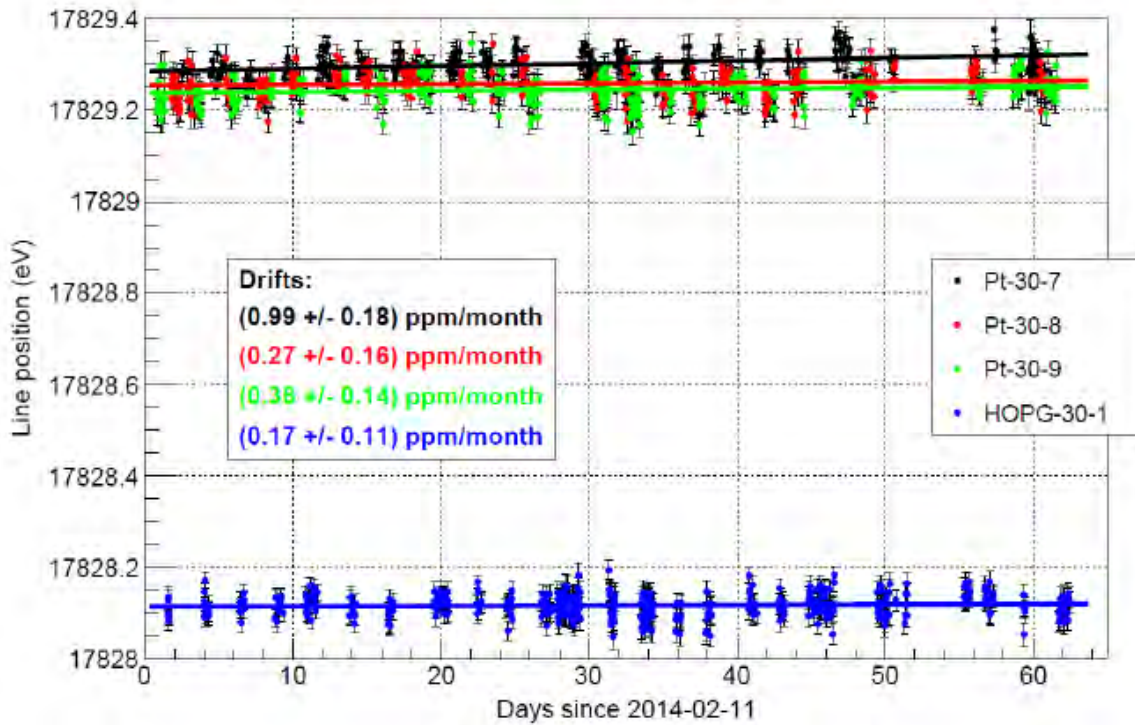
The necessary  $^{83}\text{Rb}$  activity for our work was almost fully produced at the NPI Řež cyclotron U-120M. While for the solid HV monitoring source the required activity of units of MBq, in the case of the gaseous source the activity of the hundreds MBq is expected.

### **R&D of the solid $^{83\text{m}}\text{Kr}$ monitoring source**

The valuable experiences of our previous experimental study about the photoelectron source  $^{241}\text{Am}/\text{Co}$ , intended at early stage also as a monitoring source, were collected and published, see a paper *Feasibility of photoelectron sources for testing the energy scale stability of the KATRIN  $\beta$ -ray spectrometer Appl. Rad. Isot. 69(2011)672*. The first sources for the monitoring were produced by vacuum evaporation of the  $^{83}\text{Rb}$  on the carbon foils at NPI and at ISOLDE, CERN mass-separator by implantation of the  $^{83}\text{Rb}$  ions at energy of 30 keV into the Pt and Au substrates. The stability of the K-32 electron energy of the sources was measured at the long term experiment at the Mainz University electron spectrometer. The main result sounds: the energy of the K-32 electrons from the sources is linearly dependent on the time and its change, a drift, is less than KATRIN limit of 3 ppm/month. This achievement was published in two papers: *The development of a super-stable standard for monitoring the energy scale of electron spectrometers in the energy range up to 20 keV, Meas. Technique 53(2010)573* and *Ultra stable implanted  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  electron sources for the energy scale monitoring in the KATRIN experiment 2013 JINST 8 P03009*. In such a way the monitoring concept for the KATRIN was justified. Therefore, the Mainz electron spectrometer was transported to KIT and renovated in order to serve as the KATRIN MoS. We supplied new sources holder of revolver type for the simultaneous installation up to 4 sources and XYZ table. The table allows the source alignment in space relative to the spectrometer centre. We participated on the development of the MoS detector system. Hereafter, the vacuum evaporation sources were abandoned due to dependence of the K-32 electron energy on the vacuum conditions in neighbourhood of the source. Further, the methods for the characterization of the implanted sources before their installation into MoS were developed. These are based on the silicon drift (SDD) and Timepix detectors. The activity of  $^{83}\text{Rb}$  and retention of  $^{83\text{m}}\text{Kr}$  in the source are determined with the SDD. For the retention measurement the special technique with closed (tight for the  $^{83\text{m}}\text{Kr}$  gas) and open chamber was developed. Contrary to general expectation of 100 % retention of the  $^{83\text{m}}\text{Kr}$  for the implanted sources the measurement showed in average the value of 90 %. The distribution of the radioactivity in the source area is measured with the Timepix detector implemented in close collaboration with the IEAP CTU Prague. In addition to our earlier precise measurement of the 32 keV energy transition (32151.7(5) eV) we were able to measure the precise energy of the  $^{83\text{m}}\text{Kr}$  9.4 keV transition as 9405.8(3) eV. For this a several check measurements were accomplished in collaboration with the Department of Dosimetry of the FNSPE CTU Prague. The result was published in *Precise energy of the 9.4*



keV gamma transition observed in the  $^{83}\text{Rb}$  decay, *Europ. Phys. Jour. A*(2012) 48:12. Using these transition energies the precise energies of all groups of the conversion electrons observed in the decay of the  $^{83\text{m}}\text{Kr}$  can be determined. After the MoS was commissioned at the KIT the drifts of the K-32 electron line for 8 sources prepared at ISOLDE (Pt or Ir foil substrates,  $^{83}\text{Rb}$  ions implanted with energies of 15 or 10 keV, different activities of the sources in the range of 0.6-3.3 MBq) were measured at the MoS. Nevertheless, due to the strong competition on the ISOLDE ion beam time the production of the implanted source was relocated to the mass-separator of the Bonn University. The routine process of implantation at energy of the  $^{83}\text{Rb}$  ions of 30 keV and with an efficiency of 23 % was finally achieved. Two sources prepared in the same way exhibited almost identical properties, the value of the drift in K-32 energy including. In such a way the reproducibility in the production of the sources at Bonn was proved. The 65 days measurement of the K-32 energy stability yielded for both sources a very favourable low drift of  $\sim 0.3$  ppm/month, see figure below.



The measurement period is comparable with two months of the KATRIN experimental runs. Evidently, this result is characteristic for the whole monitoring system i.e. MoS with its electric equipment and the source itself. In such a way the system MoS+electron source for the monitoring of the KATRIN HV is ready for the use. The implantations into the other substrates - ZnO and HOPG and at the lower  $^{83}\text{Rb}$  ion energies of 12, 8 and 4 keV started additionally. The  $^{83}\text{Rb}$  activity for all Bonn implantations was regularly supplied by the NPI. The MoS construction and experiences gained during the K-32 electrons energy stability measurements were published in *High-voltage monitoring with a solenoid retarding spectrometer at the KATRIN*, 2014 JINST 9 P06022. The MoS data analysis was improved. The correct account of the dead time losses was introduced and the stability of the fit process was substantially increased. The description of the spectral line with asymmetric Doniach&Sunjic shape was proved as more advantageous over the doublet Lorentz shape in *Electron line shape of the KATRIN monitor spectrometer*, 2013 JINST 8 T12002. Careful analysis of numerous MoS data reveals that the value of the K-32 electron energy drift depends very probably linearly on the volume density of  $^{83}\text{Rb}$  atoms in the substrate. The long term measurement at the MoS with two KATRIN high voltage dividers in parallel was successfully accomplished and the divider properties could be compared. The test of the “full monitoring concept”, i.e. the connection of



the MoS and MS with common high voltage was successfully performed early in January, 2015.

In collaboration with JINR Dubna the influence of the host on the value and stability of the electron binding energies of different atoms was studied and about 10 papers were published. The most relevant concerning to the krypton and rubidium atoms are: *Improved energies for the 5.2 keV M1 and 42.0 keV M2 nuclear transitions in  $^{83}\text{Rb}$*  Eur. Phys. Jour. A (2014) 50:59 and *Influence of host matrices on krypton electron binding energies and KLL Auger transition energies* Jour. Elect. Spec. Rel. Phen. 197(2014)64. The Dubna group also started to develop the  $^{83}\text{Rb}$  implantation technique with the efficiency larger than 50 %. In case of success their technique will be transferred to the Bonn mass-separator.

### **R&D of gaseous $^{83m}\text{Kr}$ source based on zeolite substrate**

The desired isotope  $^{83}\text{Rb}$  was produced at the NPI cyclotron U-120M by irradiation with protons of the natural krypton using pressurized gaseous target. Because large activity of the  $^{83}\text{Rb}$  is necessary for the gaseous krypton source the gas target equipped with cooling of its input windows by a helium gas at room temperature was developed. This allowed us to use the natural krypton in the target at higher pressure and also the larger proton beam current. As a result the time of irradiation for the production of a given of  $^{83}\text{Rb}$  activity was reduced by a factor of 3.6. With this target and infrastructure accompanied the production of  $\sim 1$  GBq of  $^{83}\text{Rb}$  is possible. The experiment KATRIN belongs to the category of the low background facilities therefore the possible release of long living  $^{83}\text{Rb}$  from zeolite into the electron beam line is dangerous. For this reason the  $^{83}\text{Rb}$  release was studied in collaboration with Münster University and the underground low background laboratory in Grand Sasso. Upper limit on the rubidium release, compatible with KATRIN demand, was obtained, see *Limits on the release of Rb isotopes from a zeolite based  $^{83m}\text{Kr}$  calibration source for the XENON project 2011 JINST 6 p10013*.

Further, in collaboration with the Max-Planck-Institute for Nuclear Physics, Heidelberg the emanation of radioactive radon isotopes from the zeolite was also measured. Owing to small amount of zeolite which will be used in the sources ( $\sim 0.1$  g) the degree of Rn emanation will be safe for the application into the WGTS. The emanation of the  $^{83m}\text{Kr}$  from many different sources prepared by deposition of  $^{83}\text{Rb}$  into zeolite of types A3, A4, A5 and XA from company Merck was studied. The sources were of different activities (1-30 MBq), ages (from fresh to one month old source), in the vacuum of different qualities and different gaseous environment ( $\text{H}_2$ , He,  $\text{O}_2$  and  $\text{N}_2$ ). The degree of  $^{83m}\text{Kr}$  release from the source based on zeolite 5A was satisfactory, about 80% when placed it in the vacuum, in contrast with zeolites of the other types for which the release in the vacuum amounted 20% or less. These and other properties of the zeolite sources were published: see *Gaseous source of  $^{83m}\text{Kr}$  conversion electrons for the neutrino experiment KATRIN 2014 JINST 9 P12010*.

Currently, at least 3 foreign institutions are using our zeolite sources in their research mostly in the dark matter experiments. Moreover, the method for the investigation of the noble gas flow in the circulation systems was suggested by us: see *A novel  $^{83m}\text{Kr}$  tracer method for characterizing xenon gas and cryogenic distillation systems 2014 JINST 9 P10010*.

The apparatus for injection of the  $^{83m}\text{Kr}$  emanated from zeolite beads into the WGTS was designed according to the KIT Tritium lab (TLK) demands and completed. The tests of the apparatus with the sources were started.

### **Miscellaneous**

Members of the team co-organized international workshop "Calibration and Monitoring", Münster, May 4-5, 2010, where they had 7 contributions. Members of the team participated each year at the summer and autumn KATRIN collaboration meetings. Altogether they

presented here 17 contributions. The extensive literature search related to the neutrino physics was started with the aim to publish the review articles about the direct methods for the neutrino mass determination. The first article was published: see *New knowledge about neutrino mass states PMFA 58(2013)28*.

## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Neutron Activation Analysis                    |

At NPI CAS, we maintain several methods of activation analysis, namely instrumental neutron activation analysis (INAA), epithermal neutron activation analysis (ENAA), radiochemical neutron activation analysis (RNAA), and instrumental photon activation analysis (IPAA). These methods were further developed and applied in various fields of science and technology in the period 2010-2014 as given below. In addition, X-ray fluorescence analysis (XRF) with both radionuclide and X-ray tube excitation sources is being performed and applied, namely for archaeological research, within the team activities.

### METHODOLOGICAL DEVELOPMENTS

There are two standardization modes largely used in INAA, namely relative standardization and  $k_0$ -standardization. The former approach is based on co-irradiation of samples and calibrants made of element certified solutions or solutions prepared by dissolution of high purity metals or well defined compounds and counting the samples and calibrants in the same conditions. In the latter approach, so-called  $k_0$  factors, which are a combination of nuclear data and experimentally determined parameters (neutron flux and detector parameters), which are presently known presently for more than 130 isotopes, are used for quantification of element contents. Since the launch of  $k_0$ -standardization in neutron activation analysis ( $k_0$ -NAA), this standardization technique has become increasingly used in many laboratories worldwide due to its favourable features. These involve mainly the possibility to determine a large number of elements without the need of irradiation and measurements of their calibrants (standards), which significantly increases the efficacy of NAA. This standardization mode also allows for so-called panoramic analysis, which yields information about contents or upper limits of more than 60 elements in a variety of matrices.

Due to extensive innovations of computers, computer programs available, and the laboratory instrumentation, it was necessary to revalidate  $k_0$ -standardization in our laboratory. Two types of reference materials (RM) were chosen for validation of  $k_0$  standardization: a set of synthetic multi-element standards IRMM-SMELS (SMELS) and matrix standard reference materials of the US National Institute of Standards and Technology (NIST SRMs). Bare triple-monitor method was used for monitoring of flux parameters at LVR-15 reactor in Řež employing most widely used Au and Zr monitors, which form upon neutron irradiation the  $^{198}\text{Au}$ ,  $^{97}\text{Zr}$ , and  $^{95}\text{Zr}$  nuclides. Quantification of results was done with the Kayzero for Windows programme. Fairly good agreement has been found between element contents determined and certified and non-certified values for both synthetic SMELS reference materials and matrix NIST SRMs, thus proving successful validation (Kubešová and Kučera, Nucl. Instrum. Meth. A 622 (2010) 403–406, Kubešová and Kučera, Chem. Listy 105, (2011) 261–268).

In the meantime a new freeware developed under the auspices of the International Atomic Energy Agency (IAEA), named  $k_0$ -IAEA, for quantification of  $k_0$ -NAA results became available. Therefore the performance of the two programs, Kayzero for Windows and  $k_0$ -IAEA, was compared, again using SMELS and NIST SRMs, and Au and Zr neutron flux monitors. Of the two programs, Kayzero for Windows strictly adheres to the  $k_0$  standardization principles, i.e., only those peaks for which  $k_0$ -values exist are used for quantification of results and the analyst may select those peaks, which are suitable for a given matrix, e.g., interference-free peaks.

On the contrary, k0-IAEA program uses the holistic interpretation of gamma-ray spectra, in which all the peaks, observed or expected, are taken into account (except of peaks that arise from random summing). However, peaks originating from (n, $\gamma$ ) reactions and characterized by  $k_0$ -values are given by far larger weight in the evaluation. In general, a good agreement was found between the elements contents determined by both programs and certified, noncertified and/or assigned values in SMELs RMs and NIST SRMs analysed. More elements were more reliably determined in SMEL SRMs and NIST SRMs from the same  $\gamma$ -ray spectra by Kayzero for Windows program. The advantages of k0-IAEA program involve the ease of data manipulation and the possibility to use reactions with fast neutrons. The declared advantage of k0-IAEA program that the holistic approach of evaluation of results minimizes the need for user interaction with the routines, its robustness with respect to interference corrections, and its reliability in identifying the origin of peaks has not been fully confirmed in this study (Kubešová and Kučera, Nucl. Instrum. Meth. A 654 (2011) 206–212).

Based on these results we decided to continue in using the Kayzero for Windows program. We have also found surprisingly different uncertainties of the results reported by Kayzero for Windows and k0-IAEA programs. Therefore, we have devised a novel Excel spreadsheet technique according to Kragten to evaluate of uncertainty of  $k_0$ -NAA results, named KRAGTEN-NPI. We believe that the proposed KRAGTEN-NPI computation tool, which calculates the uncertainty of both neutron flux parameters and element mass fractions in a simple and transparent way, overcomes the shortcomings of previous approaches, because all most significant uncertainty sources (including correlations of the relevant parameters) are taken into account (Kubešová and Kučera, J. Radioanal. Nucl. Chem., 293 (2012) 87–94).

During the above studies we have also found that that the choice of the most suitable combination of the monitor elements (nuclides) for the determination of neutron flux parameters with the use of the bare multi-monitor method depends on the reactor parameters, such as neutron flux thermalization, moderator materials, construction of the active core with special regard of the location of irradiation channels with respect to fuel elements, moderator and other reactor construction materials (Kubešová and Kučera, J. Radioanal. Nucl. Chem. 293 (2012) 665–674). In order to match specific conditions of irradiation in the LVR-15 reactor in Řež (irradiation channels located within the Be reflector), we have designed new sets of neutron flux monitors for both short- and long-time irradiation that consist of the elements Au+Mn+Rb and Au+Mo+Rb(+Zn), respectively (Kubešová et al., Nucl. Instrum. Meth. A 656 (2011) 61–64, Kubešová et al., J. Radioanal. Nucl. Chem., 300 (2014) 473–480). After validation analyses with the use of the newly developed neutron flux monitor sets, we may conclude that a composition of the monitor sets optimal for both short- and long-time irradiation in the LVR-15 reactor has been achieved and  $k_0$ -INAA method has been successfully improved.

## GEO- AND COSMOCHEMICAL RESEARCH

Neutron and photon activation analyses, particularly in their instrumental mode (INAA and IPAA, respectively), are an indispensable tool in geo- and cosmochemical research. The team of the activation analysis group at NPI has long term, well established cooperation with leading domestic institutions in the field, namely the Institute of Geology of the CAS, the Institute of Geochemistry, Mineralogy and Mineral Resources at the Faculty of Science, Charles University in Prague, the Czech Geological Survey, and the Institute of Rock Structure and Mechanics of the CAS. In the period 2010-2014, the team worked on several joint research projects with these institutions, which were supported by the Czech Science Foundation (CSF) and the CAS Grant Agency (AGA): 205/09/0991 - “Origin of moldavites – complex geochemical study” (CSF, 2009-2011); IAA300130902 - “Characteristics of the mantle sources and crystallization history of the subvolcanic alkaline rock series: Geochemical and Sr-Nd isotope signature (an example from the České středohoří Mts., Ohře/Eger Rift)” (AGA, 2009-2013); 13-22351S - “Combined use of novel and traditional stable isotope systems in identifying

source components and processes of moldavite formation" (CSF, 2013-2016); 13-27885S - "Photon activation analysis using short-lived products of photonuclear reactions for application in geochemical research" (CSF, 2013-2015). The main role of the NPI team within the projects was detailed geochemical characterization of studied materials, in terms of both major and trace elements, by INAA/IPAA. The team, however, significantly contributed to interpretation of the acquired data and their presentation at conferences and publication in papers.

Within the project 205/09/0991, a representative set of 160 samples of the Central European tektites - moldavites - covering the main parts of the Central European tektite strewn field, supplemented with samples of tektites and impact glasses from the strewn fields in other parts of the world, was prepared and characterized by various analytical methods dominated by methods of activation analysis. Within the project, several unique, previously unpublished topics were studied. These include in particular a study of lithium isotopic composition of tektites and impact glasses (Magna et al. 2011), study of the content and isotopic composition of carbon in moldavites (Žák et al., *Meteorit. Planet. Sci.*, 47 (2012) 1010–1028), determination of type of the impactor and its fraction in the impact glasses from the Zhamanshin crater (Mizera et al., *J. Radioanal. Nucl. Chem.*, 293 (2012) 359–376), gaining new supporting evidence for our new theory, which assumes participation of plant biomass in the source materials for moldavites. The research on moldavites and other tektites has continued in the framework of the follow-up project 13-22351S, which has been focused mainly on isotope analyses provided by collaborating institutes but utilizes also geochemical data provided by INAA and IPAA at NPI. Related to the moldavite research was also an investigation of chemical composition of plant phytoliths performed using INAA. Comparison of phytoliths with their source plant material showed that phytoliths are enriched in terrigenous elements such as Al, Sc, Ti, V, Cs, Fe, rare earth elements, and depleted in the major inorganic constituents of plants such as K, Ca, Mg, Mn, Cl and Br (Kameník et al., *Environ. Chem. Lett.*, 11 (2013) 189–195).

Within the reported period 2010-2014, IPAA as a complementary method to INAA was frequently utilized. It utilizes the MT-25 microtron of NPI as an irradiation source. Possibilities of IPAA compared to INAA in geochemical analysis have been well documented by analysis of a set of geochemical reference materials representing various rock types (Mizera and Řanda, *J. Radioanal. Nucl. Chem.*, 284 (2010) 157–163). Besides the above mentioned geochemical characterization of tektites and their potential source materials, IPAA was beneficial mainly in precise determination of Ti and incompatible elements Zr and Nb in studies of alkaline volcanic and subvolcanic rocks from the Ohře (Eger) Rift, a region of Cenozoic volcanic activity in northwestern Bohemia, Czech Republic. These data were inevitable for determining their mantle source and genesis of their parent magma, which was a part of the above mentioned grant project IAA300130902 and its predecessor, the project IAA300130706 (Ulrych et al., *Chem. Erde* 70 (2010) 319–333, Skála et al., *Int. J. Earth Sci.*, 103 (2014) 1233–1262). Until recently, IPAA analyses could be carried out only in the offline mode, i.e., in assay of elements providing by photoactivation radionuclides with sufficiently long half-lives, including also assay of elements with relatively short-lived photoactivation products as fluorine (Krausová et al., *Nucl. Instrum. Meth. Phys. Res. B*, 342 (2015) 82–86) and nitrogen. Currently, in the framework of the grant project 13-27885S, an automated system for rapid sample transport between the beam position and detector in the short time has been installed and the online irradiation mode is being tested (Krist et al., *J. Radioanal. Nucl. Chem.*, 2014, DOI 10.1007/s10967-014-3578-z). This will provide substantial extension of the analytical range of IPAA, particularly in express, nondestructive determination of major elements for geochemical analysis.

Outside the framework of the above listed grant projects, several individual studies utilizing INAA/IPAA were carried out, as a study of radiobarites from the Cenozoic volcanic region of the Bohemian Massif (Řanda et al., *J. Radioanal. Nucl. Chem.*, 283 (2010) 89–94), or a study of anomalous uranium mineralization in coal from Odeř in the northernmost part of the Sokolov Basin, Czech Republic (Havelcová et al., *J. Environ. Radioactiv.*, 137 (2014) 52–63). INAA was

also used to determine contents of more than 30 elements in meteorite Jesenice, which fell on April 9, 2009 over Carinthia and the Karavanke Mountains (on the border of Austria and Slovenia). The study was accomplished by an international team of scientists from the Czech Republic, Germany, Italy and Slovenia. Our INAA results showed that the bulk composition of Jesenice is very close to the published average element concentrations for L ordinary chondrites (Bischoff et al., Meteorit. Planet. Sci. 46 (2011) 793–804).

## GEOMYCOLOGY

The fundamental importance of fungi involves organic and inorganic transformations and element cycling, rock and mineral transformations, bioweathering, fungal-clay interactions, metal-fungal interactions and mycogenic mineral formation; the study of the role that fungi have played and are playing in geological processes is termed geomycology.

At NPI CAS, we focus on the phenomenon of trace element accumulation in mushrooms (macrofungal fruit-bodies). In contrast to other teams in the world, which mainly analyze the most common edible mushroom species, one of the group members (Jan Borovička) is also a mycologist and, therefore, we are able to collect and identify many macrofungi, including unusual or even very rare species. The multi-element determination by INAA provides quick and valuable results on almost all elements of interest (i.e. elements known to be accumulated in macrofungi), with the exception of Hg and Pb. Therefore, we have been able to identify various effective macrofungal accumulators, especially species accumulating Ag, As, Cl, Cu and Zn.

However, geomycology is an interdisciplinary science and the identification of hyperaccumulators represents just the first step in our research. The phenomenon of metal accumulation is studied in close co-operation with other teams. At the University of Chemistry and Technology (team led by dr. Pavel Kotrba), the chemical form of accumulated metals is studied together with the molecular aspects leading to accumulation of particular elements. At the Institute of Microbiology CAS (team led by dr. Milan Gryndler), fungal mycelia are cultivated and *in vitro* studies are performed. Furthermore, molecular methods (mainly DNA sequencing, community studies and qRT-PCR) are applied in our environmental studies. Furthermore, Jan Borovička is also employed at the Institute of Geology CAS, where other useful methods are available, especially ICP-SF-MS. Most of our studies were based on close co-operation with other teams and in some papers, possibilities of INAA and ICP-MS were compared.

In the period of 2010-2014, two main research projects funded by the Grant Agency of the Czech Academy of Science and the Czech Science Foundation, respectively, were investigated by Jan Borovička at NPI: i) Silver and zinc content of macrofungi: speciation in fruit-bodies, distribution in ectomycorrhizal and saprobic species (2007-2010), influence of environmental pollution and chemotaxonomic significance; ii) Hyperaccumulation of heavy metals in macrofungi – molecular, geomycological and ecotaxonomic aspects (2011-2015). Two research student projects funded by Charles University Grant Agency were investigated by Jaroslava Kubrová and Jan Borovička (supervisor): i) Uranium and thorium content of macrofungi from clean and polluted sites; ii) Trace elements in ectomycorrhizae.

In the period of 2010-2014, 8 research papers and 1 review were published in international journals within the scope of geomycology. We have mainly focused on the phenomenon of Ag hyperaccumulation, found and for the first time reported by our team in 2007 (Borovička et al., Mycological Research 111: 1339-1344). A complex study on the phenomenon of Ag accumulation in macrofungi was published in 2010 (Borovička et al., Science of the Total Environment 408: 2733-2744). In 2011, the first results on the chemical form of Ag in the hyperaccumulating species *Amanita strobiliformis* was published (Osobová et al., New Phytologist 190: 916-926): intracellular Ag was found to be sequestered by 3 isoforms of metallothioneins. Interaction of Ag with communities of soil saprotrophic organisms was studied in two different soils using a metagenomic approach (Gryndler et al., Biometals 25: 987-993). Organically bound (biomass of *Amanita solitaria*) and mineral forms of Ag did not

differ substantially in their effects on microbes in soil samples. The results indicate that decomposing Ag-rich fungal biomass can significantly alter soil microbiota.

Gold is another noble metal accumulated in macrofungi. A complex study focused on Au accumulation in macrofungi from an auriferous area was published by our team in 2010 (Borovička et al., *Soil Biology & Biochemistry* 42: 83-91). For the first time, gold concentrations were reported for ectomycorrhizal roots. The saprotrophic species *Lycoperdon perlatum* was found to be the most effective Au accumulator. The value of nearly 8 mg kg<sup>-1</sup> Au (in dry mass) found is the highest Au concentration ever reported for an eukaryotic organism under natural conditions.

Suspicious results on U content of macrofungi published by Campos et al. (2009, *Biometals* 22: 835–841) and interesting data obtained from on fungal-uranium interactions *in vitro* (see Gadd & Fomina 2011, *Geomicrobiology Journal* 28: 471-482) prompted us to focus on the subject of U-Th-REE accumulation in macrofungi. Results from INAA were thoroughly compared with ICP-MS in a more or less analytical paper published in 2011 (Borovička et al., *Biometals* 24: 837-845). It appeared that the data published by Campos et al. (2009) were erroneous, in part because of use of an inappropriate analytical method; and in part because of apparent contamination by soil particles resulting in elevated levels of thorium and REE. A complex study on U accumulation in macrofungi and ectomycorrhizae in U-polluted area was published in 2014 (Borovička et al., *J. Hazard. Mater.* 280: 79-88). Among others, it was found that accumulation of U, Th, Pb and Ag in macrofungal fruit-bodies apparently does not depend on total content and chemical fractionation of these metals in soils (tested by the BCR sequential extraction in this study).

The possibility to use ICP-MS at the Institute of Geology CAS prompted us to apply Pb isotopes in our geomycological studies. As recently published, Pb isotopes might be used as tracers of soil origin of the accumulated elements (Borovička et al. 2014, *Appl. Geochem.* 43: 114-120). In another paper published by our team in 2014 (Sácký et al., *Fungal Genetics and Biology* 67: 3-14) we utilized results on Zn/Cd/Ag accumulation in various *Hebeloma* species from both clean and polluted sites.

Beyond the common research at NPI, Jan Borovička also co-authored papers focused on taxonomy, ecology, and chemistry of macrofungi. Some of these studies were published in international scientific journals (*Czech Mycology*, *Mycological Progress*, and *Forensic Science International-Genetics*). One paper reporting current data on radiocaesium distribution in fruit-bodies of *Boletus badius* was published by Jan Borovička and Jaroslava Kubrová in a Czech mycological journal in 2012 (*Mykologický Sborník* 89: 92-98) as an answer to questions arisen in Czech media in 2011. The youngest member of our group, Iva Greňová (PhD student), focuses on accumulation of halogens in macrofungi; finalized manuscripts on this subject are planned to be submitted in 2015/2016.

## ENVIRONMENTAL RESEARCH

The long-lived, beta-emitting radionuclide <sup>129</sup>I (half-life 1.57·10<sup>7</sup> years) occurs in the environment as a result of both natural processes and human nuclear activities. The former processes involve mainly the spallation reaction of high energy cosmic rays with xenon in the upper atmosphere, spontaneous fission of <sup>238</sup>U, and thermal neutron-induced fission of <sup>235</sup>U. The human nuclear activities include neutron-induced fission of <sup>235</sup>U and <sup>239</sup>Pu in the explosion of nuclear devices, as well as the operation of nuclear reactors for research and power production. Neutron activation analysis in several modes (NAA with pre-irradiation separation followed by RNAA, and ENAA) was used to determine <sup>129</sup>I and the <sup>129</sup>I/<sup>127</sup>I ratio in biomonitors, namely in bovine thyroid and moss, collected in the vicinity of the Temelín nuclear power plant (NPP) in south Bohemia. The <sup>129</sup>I levels as well as the <sup>129</sup>I/<sup>127</sup>I ratios determined in this work in bovine thyroids bred in the vicinity of the Temelín NPP were found to be within those reported from various regions in the northern hemisphere unpolluted with <sup>129</sup>I, i.e., to be due to the natural fallout background levels. No significant differences of <sup>129</sup>I and the <sup>129</sup>I/<sup>127</sup>I ratios in the



thyroids collected prior to the start and after several years of the NPP operation indicate no local contamination with  $^{129}\text{I}$  due to the Temelín NPP releases. The values of the  $^{129}\text{I}$  concentrations and the  $^{129}\text{I}/^{127}\text{I}$  ratio in moss *P. schreberi*, not investigated before, may therefore be considered as baseline values for future studies (Krausová et al., J. Radioanal. Nucl. Chem., 295 (2013) 2043–2048).

Simple, direct solid sampling atomic absorption spectrometry methods are in demand for the total-Hg determination in environmental matrices. For this purpose, commercially available devices, such as AMA-254 or DMA-80 spectrometers are available. Since these devices have especially been designed for mercury determination at trace and ultratrace levels, it should carefully be examined that the upper limit of their working range (0.5 µg to 1.2 µg for AMA-254 and DMA-80, respectively) is not exceeded in analysing samples with high mercury contents, because this would lead to negatively biased results. Unlike other authors, who employed the dilution of high contents of Hg in heavily polluted samples with an inert matrix, we used low masses (10 mg to 25 mg) of well homogenized (by cryogenic grinding at temperature of liquid nitrogen), yet representative samples to comply with requirements for accurate Hg determination using AMA-254, i.e., not to exceed the upper limit of the working range of 500 ng of Hg. The accuracy of Hg determination by the AMA-254 spectrometer performed at the Institute of Chemical Technology in Prague using the above small-mass samples was confirmed by assay of much larger, otherwise identical samples by an RNAA procedure in our institute, where the cryogenic grinding was also performed (Sysalová et al., Microchem. J., 110 (2013) 691–694).

In 2011–2013, one team member was on a post-doctorate position at the University of Hawaii. The initial activity was in determination of a baseline of  $^{137}\text{Cs}$  levels in seawater of the North Central Pacific prior arrival of radionuclides from crippled reactors of Fukushima nuclear power plant. A procedure for seawater collection (20–100 L) and Cs pre-concentration was developed in cooperation with the Woods Hole Oceanographic Institution and the Czech Technical University and applied for many samples (Kameník et al., J Radioanal Nucl Chem 296 (2013) 841–846, Kameník et al., Biogeosciences 10 (2013) 6045–6052). Another task was participation in the development of a long-term monitor of submarine ground water discharges using an autonomous buoy with radon detector. The device has been in operation at Kiholo Bay (Hawaii) since 2013.

## AGRICULTURE AND NUTRITION

In co-operation with researchers of the Nuclear and Technological Institute, Sacavém, Technical University of Lisbon, and National Institute of Biological Resources, Elvas, Portugal, we used our RNAA procedure to study selenium transfer from soil or seed to wheat plants. Selenium (Se) is of utmost importance for a healthy immune system, for its protective (specific) effects against the cardiovascular disease, and, especially, certain forms of cancer. Minimum Se intakes of 40 and 30 µg per day for adult males and females, respectively, are internationally suggested average requirements. Portuguese studies on Se are scarce, yet the available data indicate that current daily intakes fail to meet the above requirements; hence, a Se-supplementation project targeting common cereals has been started. The study has shown that Se transfer from soil or seed to wheat plants increases as the plants go through the growing stages (tillering\booting\grain filling), and depends on the wheat variety. Overall, transfer coefficients from soils were lower for rye than for wheat in almost all plants' parts (Galinha et al., J. Radioanal. Nucl Chem., 294 (2012) 349–354). A subsequent study work focused on the ability of bread and durum wheat to accumulate Se via a soil-addition procedure at sowing time. Results showed that Se-supplementation at the top rate (100 g Se ha<sup>-1</sup>) can increase Se contents up to 2, 16, 18 and 20 times for Jordão, Roxo, Marialva and Celta cultivars, respectively, when compared to their unsupplemented crops (Galinha et al., J. Radioanal. Nucl. Chem, 2014, DOI 10.1007/s10967-014-3455-9).

An IPAA non-destructive procedure for nitrogen assay in malting barleys and winter wheat was developed and compared with classical destructive Kjedahl and Dumas methods. The determination has been based on counting of the non-specific 511 keV annihilation gamma rays of  $^{13}\text{N}$ , a short-lived (half-life 9.97 min) product of the photonuclear reaction  $^{14}\text{N}(\gamma, n)^{13}\text{N}$  with the threshold energy of 10.5 MeV. Since  $^{13}\text{N}$  is a pure positron emitter, its determination can be interfered by simultaneous formation of several other positron emitters. Their contributions have been eliminated by optimization of the bremsstrahlung energy, irradiation, and decay and counting times. A detection limit of 0.02 wt% has been achieved (Krausová, Doctorate thesis, to be published in 2015, Mádlíková, Diploma thesis, to be published in 2015).

Silicon is an important trace element for connective tissues. Because it also reduces the absorption of aluminium in human gastrointestinal tract, it also helps to protect the human body from the toxic effects of this metal and could be an important factor in preventing Alzheimer's disease. The recommended daily intake of silicon is about 10–25 mg, and its most readily absorbable form is orthosilicic acid  $\text{H}_4\text{SiO}_4$ . Unlike many other foodstuffs, beer contains Si in a bioavailable form. Therefore, this beverage is the most important dietary source of Si. In co-operation with the Institute of Chemical Technology in Prague, we clarified a relationship between Si concentration in various Czech lager beer samples and raw materials used for their production, and we also calculated the mass balance of silicon during the brewing process using INAA. We found that Si concentrations varied the range of 13.7 – 44.2 mg L<sup>-1</sup> and that the barley malt is the most important source of Si in beer. Thus, drinking of 0.5 – 1 L of beer daily will cover our daily Si needs, which may act as a protective factor against Alzheimer's disease (Krausová et al., J. Inst. Brew., 120 (2014) 433–437).

## NUCLEAR TECHNOLOGY

$k_0$ -INAA was employed for elemental characterization of individual components of electrical cables currently used in safety systems of nuclear power plants (NPP). The analysis yielded information about the content of 35 elements. It has been found that the presently used cables would not satisfy requirements of qualification set for the new generation of NPP by "The European Utility Requirements for LWR Nuclear Power Plants", because content of several elements exceeded the maximal admissible levels. This demonstrates that cable polymer materials for safety systems of the new generation NPP must be synthesized and controlled regarding the content of additives, which are undesired from the hygienic and radiological points of view.  $k_0$ -INAA proved to be a method of choice for elemental characterization of polymer materials of electrical cables as part of their qualification for use in NPP (Kučera et al., J. Radioanal. Nucl. Chem., 300 (2014) 685–691).

In co-operation with ÚJV Řež, a.s., gamma-and neutron doses in an experimental reactor were measured using alanine/electronspin resonance (ESR) spectrometry. The absorbed dose in alanine was decomposed into contributions caused by gamma and neutron radiation using neutron kerma factors. To overcome a low sensitivity of the alanine/ESR response to thermal neutrons, a novel method has been proposed for the assessment of a thermal neutron flux using the  $^{14}\text{N}(n, p)^{14}\text{C}$  reaction on nitrogen present in alanine and subsequent measurement of  $^{14}\text{C}$  by liquid scintillation counting (Bartoníček et al., Appl. Radiat. Isotopes 93 (2014) 52–56).

Neutron fluence and spectrum are the two main characteristics of a neutron field. A new method has been developed in collaboration with Research Centre Řež, Ltd., called the transmutation detector method that can be used to measure higher neutron fluences, where up to now the activation detector method was usually used. The methods are similar, with the main advantage of the new method that the detector's response is independent of its irradiation history. Both methods could also be used for other types of radiation and dosimetric quantities, but neutrons and fluence are most frequently used (Viererbl et al., Nucl. Instrum. Meth. A, 632 (2011) 109–111).

With regard to the use of thorium fuel for future nuclear energy production, two methods of  $^{233}\text{U}$  assay were studied with two methods of NAA with delayed neutron counting (NAA-DNC) and gamma-spectrometry (GS) to measure the  $^{233}\text{U}$  amount in neutron irradiated thorium and in a mixture of thorium and uranium in co-operation with the ÚJV Řež, plc. and the Czech Technical University in Prague using our facility for short time irradiation. Both methods studied provided results in agreement and with calculated amounts of  $^{233}\text{U}$  (Baldová et al., J. Radioanal. Nucl. Chem., 288 (2011) 37–42).

The radionuclide  $^{95\text{m}}\text{Tc}$  is frequently used radiotracer for studies concerning determination and behaviour of a long-lived fission product  $^{99}\text{Tc}$  in the environment. Therefore, several procedures of the  $^{95\text{m}}\text{Tc}$  preparation have been tested and compared in co-operation with the Czech Technical University in Prague (Fikrle et al., J. Radioanal. Nucl. Chem., 286 (2010) 661–663).

## CULTURAL HERITAGE

X-ray fluorescence analysis (XRF) was used for assays of two different types of historical samples. The first group was analysis of Bronze Age hoards from Southern and Northern Bohemia and a few findings from different parts of Czech Republic (usually from neolithic ages). The second group of interest were artefacts from second half of early Middle Ages and first half of High Middle Ages - usually jewellery and coins. The elemental composition of coins indicates an actual economical and geopolitical situation at that period in the Central Europe region. Second point of interest concerns fakes of coins. From the historical point of view it is very interesting to know the composition of contemporary fakes of coins, which contributes to overall knowledge of both “official” and illegal coinage. Knowledge of elemental composition of the historical coins, both originals and contemporary fakes can in some cases help in detecting modern fakes and thus it helps to protect cultural heritage at least of Central Europe region. All analyses were made in close cooperation with archaeological institutions from the Czech Republic (Institute of Archaeology CAS, National Museum in Prague, Hussite Museum in Tábor, etc.).

In order to evaluate the age from the equivalent dose and to obtain an optimized and efficient procedure for thermoluminescence (TL) dating, it is necessary to obtain the values of both the internal and the external dose rates from dated samples and from their environment. In co-operation with the Czech Technical University, we measured and compared the age of bricks from historic buildings using a fine-grain dating method. The dose rate fraction from  $^{238}\text{U}$  and  $^{232}\text{Th}$  can be calculated, e.g., from the alpha count rate, or from the concentrations of  $^{238}\text{U}$  and  $^{232}\text{Th}$ , measured by INAA. The dose rate fraction from  $^{40}\text{K}$  can be calculated from the concentration of potassium measured, e.g., by X-ray fluorescence analysis (XRF) or by NAA. Alpha counting and XRF are relative simple and are accessible for an ordinary laboratory. NAA can be considered as a more accurate method, but it is more demanding regarding time and costs, since it needs a nuclear reactor as a neutron source. A comparison of the above methods allowed us to decide whether the time- and cost-saving simpler techniques introduce uncertainty that is still acceptable (Bártová et al., Radiat. Phys. Chem., 104 (2014) 393-397).

In 2010, the grave of world-renowned Renaissance astronomer Tycho Brahe was opened by a Czech–Danish research consortium and samples of his bones, hair, and teeth were procured for scientific investigation. Tycho Brahe died on 24 October 1601, after 11 days of sudden illness. Shortly after his death, several conspiracy theories regarding the reason his death have been aired, presuming also poisoning by mercury. We carried out mercury determination in segmented hair samples of Tycho Brahe by RNAA. Most of the Hg values found in Brahe’s hair were in the normal range. However, the very highest value,  $16.4\text{ mg g}^{-1}$ , was slightly higher than the present normal range, and a factor of four higher than the present median value. The Hg exposure decreased in the last 2 months prior to the death of Tycho Brahe, most markedly in the last 2 weeks. The results showed that in the last 2 months of Brahe’s life, he was not exposed to lethal (or fatal) doses of Hg, as was previously speculated. Even the highest hair

Hg concentration determined, 16.4 mg g<sup>-1</sup>, is significantly below the levels of 200–800 mg g<sup>-1</sup> seen in cases of moderate intoxication. Our data therefore suggest that Tycho Brahe could possibly have been exposed to small and relatively harmless doses of Hg during the last weeks prior to his death, possibly due to his own medication *Medicamenta tria*. Measurements of samples from the femur and iliac bones, performed by AAS in Denmark, showed that

Tycho Brahe was never exposed to excess levels of Hg during the last ca. 10–15 years of his life. Thus, a murder scenario has now become a much more remote possibility than previously thought (Rasmussen et al., *Archaeometry*, 55 (2013) 1187–1195).

## MATERIAL RESEARCH AND REFERENCE MATERIALS

The synthesis of graphene materials is typically carried out by oxidizing graphite to graphite oxide followed by a reduction process. Numerous methods exist for both the oxidation and reduction steps, which causes unpredictable contamination from metallic impurities into the final material. These impurities are known to have considerable impact on the properties of graphene materials, which impacts the range of potential applications for which these graphene materials are suitable. In co-operation of Nanyang Technological University, Singapore, and Institute of Chemical Technology, Prague, several reduced graphene oxides from extremely pure graphite were synthesized using several popular oxidation and reduction methods. In our laboratory, we tracked the concentrations of metallic impurities at each stage of synthesis by *k<sub>0</sub>*-INAA. We showed that different combinations of oxidation and reduction introduce varying types as well as amounts of metallic elements into the graphene materials, and their origin can be traced to impurities within the chemical reagents used during synthesis (Wong et al, *Proc. Nat. Academy Sci. USA*, 111 (2014) 13774–13779).

At the Institute of Public Health in Prague, a reference material (RM) of butoxyacetic acid (biomarker of ethylene glycol monobutyl ether exposure) in human urine has been prepared. We participated using our previous experience with the RM preparation and certification by evaluation of stability testing, homogeneity testing, and certification of the concentration and uncertainty of butoxyacetic acid in this freeze-dried urine RM (Šperlingová et al., *Anal. Bioanal. Chem.*, 397 (2010) 433–438).

Neutron activation analysis as a primary method of measurement plays an important role in the production and certification of RM to be used in elemental analysis for various tasks including quality control (QC). In 2013 and 2014, our team successfully participated in a campaign for certification of the gold mass fraction in an Al-0.1%Au alloy organized by Institute for Reference Materials and Measurement Geel, Belgium (Bacquart et al, Certification report, EUR 26830 EN, Luxembourg, 2014).

## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Nuclear Reactions                              |

The research activities of the team are directed towards experiments concerning basic nuclear physics (nuclear astrophysics, nuclei far from the stability, reactions near Coulomb barrier) as well as to topics with more applied character (nuclear data). All the activities are performed within international collaboration. Both the home installations at the NPI cyclotron U-120M and facilities at foreign laboratories are employed.

The U-120M cyclotron provides us with beams up to  $^3\text{He}$  of very good quality ( $\Delta E/E$  better than 1/1000). The experimental area in U120M in NPI is equipped by a vacuum chamber of 65 cm diameter with planes and target holder, gas cell and isotopic gas manipulation system, a complete spectroscopic chain with Si telescopes and ACQ system based on VME.

### NUCLEAR ASTROPHYSICS

Knowledge of cross-sections of astrophysically interesting reactions in the region of stellar energies is necessary for understanding the nucleosynthesis of elements and explanation of the observed abundances of isotopes. To overcome some serious difficulties connected to experiments with direct measurements, the indirect methods are developed. We concentrate particularly on the indirect ANC and THM methods, but we also entered into a common laboratory project with GANIL (France), where we use radioactive beams to study properties of light neutron-deficient nuclei.

The ANC - Asymptotic Normalization Coefficient method deduces direct capture cross sections at low incident energies from the vertex constant of the alternate direct peripheral process. The THM - Trojan Horse Method uses the so called quasi-free (QF) mechanism in a three-body reaction to study binary reactions.

Our most important partners in the nuclear astrophysics field are from INFN-LNS (Italy) and Texas A&M University and lately GANIL. In experiments realized on the U120M cyclotron in NPI, our group members prepare the experimental setup, calculate the beam optics and supervise the beam quality, work on electronics, data acquisition, participate in data processing as well as in theoretical interpretation of experimental results and their publication. In experiments at INFN-LNS and other laboratories, our group contribute to simulations, experimental equipment settings, experiment supervision, data processing, and formulation and interpretation of the results.

We have studied  $^{14}\text{C}(n,\gamma)$  reaction in NPI U120M cyclotron using  $^{14}\text{C}(d,p)^{15}\text{C}$  reaction (*Physical Review C* 84 (2011) 024616) and in TA&MU using  $^{14}\text{C}$  beam and  $^{13}\text{C}$  target (*Physical Review C* 89 (2014) 044605). The reaction plays an important role in inhomogeneous big-bang nucleosynthesis, depletion of CNO cycle in AGB stars and other processes. Because in this case the capture is dominated by p-wave, it was possible to determine the ANC. We had to use a FR-ADWA (finite range - adiabatic model) to properly include deuteron breakup in deuteron induced reaction. We have determined the ANC for the  $^{14}\text{C}(n,\gamma)$  reaction  $C_{s1/2}^2 = 1.64 \pm 0.26 \text{ fm}^{-1}$  and  $C_{d5/2}^2 = 3.55 \pm 0.43 \text{ E-3 fm}^{-1}$  and in the second experiment the overlapping ranges  $1.88 \pm 0.18 \text{ fm}^{-1}$  and  $4.25 \pm 0.38 \text{ E-3 fm}^{-1}$ .

Earlier (*J.Phys: Conf.Ser.* 202, (2010) 012017), we have experimentally studied the reaction  $^{15}\text{N}(p,\gamma)^{16}\text{O}$ . The reaction provides a path from CN stellar cycle into the CNO bi – and CNO tri – cycle. This reaction proceeds at very low energies and is dominated by resonant captures. We discussed an interpretation of LUNA collaboration measurements that did not take into account experimental constraints on ANC in R-matrix fit. We have shown that it is necessary to include contributions from higher levels. The deduced  $S(0)=33.1 - 40.1$  keVb overlaps with the LUNA measurement (*Physical Review. C* 83 (2011) 044604).

The cross sections of d+d fusion reactions were measured via Trojan Horse Method from 1.5 MeV down to 2 keV in NPI. For the first time bare  $S(E)$  factors were determined in the region relevant to Big-Bang nucleosynthesis and thermal energies in future fusion reactors, down to the thermal energies of deuteron burning in the pre-main-sequence phase of stellar evolution. The observed  $S(E)$  and energy dependence deviate from available direct data by more than 15%. Calculated reaction rates can increase by 25% in conditions of future fusion reactors. It turns out that  $d(d,n)$  reaction is quite influential on primordial  $^7\text{Li}$  abundance and present measurement suggests an abundance decrease of  $^7\text{Li}$  by 10%. (*Physics Letters. B* 700 (2011) 111; *Astrophysical Journal* 785 (2014) 96)

Fluorine abundance is sensitive to physical conditions in stars. We studied reactions related to fluorine nucleosynthesis or destruction using the Trojan Horse Method. Reaction  $^{19}\text{F}(p,\alpha)$  at energies below 300 keV is important from the point of view of fluorine destruction in AGB stars. Part of the experimental work was done in NPI. The measurements have shown resonant structures not observed earlier, that lead to an increase of the reaction rate up to a factor 1.7 at astrophysical energies thus having a certain impact on AGB and post-AGB star nucleosynthesis. (*Astrophysical Journal Letters* 739 (2011) L54)

Trojan Horse Method was used to access low energies and to avoid the influence of electron screening to study  $^{18}\text{O}(p,\alpha)^{15}\text{N}$  reaction at astrophysical energies. Full spectroscopic study of resonances at 20 and 90 keV above threshold was performed. This reaction rate (in AGB stars, where fluorine abundance is enhanced) can modify fluorine nucleosynthesis as well as nitrogen and oxygen isotopic ratios. Reaction rate was evaluated and uncertainties from NACRE were reduced. The experiment was performed at INFN LNS. (*Astrophysical Journal* 708 (2010) 796).

$^{17}\text{O}$  is processed in CNO cycle and is important as a progenitor of  $^{18}\text{F}$  radio-isotope, that is of special interest in gamma-observations of novae. Two resonances at 65 and 183 keV were observed in  $^{17}\text{O}(p,\alpha)^{14}\text{N}$  reaction. This reaction removes the  $^{17}\text{O}$  from  $^{18}\text{F}$  production path. The reaction rates were discussed and compared to NACRE (*Nucl.Phys.* A834, 676c (2010); *Physical Review. C* 82 (2010) 032801)

LiBeB nuclei were also studied by THM method. The study of  $^{11}\text{B}(p,\alpha)^8\text{Be}$  was called for by several measurements in the past giving discrepant results. Using the Trojan Horse Method, we obtained new, more precise results, overcoming both the Coulomb barrier and the electron screening effect. This measurement overlap energy region important for LiBeB stellar burning as well as for future plants using  $^{11}\text{B}+p$  fuel cycle. (*Journal of Physics G-Nuclear and Particle Physics* 39 (2012) 015106; *Nuclear Physics. A* 834 (2010) 655c). The  $^{10}\text{B}(p,\alpha)$  was studied in *Phys.Rev. C* 90, 035801 (2014).

The THM method is new and we also worked on its development and investigation of its properties. The method was applied on the same binary reactions with different TH nuclei  $^3\text{He}$  and  $^2\text{H}$ . TH nucleus invariance was proved in the  $^6\text{Li}(d,\alpha)$  and  $^7\text{Li}(p,\alpha)$  binary reactions above and below the Coulomb barrier. A good agreement with direct data is achieved in both cases (*Physical Review. C* 83 (2011) 045801).

THM allows to study the reaction without an effect of electron screening. The electron screening effects were studied and compared to adiabatic limit (*Nuclear Physics. A* 834 (2010) 673c; *J.Phys.: Conf.Ser.* 202, 012018 (2010)). Using THM as a provider of a virtual neutron beam was also studied (*Journal of Physics G-Nuclear and Particle Physics* 37 (2010) 125105 and *Phys.Rev. C* 87, 012801 (2013)).

Our group with GANIL (France) partners have entered in a common virtual laboratory project LEA NuAG (2011-2014) (Associated European laboratory - Nuclear Astrophysics and Grids). We worked on the experiments studying light neutron deficient nuclei in GANIL and IPN Orsay.

Using the radioactive beam of SPIRAL1 facility in GANIL, we studied spectroscopic properties of four states in  $^{18}\text{Na}$  in resonant elastic scattering of on  $^{17}\text{Ne}$ . There are strong indications of a very narrow state in  $^{18}\text{Na}$  located above  $^{19}\text{Mg}$  ground state, which creates conditions for simultaneous two-proton decay of  $^{19}\text{Mg}$  to the continuum (*International Journal of Modern Physics E-Nuclear Physics* 20 (2011) 971; *Phys.Lett. B* 712, 198 (2012)).

We searched for possible resonances in  $^{10}\text{C}$  and  $^{11}\text{C}$  in reactions  $^3\text{He}+^7\text{Be}$  and  $^4\text{He}+^7\text{Be}$ , respectively, that could explain the cosmological deficit of  $^7\text{Li}$  by enhanced destruction of  $^7\text{Be}$  (the parent of  $^7\text{Li}$ ). The results do not support this conjecture as a possible solution for the  $^7\text{Li}$  problem (*Physical Review. C* 88 (2013) 062802).

We studied resonant states in  $^{15}\text{F}$  and  $^{16}\text{F}$  with  $^{14}\text{O}$  and  $^{15}\text{O}$  beams by proton elastic scattering. A large coupling to continuum for the  $l=0$  states argument was used to explain the p-n interaction symmetry breaking when compared to mirror nucleus  $^{16}\text{N}$  (*Physical Review. C* 90 (2014) 014307).

We did the test of production of  $^{15}\text{O}$  in  $^3\text{He}+^{12}\text{C}$  reaction in NPI for future intensive radioactive beams on SPIRAL2. (*Eur.Phys.J. A* 47, 72 (2011)).

## NUCLEAR DATA FOR RESEARCH AND TECHNOLOGY

### ***NPI facilities and equipment***

Isochronous Cyclotron U-120M is a basic experimental facility of the NPI. High intensity proton/deuteron beams extracted from negative mode of accelerator are used also for an applied research. Variable energy proton and deuteron beams in the energy range up to 38 and 20 MeV, respectively, are available.

There were developed two types of fast neutron generators based on proton beam from the negative-ion mode of U-120M operation:

- *high-power broad-spectrum neutron sources* produce neutrons (integral flux up to  $6 \cdot 10^{11}$  n/sr/s (mean energy of 14 MeV, extension up to 33 MeV) by 37 MeV proton beam interacting with heavy-water (flow) and/or Be(thick) target. The neutron spectra determined with 10% accuracy by dosimetry-foil activation technique are backed by the MCNPX simulation.

- *variable-energy quasi-monoenergetic neutron source* of neutrons up to 35 MeV utilizes  $^7\text{Li}(p,n)$  reaction on thin lithium target (with carbon beam stopper) induced by 20–37 MeV proton beam. Spectral flux at sample position is determined with an accuracy of 10% by the MCNPX calculations validated against experiments (proton-recoil neutron spectrometer). The neutron yield up to  $10^{10}$  n/sr/s (in peak) for 37 MeV/5  $\mu\text{A}$  proton beam is achieved.

Detector- and data acquisition systems consist of

- 1) calibrated gamma spectrometers equipped with HPGe detectors and pneumatic post system utilized in off-line activation experiments for both the neutron and charge-particle induced activation reaction,
- 2) neutron spectrometers with both the scintillator detectors and proton-recoil spectrometer based on Si detector set-up,
- 3) fADC acquisition system and time-of-flight technique, and
- 4) dedicated irradiation chamber for measurements of activation cross sections induced by charged particles (using stacked-foils technique)



### **Data for accelerator-driven neutron sources**

In the experimental validation of neutron data libraries by integral cross section measurements (broad neutron spectrum), a precise knowledge of the effective spectra at the sample position is strongly requested to allow a correct interpretation of the measured results, a complete specification of physical process, a comparison with other measurements, and theoretical predictions. The broad-spectrum neutron source based on the  $p+Be$  (thick target) reaction was investigated for 35 MeV protons by the activation technique. Resulting neutron flux up to  $10^{11}$  /cm<sup>2</sup>/s at energies up to 33 MeV and a simplified operation comparing to currently employed  $p+D_2O$  source presents an important advantage and a unique tool for high-power irradiation experiments. For comparable dimensions and source-to-sample distance the energy/angle-dependent integration effect on effective neutron spectrum over the sample and target dimensions was experimentally investigated for the first time using an MCNPX simulation of experiment (*Nuclear Data Sheets*, 119(2014)425).

The NPI quasi-monoenergetic neutron source based on the  $p+^7Li$ (carbon backing) reaction produces a spectral flux composed of a peak and a low-energy continuum. To apply the spectrum in activation cross-section measurements, not only the intensity of the neutron peak, but also the contribution of the low-energy continuum must be well determined. Simulations of the spectral flux from present source at a position of irradiated samples were performed using CYRIC (Japan) TOF-data validated against LA150h by calculations with the transport Monte Carlo code MCNPX. Simulated spectra were tested by absolute measurements using a proton-recoil telescope technique. While the MCNPX simulation well reproduced experimental data for the monopeak, the discrepancy observed for the continuum requires further investigation (*Journal of the Korean Physical Society*, 59(2011)1577).

### **Activation of high-power accelerator components**

Projected high-power neutron sources for fusion-related radiation damage studies (like IFMIF – International Fusion Material Irradiation facility) are based on deuteron accelerators and Li-stream target. Due to high beam current, the accelerator and target components (beam tubes, beam dumps, impurity in the Li stream) will be highly activated. For the safety of management, operation and also decommissioning, the accurate knowledge of the cross sections (XS) for proton/deuteron induced activation is required. The activation XS of deuteron reactions on <sup>63</sup>Cu, <sup>65</sup>Cu, were measured up to 20 MeV on NPI cyclotron using stacked-foil technique. Preliminary data on copper isotopes were used to experimentally support the evaluation of radioactive inventories in first stage of IFMIF accelerator prototype, that were tested (Karlsruhe Institute of Technology) for legal limits for the transport from Rokasho (*Fusion Engineering and Design* 83 (2008) 1543). New measured XS data on copper (*Journal of the Korean Physical Society* 59 (2011) 1928) and <sup>93</sup>Nb (*Physical Review*, C88(2013)146) and <sup>nat</sup>Fe (*Journal of the Korean Physical Society*, 59(2011)1928) were subjected to a complex theoretical analysis. An attention was paid to optical potentials for elastic scattering, breakup mechanism, direct reaction stripping and pick-up, pre-equilibrium and compound-nucleus calculations. Results improve the predictions by TALYS-1.4/TENDL package. The interpretation was done with theoreticians from IFIN-HH Bucharest and wider collaboration.

Long-term methodical experiences in activation- and fast-neutron experiments allow us to successfully participate in international collaborations. In collaboration with SPIRAL2, Ganil, France (project NFS - Neutrons for Science), the NPI team provides the design of special reaction chamber for charged-particle activation experiments. The contacts with SARAF laboratory (Soreq Applied Research Accelerator Facility, Israel) devoted to activation of Li target impurities have led in a combined experiment to study of <sup>23</sup>Na (Li target main impurity, possible activation monitor) activation by deuterons from 20MeV down to 1.7 MeV using U-120M and SARAF facilities.

### **Neutron cross sections for fusion technology**

Qualified nuclear data dedicated to materials in fusion technology are requested by world-greatest energy research projects in the framework of the Fusion for Energy (F4E/EURATOM) program. The NPI is a member of the European Consortium for Nuclear Data (ENEA Italy, KIT Germany, AGH-UST Poland, JSI Slovenia, NPI CR, CCFE UK). Being presently the only European neutron facility that possess neutron fields at IFMIF relevant energies, we have conducted a large set of experiments to measure activation cross sections on components and impurities of the low-activation steel EUROFER and on dosimetry relevant nuclides.

In particular, the activation cross sections on Au and Bi (*Workshop on Activation Data - European Activation File, 2011, Prague*), Co and Nb (*Journal of the Korean Physical Society, 59(2011)1801 and 1374*) have been measured with a quasi-monoenergetic  $p\text{-}^7\text{Li}$  neutron source. This has brought the new experimental results in the neutron energy domain between 18 and 35 MeV with the estimated uncertainty of 10%. To improve the status of the dosimetry reaction file above 20 MeV, the computational analysis of measured data (the energy differential neutron flux in the irradiated foils) including the MCNPX simulation of the experimental set-up was carried out. This approach has been validated against  $p\text{-Li}$  neutron spectra measured by different techniques. By making use of the modified unfolding code SAND-II, the dosimetry cross sections have been derived from the detected  $\gamma$ -ray activities. They were used for validation of the activation (EAF, IEAF, IRDF) - and the general purposes (ENDF) cross sections files (*Journal of the Korean Physical Society, 59(2011)1856*).

Quality assurance in measurement of the neutron cross-sections provided by quasi-monoenergetic neutron sources and the foil-activation technique has been investigated. In particular, the extraction of cross-sections from measured gamma-activities of residual nuclei is non-trivial problem due to the nature of  $p\text{-Li}$  neutron spectra, which consists of the monoenergetic peak and the continuum at lower energies. Relevant uncertainty limits of various computational approaches to extraction process were analysed for the first time and compared to other systematical and methodical uncertainties (*Nuclear Data Sheets 119(2014)425*).

### **Neutron hardness tests of microelectronics**

High flux up to  $10^{11} \text{ cm}^{-2}\text{s}^{-1}$  of fast neutrons from broad-spectrum neutron generators and well calibrated spectral flux at irradiation positions presents a unique tool for tests of radiation protection against cosmic rays and/or radiation in facilities such as CERN LHC. In particular, the expected increase of total integrated luminosity by a factor ten at the HL-LHC essentially eliminates the safety factor for radiation hardness realized at the current electronics of the ATLAS Hadronic End-cap Calorimeter (HEC). Consequently, new more radiation hard technologies were studied and tested in frame of the HECPASS Collaboration (IEP Košice, Univ. of Montreal, MPI Munich, IEAP Prague and NPI Řež). Proton irradiation experiments were done at the PSI cyclotron (Villigen), the neutron irradiation tests were done at NPI Řež. Results are regularly reported by relevant responsible person from MPI on behalf of the HECPASS Collaboration [Proceedings of CHEF 2013, 394-398, arxiv:1309.0672, and references cited here], a part of methodical findings were reported by the NPI team (*Nuclear Data Sheets, 119(2014)425*).

### **NUCLEI FAR FROM THE STABILITY**

NPI collaborates with GANIL laboratory, Caen, France for a long time. The collaboration started on the topic of halo nuclei and developed into a fruitful experimental study of nuclei near magic numbers far from the line of stability, where different effects cause the collective behavior and appearance of new magic numbers. We had one senior scientist in this

collaboration, which contributed to motivations, analysis of systematics and magic numbers. and one postdoc in GANIL, which was dedicated to the experiments for  $^{34}\text{Si}$  and  $^{44}\text{S}$ - for detector setup, setup design, detector tests, experiment preparation and supervision, data analysis and interpretation.

Nucleus of  $^{44}\text{S}$  with magic number of neutrons  $N=28$  was studied using gamma and electron spectroscopy on LISE spectrometer in GANIL. The second  $0^+$  excited state was observed and  $E0$  transition to the g.s. was measured, branching  $0^+-2^+$  yield was deduced from delayed gammas. The complete information was compared to models.  $^{44}\text{S}$  exhibits a shape coexistence of prolate ground state and spherical excited  $0^+$  state. The work completes the understanding of breaking  $N=28$  shell mechanism. (*Physical Review Letters* 105 (2010) 102501; *Physical Review C* 85 (2012) 024311)

After decade of search, an excited  $0^+_{(2)}$  state in  $^{34}\text{Si}$  at 2719 keV was observed in LISE spectrometer in GANIL, populated through the newly discovered  $1^+$  isomer in  $^{34}\text{Al}$ . The  $2^+$  state in  $^{34}\text{Si}$  decays to both  $0^+$  states. From the experimental information it was deduced that largely (0.29) deformed  $0^+_{(2)}$  state and spherical ground state coexist in  $^{34}\text{Si}$ . SM calculations suggest a 12-22% mixing of np-nh excitations across  $N=20$  shell gap with normal configuration in ground state. (*Physical Review Letters* 109 (2012) 092503)

## REACTIONS NEAR COULOMB BARRIER

The studies of nuclear transfer reactions mechanisms in the Coulomb energy region, where loosely bound nuclei are involved, attract great interest of physicists. The experiments provide new comparison of excitation functions for d,p and d,t processes in the Coulomb barrier region with transfer reactions with  $^6\text{He}$  and  $^3\text{He}$  ions on different isotopic targets (Sc, Pt). Comparing the cross section maxima for different reactions, we have observed a remarkably different  $Z$ -dependence for the deuteron and  $^6\text{He}$  projectiles (*Journal of Physics G-Nuclear and Particle Physics* 38 (2011) 035106; *Physics of Particles and Nuclei Letters* 10 (2013) 410; *Physics of Particles and Nuclei Letters* 9 (2012) 502).

## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Research with Ion and Neutron Beams            |

Material research belongs to traditionally progressive fields of technology. Its products are used in the everyday life worldwide. However, due to the continuous miniaturization, the underlying structures are far beyond the analytical limits of the most of conventional methods. Nuclear analytical methods provide this possibility as they use probes of similar or much smaller dimensions (particles, radiation). Ion beam analysis researchers and specialists in Tandetron Laboratory and at LVR nuclear reactor are dealing with the application of the energetic ion beams and neutron beams for the fundamental studies including characterization and following the physical processes beyond particle/solid interaction and simultaneously researchers using ion and neutron beams for a very wide range of applications, mainly directed to the material science.

### TECHNICAL EQUIPMENT AND INSTRUMENTATION PORTFOLIO

Laboratory of Tandetron (LT) is equipped by the accelerator Tandetron 4130 MC, put into operation in 2005. It is a source of accelerated ions of most of elements from H to Au with energies from 0.4-20 MeV and intensities up to tens of mA. LT is part of a large research infrastructure CANAM (Centre of Accelerators and Nuclear Analytical Methods). Support of the CANAM by the project LM2011019 allows for open access to the instruments of the laboratory. The operation and upgrade of the laboratory instrumentation and techniques and assistance and providing the expertise of the team members to visiting researchers forms one component of the team activities.

- Rutherford Back-Scattering spectroscopy (RBS), RBS-channeling, PIXE channeling
- Elastic Recoil Detection Analysis (ERDA), ERDA-TOF
- Particle Induced X-ray Emission spectroscopy (PIXE), Particle Induced Gamma-ray Emission spectroscopy (PIGE) and Proton Elastic Scattering Analysis (PESA)
- Ion-Microprobe with 1  $\mu\text{m}$  lateral resolution, external beam accessories for on air irradiation
- High-energy ion implantation - modification of materials, nano-structure synthesis.
- Scanning Ion Microprobe – enables precise lateral mapping of elements using our own instrumentation developed at LT
- Deposition of nanostructures and multilayer structures

Tandetron Laboratory is unique lab in the Czech Republic dealing with broad field of ion beam analytical methods. We are cooperating with highly erudite centres on the top of European research to share our research topics and instrumentation. It is worthy to mention that LT provided in last years the invention and the development of 9 functional prototypes and new software applications in nuclear instrumentation technology.

Neutron Depth Profiling (NDP) and Prompt Gamma Activation Analysis (PGAA) are well established, non-destructive technique for determining elemental composition and depth profiles of selected elements. Both techniques make use of nuclear reactions induced by

thermal neutrons and accompanied with prompt emission of charged particles and gamma-rays. At Nuclear Physics Institute the devices for NDP and PGAA analyses are arranged in tandem at the end of a 6 m long neutron guide installed at external neutron beam from LVR-15 nuclear research reactor of Nuclear Research Centre Řež, operated at 8-10 MW thermal power.

## Competence

We have collaborated with our external partners in the following research areas during the last years:

- Modification of crystalline materials and glasses by ion implantation, preparation of nano-structures with significant optical, magnetic or electrical properties.
- Preparation of nano-composites and nano-structures polymer/metal with the significant electrical and magnetic properties, MC modelling of electronic transport in such nano-structures in dependence on the metal-nano-particles morphology.
- 3D elemental mapping using ion microprobe (PIXE, PIGE), focused ion beam irradiation. PIXE, PIGE and PESA trace elements study in aerosols for the environmental studies.
- Ion beam micromachining, optical microstructure deposition.
- Study of energetic ion interaction with matter, energy losses and energy straggling, fundamental study of ion interaction with solids.
- Irradiation of the living cells using external beam of energetic ions for dosimetry.
- Study of chemical composition of the materials for nuclear power plants (nuclear fuel rods, study of heavy element diffusion in rocks for nuclear waste storage), materials for nuclear fusion.
- Characterization of materials for biomedicine, environmental research, archaeometry.
- NDP method is used for non-destructive depth profiling of technologically important light elements (He, Li, B, N) with depth resolution down to 10 nm. Major field of NDP application is depth profiling of boron, lithium and nitrogen in various materials.
- Main area of PGAA application is non-destructive determination of elemental composition of different materials.

## RESEARCH FOCUS

### 1. NANOSTRUCTURES IN CRYSTALLINE MATERIALS FOR PHOTONICS AND SPINTRONICS

The incorporation of rare earths (namely Er) in structure of lithium niobate ( $\text{LiNbO}_3$ ) and sapphire ( $\text{Al}_2\text{O}_3$ ) is interesting for optical waveguide applications. The zinc oxide ( $\text{ZnO}$ ) has attracted much attention nowadays. The wide and direct band-gap in  $\text{ZnO}$  makes it suitable as a host for optically active Er ions, since it allows for emission at wavelength 1.5  $\mu\text{m}$  as well as in the entire visible region. The efficient incorporation of the erbium into the host matrix, the particular erbium position in the structure and therefore the effect of the erbium crystal-field surroundings on the luminescence properties of the erbium ions are very important to study [1,4]. The ion-implantation technique is a way to form active optical layers in these crystals. The main attention is focused on the structural and compositional changes comparison and also on the influence of various crystals fields on the 1.5  $\mu\text{m}$  luminescence of erbium ions.

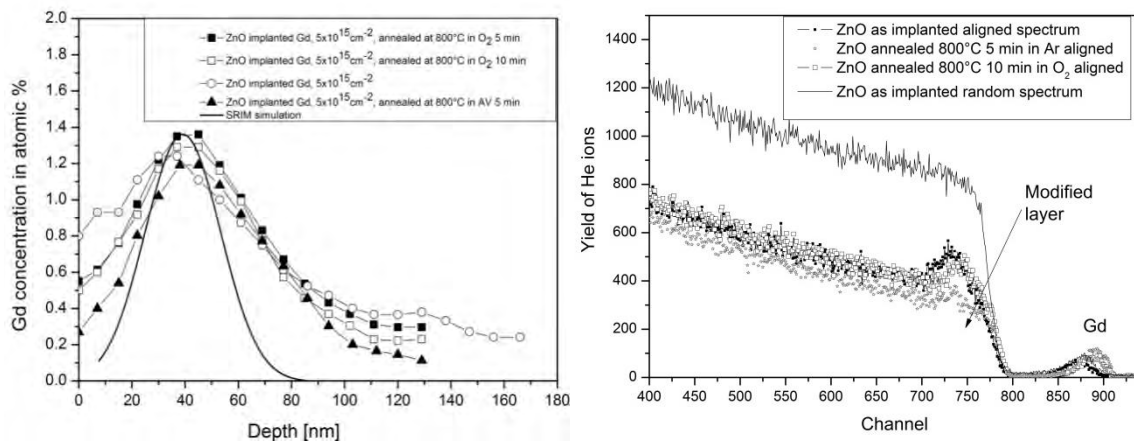
Recently, a high magnetic moment has been observed in GaN and ZnO doped with rare-earth elements. We investigated the structural changes of ZnO induced by Gd ion implantation and the effect of these structural modifications on the magnetic properties of ZnO [2].

We realized the systematic study of the structural as well as compositional changes of above mentioned crystalline materials as implanted and subsequently annealed. The study was provided in collaboration with Helmholtz Zentrum Dresden Rossendorf – HZDR, Institute of Chemical Technology, Institute of Physics ASCR and Faculty of Mathematics and Physics, Charles University). The crystalline materials were implanted into the various crystallographic cuts in cooperation with HZDR. Post-implantation annealing at 800 - 1000 °C in different atmospheres was also done. The chemical compositions and concentration-depth profiles of implanted layers were studied by Rutherford Backscattering Spectrometry (RBS) and compared to SRIM simulations at NPI. The structural properties of the prepared layers were characterised by RBS/channelling at NPI.

The relative numbers of disordered atoms in the prepared implanted layers, minimum yield and number of doped atoms in interstitial position were compared with each other and discussed for various crystals. It has been found that erbium is located in  $\text{LiNbO}_3$  and in  $\text{Al}_2\text{O}_3$  preferably in interstitial positions, unlike ZnO, where the largest amount of erbium is placed in substitutional positions after the implantation [4]. The erbium position in the host matrix was substantially influenced by the annealing procedure. Since we are interested in the relationship between structural changes and optical properties, the erbium luminescence properties were measured in the region of wavelength 1440–1650 nm for all crystals in ICHT. The annealing improved the luminescent properties significantly in all investigated crystalline materials [8, 13, 15].

As an example of the typical study we present ZnO implanted by Gd ions mainly realized in 2013 by NPI. Gd implanted depth profiles in ZnO in as-implanted and as-annealed samples are presented in Figure 1 – left and were determined by RBS (NPI). The structure of as-implanted samples was examined using the RBS-channelling method; the typical aligned spectra are shown in Figure 1 - right. It is evident that a considerable amount of damage is created in the near-surface region affected by the ion implantation, the thickness of which coincides with the ion projected range  $R_p$ . A slight recovery of the ZnO crystalline lattice was observed after the annealing at 800°C in Ar atmosphere, where the relative number of displaced atoms was reduced from 54% to 37%.

The magnetisation curves were measured at 4.5 K and 300 K in ICHT. Room-temperature ferromagnetism was measured on the as-implanted sample and also on the sample annealed in both argon and oxygen atmosphere. The origin of this ferromagnetism is most probably associated with the Gd cluster formed in the implanted ZnO crystals and persisting after the annealing procedure. [4,9].



**Figure 1**

The depth profiles of the Gd atoms implanted into ZnO to a fluence of  $5 \times 10^{15} \text{ cm}^{-2}$  from the as-implanted sample and after the annealing at 800 °C – left, the RBS-channelling spectra of ZnO implanted at Gd energy of 200 keV, a fluence of  $5 \times 10^{15} \text{ cm}^{-2}$ . A comparison of the aligned spectra for different annealing conditions – right [4].

## 2. METAL/POLYMER NANO-COMPOSITES AND NANO-STRUCTURES

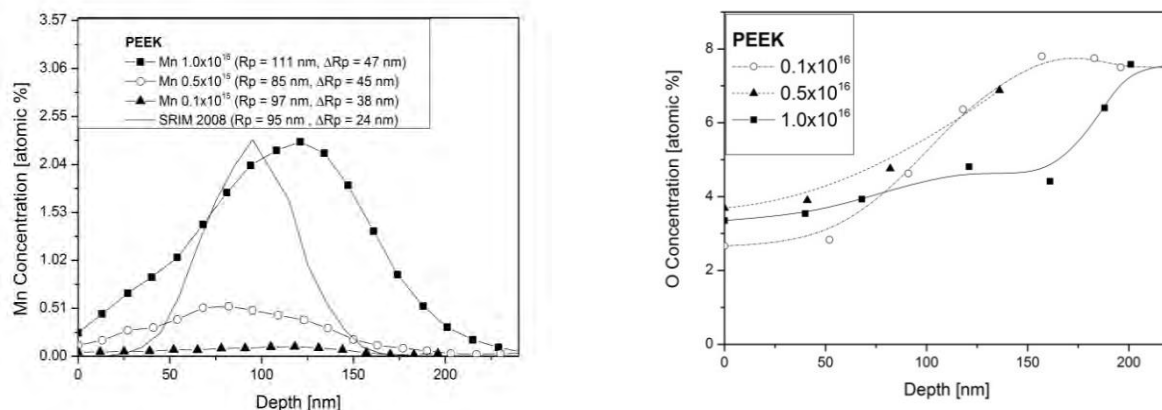
The study of electrical properties of the metal/polymer composites is of interest for a fundamental reason, i.e. the understanding of the mechanisms of electrical charge transport either through the carbon-rich phase or as a pure electron conductance through percolating metal nanoparticles, and for potential practical applications of carbon/metal composites in microelectronics or optoelectronics.

This work was focused on the characterization of the structural and physico-chemical changes caused by implantation of the different polymers with Mn, Co, Ni and Fe ions (40 – 80 keV) to different fluencies. The effect of subsequent sample annealing and possible appearance of the further structural and compositional changes depending on the previous implantation modification was examined too. The annealing influence on the implanted polymer structures is studied very rarely and we have realized a systematic study under the different implantation conditions (ion specie, ion energy, ion implantation fluencies, annealing conditions). The work was realized in cooperation with Technical-Physical Institute, Kazan, Russia (responsibility for the high fluence metal ion implantation), Institute of Chemical Technology ( sharing of the instrumentation for UV VIS, FTIR analysis, XPS), Institute of Macromolecular Chemistry AS CR (TEM analysis). The main invention, interpretation, compositional, structural analysis, electrical properties measurement, image analysis of TEM, extraction of optical parameters from UV VIS and electrical properties simulation, simulation of projected ion ranges and compositional changes including TRIDYN, SRIM were done at NPI.

Data concerning Co, Ni nano-particle preparation and characterization were provided in period 2010-2012 [10,11]. Data concerning Mn and Fe implantation into polymers are rather scarce in the literature and were obtained in 2012-2014 period [3,6]. Polymers foils were implanted with metal ions at room temperature to the fluencies ranging from  $1 \times 10^{15} \text{ cm}^{-2}$  to  $1.5 \times 10^{17} \text{ cm}^{-2}$ . The depth profiles of the implanted atoms were determined from RBS spectra. While the measured projected ranges  $R_p$  are close to those predicted by the SRIM and TRIDYN code, the measured range stragglings  $\Delta R_p$  are higher below the implantation fluence  $5 \times 10^{16} \text{ cm}^{-2}$  see Figure 2. A strong disagreement between the observed Ni-depth profiles implanted at  $5 \times 10^{16} \text{ cm}^{-2}$  –  $1.5 \times 10^{17} \text{ cm}^{-2}$  ions  $\text{cm}^{-2}$  and those calculated by the SRIM code arises from the deep structural changes in the polymer matrix caused by ion irradiation.



The TRIDYN code offers a much better explanation of the observed depth profiles for ion fluencies of up to  $0.75 \times 10^{17} \text{ cm}^{-2}$  due to the dynamical MC simulation including the dynamic changes of the elemental composition and the density during the implantation process. Mn exhibits the different behaviour comparing to Co, Ni implanted species, and most pronounced dissipation of Mn was observed in this experiment.



**Figure 2** Mn depth profiles in PEEK – left from RBS analysis, oxygen depth profiles in implanted Polyetheretherketone (PEEK) – right. Mn profiles compared to SRIM simulation.

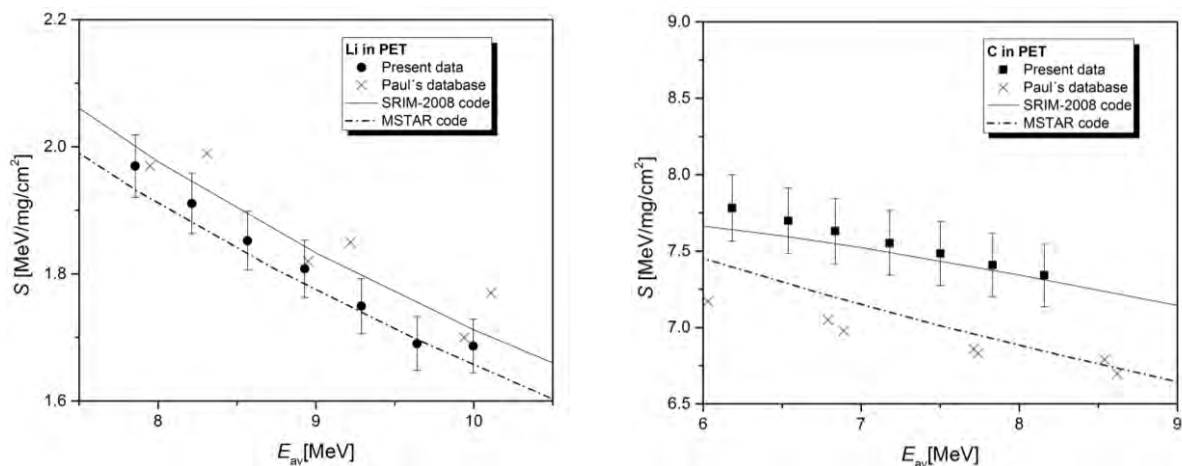
The polymer degradation is manifested by the depletion of the hydrogen and oxygen content in the irradiated surface layer. The depletion of hydrogen and oxygen in the irradiated surface layer of polymers was observed in RBS and ERDA measurements. In the case of oxygen, ion irradiation may lead to two competing processes: the desorption of oxygen-rich degradation products and the entry of oxygen from the ambient atmosphere and its trapping on the dangling bonds produced by ion bombardment. For Co, Mn implantation we observed the desorption of oxygen according the increasing ion implantation fluence, see Figure 2 -left.

At high ion fluencies, the implanted Co atoms aggregate and Co nanoparticles are formed in the near-surface layer of the polymers [10,11]. TEM analysis and the image analysis have shown that the nanoparticle mean diameter is an increasing function of the ion fluence, but the growth rate of nanoparticles depends on the polymer specie. The sheet resistance of the implanted polymers decreases with the increasing ion fluence. This trend is in accord with the gradual enhancement of UV-Vis absorbance and decreasing of optical band gap [6,14].

### 3. ENERGY LOSS STUDY IN DIFFERENT MATERIALS

This topic was invented, realized, evaluated and presented fully at NPI in 2011-2013, the complementary analysis of UV VIS and FTIR of investigated polymers were provided in 2014. The stopping power and energy straggling of  $^7\text{Li}$ ,  $^{12}\text{C}$  and  $^{16}\text{O}$  ions in thin polymer foils were measured in the incident beam energy range of 9.4–11.8 MeV using an indirect transmission method [5]. The knowledge of both the energy loss and the energy straggling heavy ions ( $Z > 2$ ) in polymer is a very important for material modification by ion implantation, for ionizing radiation dosimetry, radiation biology, radiation chemistry and radiotherapy. The experiments were carried out in LT NPI. The experimental measured stopping powers were compared with the predictions obtained from the SRIM-2008 and MSTAR codes, which use two different semi-empirical models, Bragg's rule and the cores-and-bonds (CAB) model. The measured stopping powers of Li ions in PET are in a good agreement comparing to the theoretical predictions provided by SRIM and MSTAR. In case of C, O ions we observed the better agreement with

predicted data including CAB model (SRIM simulation) in polyethyleneterephthalate (PET) see Figure 3.



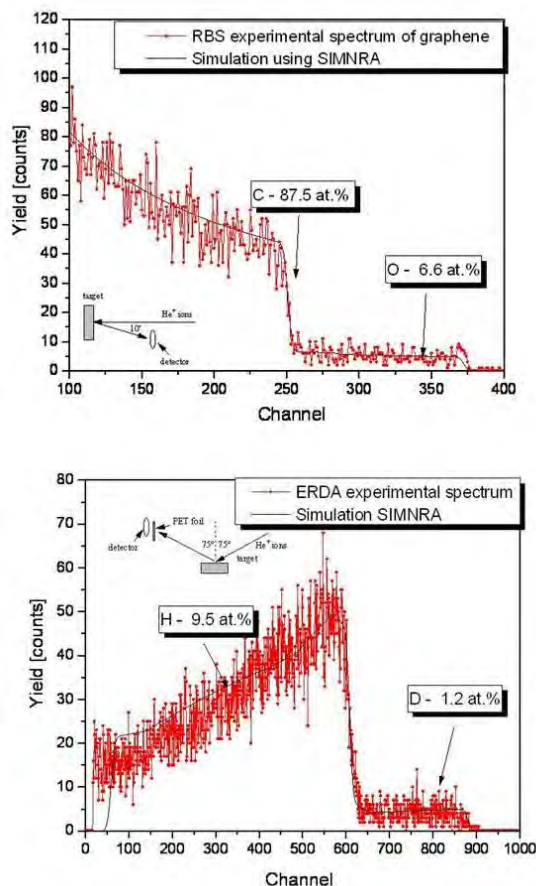
**Figure 3**

The stopping powers of a) Li, b) C ions in PET (points) and those calculated from the SRIM 2008, MSTAR codes (lines) and experimental data from Paul's database (points) as a function of  $E_{av}$  (lines).

The energy straggling data were compared with those calculated by using Bohr's, Lindhard–Scharff and Bethe–Livingston theories. For all ion-polymer combinations the measured energy straggling is much higher than Bohr's value. The deviations between experimental and theoretical values may partly be attributed to the fact that the above mentioned models take into account only the collisional energy loss straggling, but in the present experiment the ions are not fully stripped and there is a significant contribution due to charge-exchange straggling [16, 17]

#### 4. GRAPHENE BASED STRUCTURES CHARACTERIZED BY ION BEAM ANALYTICAL METHODS

Graphene, a two-dimensional (2D) sheet of carbon atoms arranged in a honeycomb lattice, attracted recently a huge scientific interest, due to its outstanding transport properties, chemical and mechanical stability and to the scalability of graphene devices to nanodimensions. Chemical synthesis of graphene relies on the usage of various chemical reagents. We demonstrated that these chemical treatments significantly contaminate graphene with heteroatoms/metals, depending on the procedures followed. Such unintentional contaminations during chemical synthesis is rarely anticipated and reported. The study was performed in cooperation of NPI Rez, Nanyang Technological University, Singapore and Institute of Chemical Technology Prague. Participation of the NPI team ensures – RBS, ERDA, PIXE, PIGE analysis of heteroatoms and incorporated metals concentration, participation of the Nanyang Technological University team included partially deposition of the graphene structures by various chemical methods, and participation of the ICHT team includes graphene deposition, XPS and Sem-EDX analysis [18, 19].



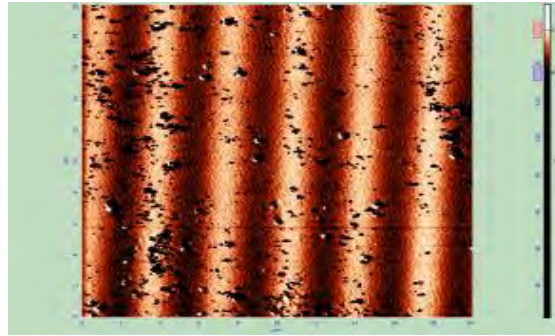
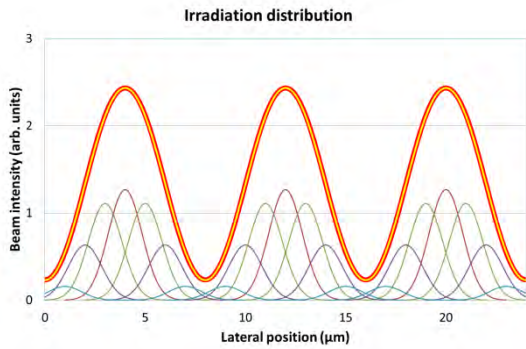
The most widely studied graphene derivatives are halogenated and hydrogenated graphenes. Fully hydrogenated graphene with is called graphane. ICHT team prepared hydrogenated graphene. NPI team studied exact yield of hydrogenation using deuterium labelling and consequent analysis by nuclear spectroscopic techniques (ERDA and RBS). The structure and composition of synthesized hydrogenated graphene was analysed by SEM, EDS, STEM, high resolution XPS, Raman spectroscopy, combustion elemental analysis, FTIR spectroscopy etc. in ICHT. We demonstrated that the deuterium labelling is highly useful for exact measurement of hydrogen concentration in the form of C-H bonds in hydrogenated graphenes. The nuclear analytical methods like RBS and ERDA were used for exact quantification of deuterium concentration within hydrogenated graphenes see Figure 4 [20].

**Figure 4** RBS (up) and ERDA (bottom) analysis of graphene labelled by deuterium.

## 5. MICROBEAM APPLICATION ON ION BEAM WRITING

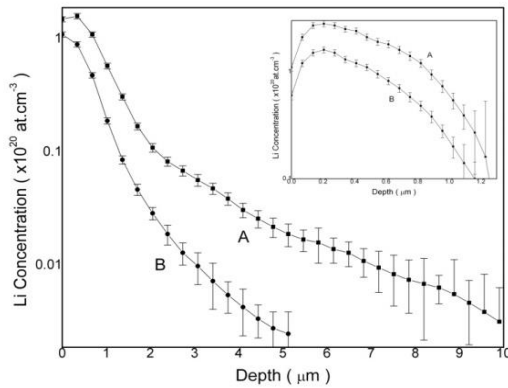
Ion beam implantation is able to modify the optical properties of optical materials, such as some polymers, glasses and crystalline materials. Numerous practical applications exist, optical gratings are also among the possible applications. Although these gratings are mainly produced as surface relief gratings, ion beam implantation can effect in the change of the refractive index. However, previous experiments showed that during ion implantation a surface structure may also appear due to the induced volume change, resulting mixed-type gratings investigated the refractive index depth profile in PMMA due to proton irradiation, and found that the highest increase of the refractive index occurs at the end-of-range (Bragg-peak) of the penetrating protons. This allows us to produce diffractive optical elements by modulating the refractive index of the material well below its surface by use of high energy ion implantation. The aim of the research was to imitate interferometrically produced optical gratings by producing quasi-sinusoidal refractive index profiles making by modulating irradiation fluence across the grating lines, utilizing that the intensity distribution of the ion microbeam is close to Gaussian [21, 22].

Transmission phase optical gratings with grating constants ranging from 2  $\mu\text{m}$  to 15  $\mu\text{m}$  were designed and fabricated in Pyrex glass by 2 MeV  $\text{H}^+$  and 6 MeV  $\text{C}^{3+}$  microbeam irradiation. The resulting mixed gratings (index of refraction and surface relief) were studied with atomic force microscopy and phase contrast and interference contrast optical microscopy. Measured diffraction efficiency distributions in the various orders confirmed that the obtained grating profiles were close to the sinusoidal Figure 5.



**Figure 5** The irradiation distribution for the  $\Lambda=8\ \mu\text{m}$  grating constant. The red-yellow-red line is the expected quasi-Gaussian distribution achieved by scanning the beam on different pixels multiple times (shown by thin lines of various colours) -left. AFM image of the ion micromachined gratings - right

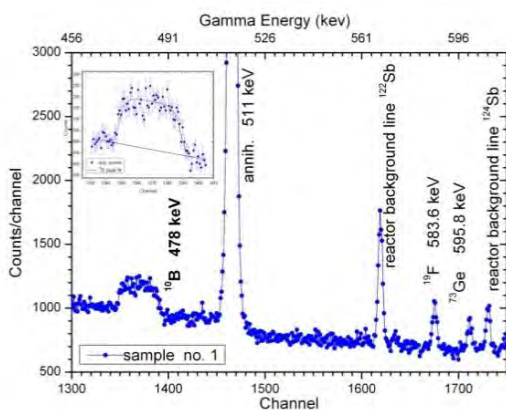
## 6. NEUTRON BEAM APPLICATIONS



Major field of NDP application is depth profiling of boron, lithium and nitrogen in various materials [23-28]. An example is the first study of lithium diffusion in synthetic polymers stimulated by in situ electron irradiation [28].

**Figure 6** The depth profiles of  $^6\text{Li}$  from polyimide samples doped for 1000 (A) and 2000 s (B). The profiles were determined using LIBOR code (prepared in NPI) from the spectra of  $^3\text{H}$  and  $^4\text{He}$  (inset).

Main area of PGAA application is non-destructive determination of elemental composition of different materials [29-30]. The device was used, e.g., for determination of concentration of boron dopant in graphene [30].



**Figure 7** PGAA spectrum of prompt gamma-rays from graphene doped with boron with fit of Doppler broadened 478 keV line from neutron induced reaction on  $^{10}\text{B}$  (lower) [30].

Besides the research utilizing nuclear analytical methods, LT deals also with a study (fabrication and characterization) of novel materials with a high application potential, such as materials for biosensors, gas sensors, tissue engineering, and

hybrid (metal-organic) thin films. The study is carried out on laboratory-prepared systems, i.e., vacuum deposition facilities, low energy ion beam deposition complex (used for sputtering and implantation), and devices for post-deposition sample processing (etching, annealing, plasma treatment, etc.). The biosensors are prepared on thin polymeric foils, irradiated with swift heavy ions and etched in a special way to develop pores with a certain (conus-type) shape [31-34]. The hybrid films are fabricated by alternate or simultaneous deposition of transitional metals

(e.g., Ni, Cu) and fullerenes (e.g., C<sub>60</sub>); the hybrid films exhibit unique properties, such as a strong charge transfer, biotolerance or selforganization tendency [35-40].

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## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Neutron Diffraction                            |

### INTRODUCTION

The neutron diffraction team participates in the research programme of a large research infrastructure – the Centre of Accelerators and Nuclear Analytical Methods (CANAM) – providing unique experimental infrastructure in nuclear physics and neutron science to academic and industrial research community. Research activity of the team is mainly oriented on experimental physics with neutrons, employing the neutron beams of the research reactor LVR-15 in Řež. Mission of the team members is therefore twofold: (i) to provide the experimental infrastructure and expertise in neutron scattering methods to the research community in the Czech Republic and abroad, and (ii) to carry out their own research, usually on the basis of long-term collaborations with regular facility users. Results of this research in the period 2010-2014 can be divided in two major topics - materials research with neutrons, and neutron scattering instrumentation and methods.

### 1. MATERIALS RESEARCH WITH NEUTRONS

Materials research with neutrons has been usually carried out in collaboration with partners from other research institutes. In many cases, like those described the examples below, this collaboration goes far beyond the usual user support in conducting the experiment and data reduction. The team members are much more involved in the underlying science and participate actively in data analysis, physical interpretation of the experimental results as well as writing publications. This approach gave rise to a growing number of long-term collaborations with researchers from both Czech and foreign laboratories, which are mentioned at the end of each example.

#### 1.1 Deformation mechanisms of metals under thermo-mechanical loading

*P. Lukáš, J. Pilch, P. Beran, P. Strunz,*

*PhD students: J. Čapek, G. Farkas*

Diffraction experiments provide extremely valuable information about the structure and microstructure evolution upon in situ thermo-mechanical treatment of the material and these data can be currently correlated with the measured conventional thermal and mechanical response of the material. In general, this technique yields very useful information on deformation mechanisms and phase transformations.

The very high resolution of our neutron diffractometer TKS-400 enables us to apply the methods of profile analysis to treat the obtained diffractograms. The microstructural parameters of the examined material obtained in such a way can be directly compared with parameters of micromechanical models. This approach brings a deeper understanding of processes ongoing in materials upon deformations, thermal treatments or phase transformations.

The above described methods were mainly applied to investigation of deformation mechanisms of *magnesium alloys*, including innovative application of acoustic emission



method simultaneously with neutron diffraction. Complementary dataset about the loading mode dependence of twinning was obtained, since acoustic emission is sensitive to twin nucleation whereas diffraction to twin growth. Theoretical calculations of Schmid-factor dependence of twin nucleation complete the experimental results which clearly explain the different behaviour of this material in tension and compression [1]. (Collaboration with the Faculty of Mathematics and Physics, Charles University).

## **1.2 Microstructure of novel materials**

*P. Strunz, V. Ryukhtin, P. Beran, J. Šaroun*

The small-angle neutron scattering (SANS) method provides valuable information about material microstructure in a wide range of size scales ranging from units of nanometres to several microns. Covering this broad range requires a combination of measurements at various types of SANS instruments. The double-crystal SANS diffractometer MAUD at the reactor LVR15 in Řež is unique in covering the gap between about 100 nm and 1  $\mu\text{m}$ , which is not efficiently accessible by other existing SANS techniques. In addition, diffraction experiments provide necessary complementary information on phase composition, grain size, microstrains and lattice constant misfits. The studies carried out by the team members often combine the experiments at the instruments MAUD and MEREDIT in Řež with the measurements at other European facilities.

### **High-temperature materials**

*Experimental alloys based on the Co-Re system*

The results of research on Co–Re alloys belong to the most significant and interesting scientific outputs of the team in the last years. Co–Re alloys development was prompted by a search for new high-temperature material for future gas turbines. For the first time, in-situ neutron diffraction at very high temperatures (up to 1490°C) was used to investigate phase transformation in a Co–Re base alloy developed for application at high temperatures. The observed hcp to fcc matrix transformation [2] exhibited a large hysteresis. The hysteresis is a result of composition interplay between Co-matrix and other phases. Stability of carbides ( $\text{Cr}_{23}\text{C}_6$ , TaC) and  $\sigma$  phase was investigated as well [2, 3]. The TaC phase is stable up to at least 1300°C and, therefore, it is a very promising strengthening phase at high temperatures.

*Ni-base superalloys*

Further important results were achieved in the research of Ni-base superalloys, frequently used high-temperature materials for turbine blades nowadays [4-6]. For example, an additional  $\gamma'$  precipitation with slow kinetics was detected and characterized (formation, dissolution, kinetics) in IN738LC high-temperature superalloy for the first time [5]. It was found that the small precipitates arise regardless the application of the mechanical load. Nevertheless, they influence mechanical parameters and explain an anomaly observed around 700°C. Also, the temperature dependence of the lattice misfit between  $\gamma$  and  $\gamma'$  phases, which is related to the coherency stresses and thus to the  $\gamma/\gamma'$  interfacial energy, was determined in Inconel-type superalloy [6].

### **Nanostructures made from metallic materials**

*Metal-matrix composites*

The Al-Pb binary system is a suitable model system for testing liquid phase dispersion strengthening in bulk materials for structural applications. The material microstructure was measured by SANS during the subsequent in-situ thermal cycling, which enabled to monitor changes of morphology of the Pb particles and their solid-liquid phase transition [7].

*Nano-porous membranes*

Using a selective phase dissolution technique, nano-porous membranes with a number of prospective applications can be produced from simple two-phase metallic alloys, which contains through-thickness elongated channel-like pores of only a few hundred nanometre in diameter. Complementary SANS experiments carried out at the medium resolution SANS instrument at HZB Berlin and high-resolution SANS instrument MAUD at LVR15 in Řež enabled to determine microstructural parameters of the membrane (pore-to-pore distance, raft thickness, pore volume fraction, specific interface) and, through contrast variation, to measure kinetics of pore filling by liquid and their subsequent emptying by evaporation [8].

The research in these fields was carried out in international collaborations with TU Munich, TU Braunschweig, EMPA institute (Switzerland) and HZB Berlin as well as in collaboration with domestic academic institutions.

### **Other**

In addition to the above topics, team members actively participated in the research of other interesting materials and their microstructure, such as

- Pores morphology of natural rocks (collaboration with the Czech Technical University in Prague).
- Structure of precipitates in NiTi-based wires (collaboration with the Institute of Physics, Prague).
- Magnetic flux line lattices in unconventional superconductors  $\text{Sr}_2\text{RuO}_4$  (collaboration with prof. H. Furukawa, Ochanomizu University, Tokyo, Japan).

## **1.3 Crystallography**

*P. Beran, P. Strunz*

Results obtained from structural and phase ratio determination play an important role in materials science and help to develop, optimize and tailor material properties for application needs. The neutron diffraction methods can reveal not only crystallographic structure, but also bulk microstructure characteristics such as the size and preferred orientation of constituent single crystal domains and moreover arrangement of magnetic moments. Examples of the research carried out by the team are:

### *Lithium batteries*

Lithium ion battery test cell for in-situ neutron diffraction measurements has been successfully designed and developed in collaboration with Uppsala University and then tested at the MEREDIT instrument in Řež. Results of this research will help to carry out in-situ experiments with neutrons for real-time monitoring of the structural changes in the battery material during within its live cycle [9]. (Collaboration with Uppsala University)

### *Graphene*

Although graphene becomes commonly available in large amounts in present days through mass production technologies, there is still a lack of precise and reliable techniques for non-destructive and fast determination of its structural properties on the bulk scale. Results of neutron diffraction experiments carried out at the MEREDIT instrument and laboratory X-ray diffractometer were compared to other analytical methods being routinely applied for graphene characterization (TEM, AFM, etc.). This study brings new deep insights into the basic structural properties of graphene in a bulk form and clearly demonstrates the advantages of diffraction methods for accurate determination of the thickness and lateral parameters of the graphene sheets [10]. (Collaboration with Institute of Chemical Technology in Prague.)

## *Magnetic materials*

Neutrons are particularly well suited for studies of magnetically ordered materials. Determination of spin arrangement in the crystal lattice is indispensable in development of materials with high application potential, such as *magneto-caloric materials*. The system FeMnP<sub>0.5</sub>Si<sub>0.5</sub> with enhanced magneto-caloric properties was studied from the point of view of nuclear and magnetic structure. The neutron diffraction measurement at the instrument MEREDIT helped to characterise the symmetry of magnetic ordering (ferromagnetic along x axis), but also to analyse different contributions of individual mixed sites (Fe/Mn) to overall magnetic structure [11].

Studies of magnetic ordering are interesting also from the point of view of fundamental condensed matter physics. Combination of X-ray single crystal diffraction and neutron powder diffraction (MEREDIT@LVR15, Řež) techniques was applied on the quasi-crystal approximant Tb<sub>14</sub>Au<sub>70</sub>Si<sub>16</sub>. The results enabled, for the first time, to construct a model of *magnetic structure of a quasi-crystal approximant* [12]. (Collaboration with Uppsala University)

## *Other*

The neutron powder diffraction experiments carried out at MEREDIT often complemented the large-scale microstructure measurements by SANS. This was also the case of the above examples on Co-Re-based alloys [3].

## **1.4 Non-invasive analysis of residual stresses**

*M. Vrána, P. Mikula, Ch. Hervoches*

Neutron diffraction permits to measure very accurately the distances between atoms and their changes due to elastic deformation. Neutrons are therefore very well suited as a probe for non-invasive determination of residual stresses in large material depths up to several centimetres. This is very important for the assessment of structural integrity and lifetime of critical engineering components, by evaluation of stresses developed during material processing (e.g. welding, rolling or case hardening) or long term use. For this type of measurements, the team employs the neutron diffractometer SPN-100, which provides necessary equipment for sample positioning and a small gauge volume necessary to map spatial distributions of residual stresses. Below are the examples of research carried out at this instrument in the course of 2010-2014.

### *High Strength Steels Welds*

Residual stresses were studied with the aim to find optimum composition of the additive material in order to decrease residual stresses in the vicinity of the foot of the welding joint and consequently to increase the fatigue strength. The aim was to test the concept of so called LTT (low transformation temperature) metal used for electrodes which (according to a theory) decreases the level of residual stresses and increases the fatigue strength [13]. (Cooperation with Welding Research Institute – Industrial Institute, Slovakia)

### *Near-surface residual stresses steel coated by tungsten carbide*

Residual stresses in inoxidizable martensitic steel 13Cr4Ni with the surface hardened either by tungsten carbide coating were studied by neutron diffraction. The achieved results gave indications which can be used in the monitoring of the coating characteristics, in particular the adhesion [14]. (Cooperation with Rogante Engineering Office, Italy)

### *Correlation of magnetic properties and residual stress distribution in welded steel*

Residual stress distribution in the welded AISI 1008 steel sheets was monitored by the X-ray and neutron diffraction technique. Alternatively, surface and bulk magnetic properties, namely Barkhausen noise and quasi-dc permeability, were measured in the same material. The study showed good agreement between the diffraction and magnetic measurements, which is

important as an independent validation of the magnetic methods [15]. (Collaboration with National TU of Athens, Greece)

## **2. NEUTRON SCATTERING INSTRUMENTATION AND METHODS**

The team members built on the long tradition of the group in developing new experimental techniques, Bragg diffraction optics and specialised methods and software for data analysis and Monte Carlo simulations. Two major activities in this field - regarding neutron optics and instrumentation for the European Spallation Source (ESS) - are described in the paragraphs below.

### **2.1. European Spallation Source**

*P. Lukáš, J. Šaroun, P. Beran, J. Pilch, P. Strunz, P. Šittner, L. Kadeřávek, V. Ryukhtin*

The neutron diffraction team has been deeply involved with the project of European Spallation Source (ESS), which is a large international research infrastructure under construction in Lund (Sweden). Since 2010, the project “ESS Scandinavia” has been funded by the Czech government (MEYS, LM 2010011) in order to support participation of the Czech Republic in the design and construction of ESS. The team lead by P. Lukáš became responsible for realization of this task. In collaboration with colleagues from the Faculty of Mathematics and Physics at the Charles University and from the Institute of Physics CAS, they developed the first concept of a neutron diffractometer for ESS, addressing the growing demand of the materials engineering research community for complex in-situ and in-operando experiments with neutrons, under industrially relevant heating/cooling rate, deformation rate and time scale conditions. Given the support from ESS, the concept has been further elaborated and finally resulted in the joint instrument construction proposal together with the German partners from the Helmholtz Zentrum Geesthacht (HZG). After successful reviews by international science and technical advisory panels, the project named as “Beamline for European materials Engineering Research (BEER)” has been eventually endorsed by the ESS steering committee in early September 2014. The neutron diffraction team contributed to the project mainly by developing the science case for the above in-operando experiments, by the pre-design study of the related special sample environment and by detailed conceptual design of the neutron optics and neutron transport systems, based on a large set of neutron transport simulations, numerical optimizations and simulated performance characteristics. During the evaluated period, the ESS project became one of the key research activities of the team, attracting also young scientists and leading to expansion of the team over this period. Since 2014, the team has become even more engaged in the ESS project, taking over responsibilities within the instrument construction consortium related to their expertise (mainly neutron optics and sample environment). It is therefore assumed that construction of the diffractometer BEER for ESS will remain one of the key topics for the team also in the next period.

### **2.2. Bragg diffraction optics**

*P. Mikula, J. Šaroun*

Since 2010, intensive collaboration with colleagues from KAERI Daejeon (Korea) resulted in a number of outstanding results in the field of Bragg diffraction optics, documented by series of articles and conference papers [16-21). These results can be divided in two categories:

1. *Use of Bragg diffraction optics for a modernisation of diffractometers dedicated to residual strain/stress measurements.* Here the application of neutron focusing techniques proposed by the NPI team allowed to reach world class instrument performance parameters. At present, the dedicated instrument in KAERI Daejeon thus enables stress investigations in steel samples

in the depth up to 80 mm or kinetic processes of structural changes in the time scale of several seconds [16-17].

*2. Experimental studies of new types of high resolution neutron monochromators/analysers employing dispersive configurations and multiple Bragg reflections.* This research aims at the development of new types of the double bent crystal monochromators, which can provide high resolution thermal neutron beams either of millimetre width or cross-section of several square centimetres without any mechanical slit and collimator systems. The resolution can be easily manipulated only by adjustment of bending radii of the crystals. All these investigations are really pioneering in the field of neutron diffractometry. Microfocusing of the neutron beam can be exploited in powder diffractometry with samples of small dimensions. On the other hand, the highly collimated beam of the large cross section either in the case of multiple reflection monochromators or dispersive double bent crystal settings permits observation of edge refraction effects and therefore, can be successfully used e.g. in phase contrast radiography measurements [18-22].

These results contributed to the growing credit of the NPI group in this field among the world neutron scattering community, firstly the collaborating group at the HANARO reactor in KAERI, but also at other neutron centres in Asia and Europe, which was underlined by participation in the international projects like the EU FP7-NMI3-II initiative in 2012-2015 (WP17 - Neutron imaging) or European Spallation Source.

### **2.3. New instrument concepts and data analysis methods**

*J. Šaroun, P. Mikula, P. Strunz*

Since 2010, development of the Monte Carlo simulation software for modelling neutron scattering experiments and data analysis (RESTRAX & SIMRES) has been focused on time-of-flight methods, which was motivated by the team's strong involvement in the ESS project (see 2.1). However, this work has a wider international context. The program SIMRES has been used by the author (J. Šaroun) and other users abroad in a number of instrument upgrade programs lead by major large scale facilities, for example the project ThALES at the Institute Laue-Langevin in Grenoble (ILL) [23]. The simulations also support research in the field of Bragg optics (2.1), for example by modelling of multiple Bragg diffraction in elastically deformed single-crystals, which is not possible by any of the other available simulation programs [21]. Application of the neutron ray-tracing simulation methods to residual stress analysis gave rise to a continuing collaboration with colleagues from TU Munich and Karlsruhe Institute of Technology (KIT) resulting in the progress in solving the problem of the surface effect [24,25], opening the way to the studies of medium (millimetre) range sub-surface stress distributions by combining X-ray and neutron diffraction data.

Many of the publications on SANS investigations of precipitation in high-temperature materials are based on data interpreted with the help of the software developed by P. Strunz especially for the coherent anisotropic microstructures occurring in this kind of materials [4,7,8]. This approach permits to assess physical microstructure characteristics relevant particularly for these materials, which is not possible by other more general software available elsewhere.

### **2.4. Neutron scattering instrumentation at LVR15**

Continuous effort has been spent on the improvement of experimental base of the neutron diffraction group. Even though this activity does not generate scientific results per se, it is crucial for competitiveness of research carried out by both the team members and external users of the facility. Since 2010, new in-pile collimators equipped by sapphire filters were constructed and installed on last two of the instrument suite, which lead to about a factor of two reduction in the background level. Later, the old 1D detectors were replaced by three larger (200 x 200 mm<sup>2</sup>) 2D position-sensitive detectors equipped with new shielding, which increased the data acquisition rate for diffraction experiments by a factor of four. This was accompanied by modernisation of the instrument control electronics and software, which allows easier

implementation of growing variety of sensors and devices needed for carrying out complex in-situ experiments. To extend experimental possibilities of the neutron diffraction instruments, the suite of sample environment devices has been extended by a compact light furnace ( $T < 1000^{\circ}\text{C}$ ) and closed-cycle cryostat ( $T > 4\text{K}$ ) for powder diffraction.

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## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Dosimetry of Ionizing Radiation                |

The research topics of the team concentrate to three overlapping and complementary areas: dosimetry of complex radiation fields, radiation biophysics and biology and environmental dosimetry.

### DOSIMETRY OF COMPLEX RADIATION FIELDS

The main research activities in this domain focus on studies of cosmic radiation, related radiation protection issues on board aircrafts and spacecrafts, dosimetric and microdosimetric description of therapeutic charge particle beams, and methodology of passive dosimetry using track-etched detectors.

Iva Ambrožová coordinates participation of the research team in international experiments focused on passive dosimetry on board the International Space Station (ISS), such as project Matroshka-R: Study of cosmic rays on ISS Russian segment, European Space Agency (ESA) projects Dosis and Dosis 3D and others. Our passive detectors have been placed on the surface and inside the tissue equivalent phantoms and at different locations inside and outside ISS. Analysis of the results, obtained in the experiments since 2005, has enabled to study the dependence of dosimetric quantities (linear energy transfer spectra, dose and dose equivalent) on various parameters, such as phase of solar cycle, shielding characteristics, or ISS orbit parameters. In addition to experimental measurements, theoretical calculations were also carried out using PHITS code and compared with the measurements obtained in experiment Matroshka-R 2006. The effect of different parameters, which affect the accuracy of the calculation of absorbed dose and dose equivalent, has been determined [1]. The PHITS code was also used for simulations of the Protective curtain experiment onboard the Service module of ISS. The experiment was aimed on measurement of the dose-reducing effect of the additional shielding made of hygienic water-soaked wipes and towels placed on the wall in the crew cabin of the module. Using our simulations, we found this type of shielding very efficient when applied on spacecraft at low-Earth orbits where the trapped protons dominate. However, for deep-space manned missions, where astronauts are exposed mainly to galactic cosmic rays, other shielding technology should be used [2].

We continuously extend our unique expertise in methodology of linear energy transfer (LET) spectrometry by track-etched detectors. We classified the sources of the measurement uncertainty of a LET spectrum and developed a model for calculation of a combined uncertainty. The model was applied to a spectrum measured with a track-etched detector in space. For some spectrum bins, the largest contribution to the combined uncertainty was due to the uncertainty associated with the randomness of particle detection. For the others it came from the uncertainty of the calibration curve. The analysis showed that sources of uncertainties other than the randomness of particle detection should not, in general, be neglected [3,4].

Our team members perform dosimetry studies in complex radiation fields on board aircrafts; compliant with needs of radiation protection of crew and passengers. Due to the increased level of cosmic radiation at flight altitudes the annual effective doses of aircrew members often exceed the limit of 1 mSv for the public, and thus it is recommended to monitor them (see ICRP Publication 60). Annual effective doses received by aircrew are routinely calculated using the



computer codes CARI (versions 5E and 6) and EPCARD. The codes, which take into account flight parameters such as altitude, geographic position, and solar activity, are validated by experimental measurements every five years. Dose and ambient dose equivalent rate distributions on-board Czech Airlines' narrow body short- and middle-range aircraft were measured in June, July and August 2011 using six to eight planar silicon diode detectors of the Liulin type. We found that ambient dose equivalent is higher in the front and the back of the cabin and lesser in the middle of the cabin. Results of the measurements were found to be in a good agreement with performed EPCARD calculations and other published data [5].

We allow a free access to our long-term measurements with the silicon spectrometer Liulin onboard aircraft by means of a database available online at <http://hroch.ujf.cas.cz/~aircraft/>. The database covers measurements since 2001, which is longer than usual duration of a solar cycle period. The database comprises over  $10^5$  individual records of energy deposition spectra, absorbed dose rates, and ambient dose equivalent rates including also information about flight parameters. The database represents a unique and useful tool for verification of the routine dosimetry of aircraft crews [6].

We apply our experiences in dosimetry and microdosimetry to provide information about quality of therapeutic ion beams for cancer therapy. Various detection systems (thermoluminescence detectors, track-etched detectors, silicon detector Liulin, tissue-equivalent proportional counter type HAWK) were irradiated in heavy ion beams at accelerator HIMAC in the National Institute of Radiological Sciences, Japan. We obtained spectra of linear energy transfer along the Bragg curve and depth dose distributions for each ion beam of different energies and configurations. We obtained valuable information about the contribution of fragments of the primary ions or target fragments to dose [7,8,9]. Particular attention have been devoted to measurements in carbon ion beam in monoenergetic (MONO) and spread out Bragg peak (SOBP) configurations. The LET spectra in the beam and out of the beam have been measured using strips of track-etched detectors and confirmed by calculations using Geant4 toolkit [10,11,12,13].

The institute is a voting member of EURADOS platform. The researchers of this team actively contribute to activities of EURADOS work groups WG6 – Computational dosimetry, WG9 – Radiation protection dosimetry in medicine and WG11 – High energy radiation fields. To demonstrate our involvement in EURADOS activities, let us mention the invited lecture of Marie Davidková „Introduction to microdosimetry“ presented in the frame of the 6th EURADOS Winter School on Microdosimetry, Annual Meeting 2013, Spain. Iva Ambrožová is leading the task on cosmic rays dosimetry on board aircrafts of EURADOS WG11 – High energy radiation fields. Ondřej Ploc and Ján Kubančák actively contribute to activities of WG9 – Radiation protection dosimetry in medicine focused to determination of out-of-field doses during radiotherapy. The importance of this issue is given by the fact that doses delivered outside the radiation field during radiotherapy can potentially lead to secondary cancer development. Recent international experiments have been performed in therapeutic active scanning proton beams in Trento, Italy (2013) [14] and Krakow, Poland (2014). We contribute to these experiments with measurements using passive detectors (thermoluminescence and track-etched detectors) and tissue-equivalent proportional counter type HAWK. In collaboration with Alexander Molokanov, out-of-field doses in therapeutic proton beam in the Joint Institute for Nuclear Research have been also measured. In that case, SOBP configuration was achieved using a passive modulator [15].

The contribution of neutrons to out-of-field doses during radiotherapy has been also evaluated. Measurements of neutron spectra were carried out around radiotherapeutic linear accelerator (LINAC) producing undesirable photoneutrons. In the Bonner spheres passive track etch detector with  $^{10}\text{B}$  radiator was used to avoid overloading of the active detector during very short period of neutron generation. It has been shown that a flattening filter is the main source of photoneutrons generated in the therapeutic LINAC and that the collimator jaws decrease the number photoneutrons going outside from the LINAC gantry [16].

As a new perspective in passive dosimetry, we started collaboration with colleagues from the German Cancer Research Center (DKFZ), Division of Medical Physics in Radiation Oncology in Heidelberg. We have tested capacities of combination of track-etched detectors and fluorescent nuclear track detectors for single track coincidence measurements. The feasibility study has shown a possibility to gather a variety of information about a detector material such as detection efficiency, spectroscopic properties, agreement of track positions, etc. on an individual track level [17].

## **RADIATION BIOPHYSICS AND RADIOBIOLOGY**

Biological effects of ionizing radiation depend crucially on microscopic radiation quality, namely the spatial structure of energy depositions along the particle track. As a part of our basic research, we seek to define links between radiation track structure and biological consequences of irradiation.

First, our long-term interest are the biological consequences of radiation action on subcellular level. In these studies we use DNA plasmids. In cooperation with Prof. Lembit Sihver from Chalmers University of Technology, Sweden, we studied primary DNA damage caused by heavy ions, 290 MeV/u C ions and 500 MeV/u Fe ions. The DNA plasmids were in solutions with different scavengers and scavenging capacities to analyze indirect effects of radiation. We concluded that radiation-induced yields of double strand breaks (DSB), the typical clustered DNA damage, depend only on the concentration of hydroxyl radical in the solution. On the other hand, the yields of non-DSB clusters depend on more factors, which are likely connected to properties of the individual scavengers [18]. The studies of direct and indirect effects of radiation continued in the project aimed on proton-induced effects. The plasmid DNA damage has been measured in solution of coumarin-3-carboxylic acid scavenger to control an extent of the indirect effect. The scavenger was also used for precise measurement of hydroxyl radical yields, which were compared with Monte Carlo simulations. The results revealed that in given conditions, the indirect effects caused by radical attack are responsible for most of the DNA damage [19]. The collaboration with Prof. Sihver has continued within the project dedicated to extension of the information about radiation-induced DNA damage with help of atomic force microscopy. This project has started in 2014 and is partially supported by ESA.

In collaboration with the group of Dr. Juha from the Institute of Physics CAS, we participated on the studies with dry DNA plasmid layers irradiated with soft X rays, where the indirect effect is fully suppressed [20]. In order to include also protons, a set of experiments was performed at U120-M cyclotron in Řež and at the LCAR laboratory of the University of Paul Sabatier in Toulouse – the paper summarizing obtained results has been submitted recently.

Thanks to the strong effort of researchers, we have successfully started experimental studies on cellular level. In our own experiments we work at the moment only with normal neonatal and adult human skin fibroblasts, which represent normal cell line. We can monitor the response of the whole cell culture. Except cell survival, we can follow level of apoptosis, senescence and DNA damage expressed as micronuclei formation in dividing cells. During two years of scientific stay, biochemist Alexandra Litvinchuk strengthened significantly our team. She introduced in the laboratory new techniques including polymerase chain reaction (PCR), which allows us to follow gene expression in irradiated cells. The goal of these studies is to describe effects of low energy ions to cell population. For that purpose we designed a particular setup for irradiation of cell monolayers at microbeam of the NPI Tandatron accelerator 4130. The first results on low energy protons and alpha particles have been obtained [e.g. 21,22].

More detailed analysis of cell response to radiation is carried out in collaboration with biologists from the Institute in Biophysics CAS in Brno, namely team of Martin Falk. Using advanced immunofluorescence techniques, they were able to obtain information about cell DNA damage and repair [23,24,25,26]. We assured in these studies cell cultivation, sample preparation and irradiation, including dosimetry measurements and sample post-irradiation fixation.

During the last two years, we performed the first radiobiological experiments in clinical proton beam at the Proton Therapy Center in Prague (PTC). Our experimental work is focused on biological efficiency of spread out Bragg peak of actively scanning proton beam. We perform precise dosimetry measurements to position cell monolayers at the beginning, at the middle and at the distal edge of the SOBP and we follow different biological endpoints in irradiated normal human skin fibroblasts [27,28]. The international interest to perform such studies can be demonstrated by four experimental campaigns in PTC in collaboration with prof. Kevin Prise from the Centre for Cancer Research & Cell Biology, Queen's University Belfast, UK.

We continue long-term development of tools for theoretical modeling and prediction of biological effects of ionizing radiation at molecular level. A new module for modeling of charge migration and localization in DNA has been developed and implemented into our RADAMOL simulation tool [29]. Free electrons and holes are formed by direct ionizations of the macromolecule. Subsequent processes of charge migration (distance, migration between strands of DNA or intrastrand between deoxyribose and bases) have been described according to current knowledge. Series of calculations for oligomer DNA and DNA complexes with the lac repressor protein have been performed and distributions of deoxyribose and base damage were compared with calculations where migration processes were not taken into account. We demonstrated the importance of charge transfer on distribution of primary DNA damage. Charge migration has to be considered and followed when modeling systems, where unscavengeable effect of ionizing radiation is significant. Such conditions are relevant especially in living cells.

In order to share our experiences in the domain of DNA radiation damage modeling with wide scientific community, we started collaboration with Sebastien Incerti, the director of research at the Université Bordeaux/CNRS. S. Incerti is an expert in Monte Carlo simulations, developer of Geant4 toolkit and spokesperson of Geant4-DNA collaboration (<http://geant4-dna.org/>). Václav Štěpán became a member of Geant4-DNA development team and contributed to development and benchmarking of the stochastic modelling of chemical stage in Geant4-DNA, as released in Geant4 version 10. Marie Davídková is a member of the Geant4-DNA collaboration and contributes in areas of Geant4-DNA application, outreach and support [30,31].

## ENVIRONMENTAL DOSIMETRY

The last, not least, research direction of the team is environmental dosimetry. The main research topics of the group of environmental dosimetry are: occurrence of radionuclides in the environment, studies of anthropogenic influences on the environment, development of new methods of radionuclides determination, radiocarbon dating, and applications of developed analytical methods in research and industry. In general, developed analytical methods are aimed on chemical forms of uneasily determinable radionuclides (almost clear beta emitters), especially:  $^{14}\text{C}$ ,  $^3\text{H}$ ,  $^{129}\text{I}$ ,  $^{90}\text{Sr}$  together with  $^{89}\text{Sr}$ .

### A) $^{14}\text{C}$

For the precise determination of  $^{14}\text{C}$  in various sample types, our laboratory still partially applies a “conventional” approach based on conversion of the carbon from sample into benzene ( $\text{C}_6\text{H}_6$ ) chemical form, which is then measured using a low-background scintillation spectrometer. The disadvantage of the method is a high demand on the quantity of sample carbon, since about several grams are required. In the last three years, our laboratory has been working intensively on processing of microsamples for the Accelerator Mass Spectrometry (AMS) measurement. The sample processing includes isolating and purifying relevant forms of carbon, combustion, and conversion to graphite of resulting purified  $\text{CO}_2$ . Graphite is the form directly used for the AMS measurement. Only milligrams of carbon per sample are required there, which extends substantially the possibilities of  $^{14}\text{C}$  analyses for various purposes. Regrettably, there is no

AMS device in our country. The samples prepared in our laboratory are being sent for measurement to research facilities abroad, mostly to DeA ATOMKI HAS, Debrecen, Hungary. Determination of  $^{14}\text{C}$  in various sample types might yield important data serving multiple purposes, such as: age determination, study of recent atmospheric  $^{14}\text{CO}_2$  and  $\text{CO}_2$ , and  $^{14}\text{C}$  in the surrounding of nuclear power plants (NPP).

Age determination (radiocarbon dating) is an important tool for archaeology, geology, palaeoclimatology, botany, palaeontology, etc. In this field, we collaborate with the Institute of Archaeology CAS in Prague (joint radiocarbon laboratory under the international code label CRL). The radiocarbon dating method, in general requires a very precise determination of relatively low  $^{14}\text{C}$  activities, the relative uncertainty being within the order of  $10^{-3}$  for samples with age up to one half-time. A certain part of the samples sent for  $^{14}\text{C}$  dating serves to archaeologists for verification purposes. The age of the archaeological objects under study is often known from historical record, estimated from the findings of pottery, or determined in parallel, using some other dating method (dendrochronology, thermoluminescence, imbalances between some radionuclides of natural decay chain etc.). From the view of a laboratory that deals with  $^{14}\text{C}$  determination, the comparison with other dating methods is a valuable aspect for the control of the analytical techniques. In the last years, age estimation based on the so called „bomb peak“ is being increasingly used for samples younger than 1960, enabling time resolution of just single years. Besides the use in forensic medicine, public administration authorities (namely, the Czech Environmental Inspectorate, South Moravian Regional Authority) also started showing demand for this method.

In co-operation with other institutes of the CAS (Institute of Geology, Institute of Inorganic Chemistry, Institute of Botany), we were involved in the research of flood events in the floodplains of Strážnické Pomoraví and of the possible human impacts on this territory over the past periods [32,33,34]. In co-operation with the Institute of Archaeology CAS, our laboratory participated in many research topics and contributed to the preparation of several manuscripts for journals with impact factor. For example, we carried out age determination of a large number of samples from the first known Slavic settlement in our territory (in Roztoky near Prague). Our results indicate that the settlement was only inhabited for a relatively short time within the supposed period 530–652 AD [35].

Precise determinations of  $^{14}\text{C}$  activity in the air and other recent samples facilitates study of the impact of fossil fuel combustion on increasing atmospheric  $\text{CO}_2$  concentration, by specifying the parameters of carbon and  $\text{CO}_2$  transport in environments. The precise models of the  $\text{CO}_2$ /carbon transport might help in the future to avoid detrimental consequences of underestimating or overestimating the human impact on climate change. Our main achievements from the years 2010–2014 contain several published studies on the behaviour of  $^{14}\text{C}$  in the atmosphere. Using our results and data from the German monitoring station Schauinsland, normalised volume activity of atmospheric  $^{14}\text{CO}_2$  has been calculated. The pattern of the parameter obtained from our calculation has confirmed a relatively stable amount of  $^{14}\text{CO}_2$  in the troposphere after 1992 and the resulting dominant influence of the global Suess effect on the decrease of atmospheric  $^{14}\text{CO}_2$  in the following years. That means, the decrease of activity observed on global level is caused predominantly by the increasing release of fossil  $\text{CO}_2$ , without the detention time of  $^{14}\text{CO}_2$  in the atmosphere being significantly increased [36,37].

The modified approach based on calculation of  $^{14}\text{CO}_2$  content in the troposphere was used for the past trend of  $^{14}\text{C}$  activities, together with available reconstructions of  $\text{CO}_2$  concentrations in the past [38]. This way, some new findings were achieved and some expectations were confirmed concerning the behavior of atmospheric  $^{14}\text{CO}_2$  in the past. Namely: a) within the period 50–22 ka (thousands of years), the activity of  $^{14}\text{CO}_2$  was prevalingly given by the rate of its cosmogenic formation. b) during the period of the Late Glacial, approx. 22–11 ka, the activity of atmospheric  $^{14}\text{CO}_2$  was almost exclusively influenced by input of  $\text{CO}_2$  with a depleted amount of  $^{14}\text{C}$  (a surprisingly strong anti-correlation between the  $\text{CO}_2$  concentration and  $^{14}\text{C}$

activity was found here), c) the dominant influence of atmospheric CO<sub>2</sub> on the <sup>14</sup>C activity continued throughout most of the following Holocene until 2 000 years BP.

In light of the dose impact on population, <sup>14</sup>C represents the most important radionuclide released into atmosphere by nuclear power plants with pressurized water reactors during normal operation. Our study of <sup>14</sup>C activity in biota followed its possibly enhanced levels in surroundings of NPPs Temelín and Dukovany. We focused mainly on the method of selecting suitable samples, attempting to reduce the variance of observed activities. Within the frame of this study we also aimed on the method of selecting suitable reference sites, the Suess effect of which would be comparable to that in the surroundings of the nuclear power plants [39]. In 2014, our laboratory has performed an analysis of <sup>14</sup>C in annual rings sampled from conifers near Temelín NPP and near Košetice, close to the CHMI monitoring station. From the annual-ring sequence from Košetice, we obtained a relatively long record of <sup>14</sup>C activities, ranging as far as to 1940s. Thus, besides the possibility to follow back the trend of <sup>14</sup>C activity around NPPs, we have also obtained the first <sup>14</sup>C activity curve to cover the whole period of the „bomb peak“. Taking into account the slight geographical differences in activities mainly before 1964, we now have a national calibration curve. This would enable, for samples originating from our territory, a partial refinement of the age estimations based on bomb peak. For analyses of annual rings, we used our previously validated methods of microsample pretreatment, combustion and graphitization. The results are currently being prepared for publication.

#### B) Tritium

In co-operation with the National Radiation Protection Institute (NRPI), a research was conducted with focus on a possible enhancement of activities of organically bound tritium (OBT) in the surroundings of the Dukovany NPP. Activities of OBT exceeding the background levels by two orders of magnitude were found in the surroundings of the Mohelno reservoir. Into this reservoir, the waste waters from the power plant are released that contain tritium in the form of HTO. Since the reservoir is situated in a deep valley with only limited ventilation, the enhancement of OBT activity is noticeable also at neighboring sites without a direct communication with the reservoir water. This unique area makes it possible to carry out directly in the field observations on the uptake of <sup>3</sup>H by plants or to trace the transport of tritium in this interesting system [40].

#### C) Other radionuclides

Our laboratory participated in a project, aimed on the activity levels of <sup>129</sup>I in the surroundings of Temelín NPP and at reference sites within our territory. Within the frame of this project, the first data have been obtained on the activity level of this radionuclide in our country, however, no significant surplus of <sup>129</sup>I has been observed in the vicinity of the power plant [41]. The main coordinator of this project was the Neutron Activation Analysis team of our institute, the estimated participation of our laboratory makes up about 15%. Our laboratory has validated and established a method of liquid scintillation measurement of <sup>90</sup>Sr together with <sup>89</sup>Sr. This enables a direct measurement of both radionuclides without the need to wait in the presence of <sup>89</sup>Sr for a radioactive equilibrium between <sup>90</sup>Sr and its daughter nuclei <sup>90</sup>Y. The advantage of this method is the possibility to perform a measurement with just a few hour delay – for example in the case of an accident accompanied by release of these radionuclides, where a substantial time pressure on delivery of results might be expected. Orders made by the companies ETE, EDU, Canberra-Packard and Envinet in the period 2010-2014 testify an interest in the method developed by our team.

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## Research Report of the team in the period 2010–2014

|                 |  |
|-----------------|--|
| Institute       | Nuclear Physics Institute of the CAS, v. v. i. |
| Scientific team | Radionuclides and Accelerators                 |

The team is composed of researchers of two institute's departments – Department of Radiopharmaceuticals and Department of Accelerators. These organizationally independent units closely interrelate, share many research topics and present common outputs and results.

### 1. EXCITATION FUNCTIONS MEASUREMENT

Reliable cross-section data are relevant in several fields: testing of the predictive nuclear reaction model codes, cyclotron beam monitoring, production of medical radionuclides, thin layer analysis for the wear measurement and estimate of irradiated parts activation. Rather large range of available energies ( $K = 40$ ) and particle beams of the cyclotron U-120M (p, d, He-3 and  $\alpha$ ) makes it a versatile tool for obtaining such data.

We have measured cross-sections of proton- and deuteron-induced nuclear reactions on natural molybdenum. The data are relevant for cyclotron-production of Tc-99m, beam monitoring via Mo-nat(p,x)Tc-96m+g and Mo-nat(d,x)Tc-96m+g reactions, thin layer analysis (TLA) for wear measurements of alloys containing molybdenum and for production of Tc-95m as a tracer of Tc-99g in environmental samples. The elemental cross-sections for Mo-nat(p,x)Tc-99m and Mo-99 can be converted to isotopic cross-sections. The whole data set is also a good benchmark for existing nuclear reaction model codes. Data were compared with previously published results. Detailed analysis of interferences in measurement of cross-sections for formation of Tc-99m was performed and their correction described (O. Lebeda, M. Pruszyński: Appl. Radiat. Isot. 68 (2012) 2355–2365; O. Lebeda, M. Fikrlé: Appl. Radiat. Isot. 68 (2012) 2425–2432).

We performed the first measurement of excitation functions of proton-induced reactions on natural neodymium. Besides the lack of experimental data, the work was motivated by the need to estimate natural neodymium activation by cosmic protons, when mined and processed on the Earth's surface for the low-background search for neutrinoless double-beta decay of Nd-150. Results were compared with prediction of the TALYS code adopted from the TENDL library with relatively good agreement for the (p,xn) reactions. The work was performed in collaboration with group of Prof. Kai Zuber from Technical University Dresden that provided target material and characterized it, and cross-checked the primary data evaluation (O. Lebeda, V. Lozza, P. Schrock, J. Štursa, K. Zuber: Phys. Rev. C 85 (2012) 014602; O. Lebeda, V. Lozza, J. Petzoldt, J. Štursa, V. Zdychová, K. Zuber: Nucl. Phys. A 929 (2014) 129–142).

In the years 2011–2014 we also measured He-3 induced reactions on Rh-103, Tb-159 and Ho-165. Results are partly evaluated and are to be published later, as well as new measurements of for the Y-89(d,x) and As-75(p,x) reactions. In parallel, the experiments will yield mutual comparison of two monitoring reactions measured simultaneously (protons on titanium and copper, deuterons on aluminium and titanium). The data were obtained within two IAEA research contracts no. 16667 and 17461.

## 2. PRODUCTION OF RADIONUCLIDES

Production of radionuclides for medicine, calibration sources and as tracers is one of the major tasks on the cyclotron U-120M. Target holders, targets, their processing, recycling of enriched materials, and chemical separation of the products including analytical methods are studied, starting from design of targetry and ending in a tested preparation suitable for further research (labelling, measurements etc.). We are focused mainly on novel medical radionuclides, novel production routes and also on production of radionuclides for physical research.

By 2011, we finished a project focused on cyclotron production of novel positron emitters, Y-86 (14.76 h) and I-124 (4.176 d). Production of both radionuclides was established. Originally planned production of Y-86 on a solid target was modified after the first experience, and we tested and then successfully introduced production of selected radionuclides in a solution targets (MŠMT project no. 2B06165).

In 2011–2012 we tested direct cyclotron production of Ga-68, one of the emerging medical radionuclides for positron emission tomography, using solution target. The radionuclide, now already established in clinical practice, is obtained by eluting Ge-68/Ga-68 generators that are very expensive due to long-lived parent, Ge-68. Direct production of Ga-68 via Zn-68(p,n) reaction may become very interesting alternative for centers operating compact medical cyclotrons.

In 2012–2014 we have established regular production of Cu-61 (3.33 h) and Cu-64 (12.70 h) via Ni-nat(d,x) and Ni-64(p,n) reactions, including separation from target material. The former is relevant as novel PET radionuclide, the latter is theranostic radionuclide per se. Quality of the produced radionuclides regarding radionuclidic and radiochemical purity as well as specific activity is appropriate for medical use and for labelling of monoclonal antibodies and their fragments (TAČR project no. TA02010797; O. Lebeda, J. Ráliš, D. Seifert: Eur. J. Nucl. Med. Mol. Imaging 40 (Suppl. 2) (2013) S323).

Since 2010, much attention was paid to cyclotron production of Tc-99m. In 2011, we performed extensive measurements of thick target yields of various Tc radioisotopes formed by activation of highly enriched targets from Mo-95, Mo-96, Mo-97 and Mo-98. This data base allows for calculation of radionuclidic impurities content in cyclotron-produced Tc-99m from isotopic composition of the target, its thickness, beam incident energy and irradiation and cooling times. The predictive power was tested on a highly enriched Mo-100 target of known isotopic composition irradiated with 24 MeV protons (O. Lebeda, J. Ráliš, J. Štursa, E.J. van Lier, A. Zyuzin: Nucl. Med. Biol. 39 (2012) 1286–1291).

The next step was testing separation of Tc-99m, including target dissolving, deposition of sodium pertechnetate on solid phase extraction column and its elution with water. Moreover, we have also tested compatibility of the cyclotron-produced Tc-99m with many commercially available kits for established radiopharmaceuticals. In all the cases, we have not observed any difference between generator- and cyclotron-produced Tc-99m. Majority of kits combined with cyclotron-produced Tc-99m provided entirely or almost entirely quantitative labelling yields. The research was performed in collaboration with Canadian company ACSI (O. Lebeda, J. Ráliš, A. Zyuzin, E.J. van Lier: Eur. J. Nucl. Med. Mol. Imaging 39 (Suppl. 2) (2012) S412; A. Zyuzin, E.J. van Lier, J. Sader, B. Guerin, L. Matei, O. Lebeda, J. Ráliš, P. Hradilek: J. Label. Compds. Radiopharm. 56 (Suppl. 1) (2013) S470; O. Lebeda, J. Ráliš, P. Hradilek, P. Hanč, E.J. van Lier, A. Zyuzin, M. Moša: Eur. J. Nucl. Med. Mol. Imaging 40 (Suppl. 2) (2013) S424–S425; O. Lebeda, J. Ráliš, A. Čepa, P. Hradilek, T. Vrba, A. Zyuzin, E.J. van Lier: Eur. J. Nucl. Med. Mol. Imaging 41 (Suppl. 2) (2014) S434).

Finally, we proposed a set of quality control tests for the cyclotron-produced Tc-99m. Head of the department proposed as a member of the Group 14 of the European Pharmacopoeia Committee to include a new monograph “Sodium pertechnetate (99mTc) injection (cyclotron-produced)” in the European Pharmacopoeia. The proposal was approved and the monograph is under intense preparation. After thorough discussions with leading research centres in

Canada (TRIUMF, Alberta) and colleagues in the Group 14 and based on our data and data provided by other research centres, the drafted text is close to finalization.

A new gaseous target system with helium-cooled entrance window significantly increased the available production rate of Rb-83. This radionuclide plays an important role as a calibration source in the experiments KATRIN and XENON. For the purpose of the both experiments, we prepare emanation generators Rb-83/Kr-83m where the parent nuclide is fixed in zeolite, while allowing for efficient emanation of Kr-83m. We also perform filling of furnaces for production of implanted Rb-83/Kr-83m calibration sources. The current target system covers easily maximum expected activity needs of the experiment KATRIN (Manalaysay A., Marrodán Undagoitia T., Askin A., Baudis L., Behrens A., Ferella A.D., Kish A., Lebeda O., Santorelli R., Vénos D., Vollhardt A.: *Rev. Sci. Instr.* 81 (2010) 073303; Venos D., Zboril M., Kaspar J., Dragoun O., Bonn J., Kovalik A., Lebeda O., Lebedev N.A., Rysavy M., Schlosser K., Spalek A., Weinheimer Ch.: *Measurement Techniques* 53 (2010) 573–581; Hannen V., Aprile E., Arneodo F., Baudis L., Beck M., Bokeloh K., Ferella A.D., Giboni K., Lang R.F., Lebeda O., Ortjohann H.-W., Schumann M., Spalek A., Venos D., Weinheimer C.: *J. Inst.* 6 (2011) P10013; Slezák M., Vénos D., Lebeda O., Trojek T.: *Eur. Phys. J. A* 48 (2012) 12; Rosendahl S., Bokeloh K., Brown E., Cristescu I., Fieguth A., Huhman C., Lebeda O., Levy C., Murra M., Schneider S., Vénos D., Weinheimer C.: *J. Inst.* 9 (2014) P10010; Vénos D., Slezák M., Dragoun O., Inoyatov A., Lebeda O., Pulec Z., Sentkerestiová J., Špalek A.: *J. Inst.* 9 (2014) P12010).

### 3. LABELLING OF COMPOUNDS

Consequent use of novel or established medical radionuclides is research of their labelled compounds as potential radiopharmaceuticals as well as estimating their properties in vivo (biodistribution, tumour accumulation, clearance etc.) regarding this aim. There were several projects focused on this purpose.

The first large group of labellings was focused on production of potential therapeutic radiopharmaceuticals based on monoclonal antibodies and their fragments. We studied preparation of a potential therapeutic agent, EGFR targeting antibody nimotuzumab that has clinically very promising properties regarding minimal side effects combined with beta emitter Lu-177 using standard chelators with promising results (Beckford D.R., Eigner S., Beran M., Eigner-Henke K., Lázníček M., Melichar F., Chinol M.: *Cancer Biother. Radiopharm.* 26 (2011) 287–297; Beckford Vera D.R., Eigner S., Eigner Henke K., Lebeda O., Melichar F., Beran M.: *Nucl. Med. Biol.* 39 (2012), 3–14). Lu-177 and Y-90 labelled monoclonal antibodies and peptides as potential radiotherapeutics were studied in the framework of the IAEA co-ordinated research project no. 16620 (2011–2014).

Much attention was paid to testing of a new, copper-specific chelator “phosphinate”, commercially available like SCN-PCTA a SCN-DO3A and its use for labelling of the antibody IgG M75 against carbonic anhydrase IX. It was demonstrated that the chelator has very good properties for the intended purpose. This work, performed within the grant project of the Technology Agency of the Czech Republic TA02010797, was completed by biodistribution of the labelled antibody IgG M75 in mice that showed significant uptake in tumour tissue of the chosen xenografted mice model (biodistribution study was executed in ÚJV, a.s., commercial partner of the project). Similar results were obtained, when the IgG M75 was labelled with iodine radioisotopes.

Important results were obtained with puromycin, an antibiotic that inhibits in larger amount proteosynthesis, modified and labelled with Y-86, Ga-68 and Sc-44 (the latter radionuclide, unique in a world measure, was provided by group of Prof. Rösch from Mainz University from the only existing Ti-44/Sc-44 generator). This compound is namely optimal for imaging of proteosynthesis, since in contrast to current protheosynthesis tracers (aminoacids) it has single metabolic pathway. As such, it is very promising tool not only for tumour imaging and staging, but also for imaging of infectious diseases (Eigner S., Beckford Vera D.R., Fellner M.,

Loktionova N.S., Piel M., Lebeda O., Rösch F., Roß T.L., Eigner Henke K.: *Mol. Imaging Biol.* 15 (2013) 79–86; Eigner S., Beckford D.R., Fellner M., Loktionova N., Piel M., Melichar F., Rösch F., Roß T., Lebeda O., Eigner-Henke K.: In Baum, Richard, P. (ed.). *Recent Results in Cancer Research Theranostic, Gallium-68, and Other Radionuclides*. Berlin: Springer, 2013. pp. 269-283. ISBN 978-3-642-27993-5).

Trastuzumab and nimotuzumab conjugates were labelled with Y-86 and Sc-44 in the framework of bilateral project of the Czech Academy of Science with the Institute of Nuclear Chemistry of the Mainz University (M100481201). As a “side-product” of the project, we preliminarily tested the possibility to image Y-90 thanks to very low probability of positron branching ratio in its decay resulting from the internal pair production. Appropriate choice of the material for suppressing the bremsstrahlung, one may achieve an interesting tool for PET imaging of Y-90.

#### **4. AUTOMATION AND NEW SYSTEMS FOR RADIOPHARMACY AND NUCLEAR CHEMISTRY**

Automation and new technologies in separation of radionuclides, preparing and purification of labelled compounds as well as in radioanalytical methods are important trends in nuclear chemistry and radiopharmacy. In co-operation with academic and private subjects, we started to work in that highly important field since 2012.

The large grant project of the Technology Agency of the Czech Republic (no. TA02010797) was focused primarily on development of an automated system for processing solid cyclotron targets for production of copper isotopes and development of an automated microfluidic systems including the disposable and dedicated microfluidic chips. The project was successfully completed by the end of 2014 as a result of collaboration of the four subjects: Nuclear Physics Institute, ÚJV, a.s., Envinet, a.s. and Institute for Molecular Genetics CAS under the leadership of our institute.

The developed automated unit for processing solid cyclotron targets for production of copper isotopes (CuSepU) is a universal tool for processing solid targets, not solely the targets for copper isotopes production. The system allows for automated transport of a target from the target holder in a container, opening of the container in a unit, etching of the target layer of defined thickness and finally separation of the radionuclide from the target matrix via ion-exchange chromatography, solid phase extraction chromatography etc. according to the needs of the particular target.

The automated unit for controlling processes performed on a microfluidic chip allows for various mixing the solvents/solutions with various speed/times. The technology of the chips production was mastered including their bonding that stands pressures up to 200 bar.

Another project related to radiopharmaceutical technology is focused on development and testing of so-called “fluorine conversion box” that transforms nucleophilic F-18 produced in the most widespread water targets (enriched with O-18) into electrophilic form. This form is highly desirable for preparation of a large class of F-18 based PET tracers that cannot be efficiently or at all prepared by nucleophilic substitution. The developed system is based on an electric discharge chambers producing F-18 cations stabilized in a suitable chemical form and immediately used for the labelling. The project is funded by the Technology Agency of the Czech Republic (no. TA03010315) as collaboration of our institute and ÚJV, a.s. in years 2013–2015. Our team is responsible for the design, manufacturing and testing of the box itself, where the significant progress was made, while ÚJV, a.s. will test the system in the real conditions of production of a model F-18 radiopharmaceutical.

## 5. FLUORESCENT NANODIAMONDS

Fluorescent nanodiamonds (fNDs) with good luminescent properties are promising biocompatible probes for multimodal optical imaging of biological processes in vitro and ex vivo in real time. In the framework of the projects FP7-245122-DINAMO and GAP108/12/0640, our team was responsible for the research and development of production methods of fluorescent NV centres by various forms of ionizing radiation (heavy charged particles in cyclotron beams and electrons in microtron beam). The major task was to develop target holders and to compare different irradiation techniques (solid targets, solution targets, Bragg peak vs. non Bragg peak) in order to maximize fraction of fluorescent particles, to obtain more homogenous distribution of NV centers per particle and fewer lattice damages. It was revealed that the irradiation of aqueous colloidal nanodiamonds provide superior results to compressed solid targets and that high-mass solid targets irradiated with electrons show comparably good properties with those irradiated on cyclotron. In general, we developed a method for reproducible production of bright luminescence nanodiamond particles that were provided to other project participants (Institute of Organic Chemistry and Biochemistry CAS, Institute of Macromolecular Chemistry CAS and Faculty of Science of the Charles University as partners in GAP108/12/0640; Interuniversitair Micro-Electronica Centrum vzw, Belgie, University of Stuttgart and Julius-Maximilian-Universität Würzburg, Německo, Robert R. McCormick School of Engineering and Applied Science Northwestern University, USA, School of Medical Science, Griffith University, Austrálie, Institute of Organic Chemistry and Biochemistry CAS, Institute of microbiology CAS, Generi Bio, SME, Czech republic in the FP7-245122-DINAMO). Results were published in several peer-reviewed journals (Petráková V., Taylor A., Kratochvílová, I., Fendrych F., Vacík J., Kučka J., Štursa J., Cígler P., Ledvina M., Fišerová A., Kneppo P., Nesládek M.: *Advanced Functional Materials* 22 (2012) 812–819; Havlík J., Petráková V., Řehoř I., Petrák V., Gulka M., Štursa J., Kučka J., Ráliš J., Rendler T., Lee S.Y., Reuter R., Wrachtrup J., Ledvina M., Nesládek M., Cígler P.: *Nanoscale* 5 (2013) 3208–3211; Řehoř I., Macková H., Filippov S., Kučka J., Proks V., Šlegerová J., Turner S., van Tendeloo G., Ledvina M., Hrubý M., Cígler P.: *ChemPlusChem* 79 (2014) 21–24; Řehoř I., Šlegerová J., Kučka J., Proks V., Petráková V., Adam M.-P., Treussart F., Turner S., Bals S., Šácha P., Ledvina M., Wen A.M., Steinmetz N.F., Cígler P.: *Small* 10 (2014) 1106–1115; Moore L., Grobárová V., Shen H., Man H.B., Míčová J., Ledvina M., Štursa J., Nesládek M., Fišerová A., Ho D.: *Nanoscale* 6 (2014) 11712–11721).

## 6. CYCLOTRON U-120M AND MICROTRON MT 25

The smooth operation of the current cyclotron U-120M is condition for successful performance of many experiments and radionuclide production in general. The project CANAM (Center of Accelerators and Nuclear Analytical Methods, MŠMT project no. LM2011019, 2012–2016) enabled introduction of open access to the instrument. It has also significantly contributed to funding of upgrade of several cyclotron subsystems, like purchasing of new vacuum aggregates and components, modernization of resonance system, installation of a new control panel, new integral beam probe including rotational solid-state target holder, design and construction of a new beam current integrator that allows for continuous beam current monitoring and data storing, modernization of the elements of the ion-optic beam line allowing for easier and rapid extraction and shaping of the beam.

Mathematical model of the cyclotron beam dynamics has been continuously improved and applied for solving of many particular tasks.

Standard part of the team work is design, construction, testing and operation of cyclotron targets, external and internal, solid, liquid, solution and gaseous.

Cyclotron U-120M provided beam time for many departments of the institute and within CANAM also open access for many foreign researchers. We can explicitly mention experiments for astrophysics that require usually 7–10 days of continuous beam time 2–4 times per year and operation of neutron generators for department of nuclear reactions, production

of Rb-83 for KATRIN, beam time for excitation functions measurement, testing of electronics (e.g. Radiation Hardness of Si Pixel Chips and Components for ALICE Inner Tracker System Upgrade for CERN and semiconductor diamond detectors for GSI), irradiation of biological samples for estimating DNA radiation damage and general impact of particular radiation on the samples etc.

Also microtron MT 25 was upgraded, new pneumatic rabbit for instant transport of the irradiated target to detector was designed, constructed and implemented. Its potential as a neutron source (Králík M., Šolc J., Chvátil D., Krist P., Turek K., Granja C.: *Rev. Sci. Instr.* 83 (2012) 083502) and new control systems were studied (Krist P., Bíla J., Chvátil D.: *J. Inst.* 8 (2013) t05003). Microtron MT 25 was much involved in preparation of fluorescent nanodiamonds (cf. section 6) and plays key role in the project Photon activation analysis using short-lived products of photonuclear reaction for applications in geochemical research (GA13-27885S, 2013–2015). It was also used for testing Timepix detectors (Granja C., Krist P., Chvátil D., Šolc J., Pospíšil S., Jakubek J., Opalka L.: *Radiation Measurements* 59 (2013) 245–261).

## **7. NEW CYCLOTRON TR24**

Since 2012, much attention was paid to a project of purchasing of a new compact cyclotron. The Canadian cyclotron TR24 was chosen as an optimum between beam energy, current and price. Since 2012, many team members were involved in preparing tenders, reconstruction of the former van de Graaf accelerator building. Much time was spent over calculations of optimal shielding, choice of appropriate infrastructure and new building construction, including subsystems inevitable for the cyclotron operation (power and water supplies, air-conditioning system, cyclotron vault disposition, entrance door etc.) and frequent communication with the cyclotron supplier and with designer.

Design and implementation of a new ion beam line with external chopping system modifying the extracted beam time structure TOF measurements was discussed in detail, preliminary solutions were suggested and the most feasible one chosen for further development.

Reconstruction of the building was finished and new cyclotron was installed in the vault in that it was then closed. Commissioning of the cyclotron is expected to take place in spring/summer 2015.