

## Description of the main research directions investigated by the institute

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 in 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 ultra-relativistic 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. As concern instrumentation and IT support, NPI group has been involved in upgrade project of the ALICE detector Inner Tracking System (ITS), where they contribute in many aspects, e.g., tests of radiation hardness of various electronic components at the local NPI cyclotron facility, analysis of data from test beams, software development and detector commissioning. Further, the ALICE group contributes to maintenance and monitoring of the local installations of the global distributed computing resources, a local storage cluster at NPI and the CERN Tier2 center at the Institute of Physics of the Czech Academy of Sciences.

#### *STAR*

Experiment at RHIC BNL studies hot and dense nuclear matter formed in ultra-relativistic 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. Concerning instrumentation and IT support, NPI group was responsible for maintenance and operation of the STAR detector Zero Degree Calorimeter.

#### *FAIR*

Experiment HADES at FAIR/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, operation and calibration of TOF, FW and ECAL detectors. Its research activities concentrated on study of dilepton and strange particles yields in different combinations of projectile and target. Instrumentation activities concerned the development and construction of ECAL detector as parts of the extensive HADES upgrade for the first phase of the FAIR project. Member of the group is technical coordinator of the ECAL project. NPI group is also involved in the development of Projectile Spectator Detector (PSD) for the Compressed Baryonic Matter (CBM) experiment at FAIR. Scientists from the RHIC group are founding

members of the CBM experiment as a successor project to the HADES. The CBM experiment is under preparation at FAIR 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. Members of the Department of dosimetry NPI are contributing to experiment BIOMAT with research and development work in the field of dosimetry and applications of ionizing radiation for materials research.

#### *KATRIN*

KATRIN project under construction at KIT until 2019 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. The significant NPI contribution to KATRIN is a production and delivery of advanced  $^{83}\text{Rb}$  calibration sources being produced at NPI cyclotrons. Currently members of the NPI team help to ensure the operation of KATRIN experiment and participate on the beamtimes.

#### *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 past five years, impressive progress in construction was achieved while NPI has been involved in delivery of several technologies for neutron target station (He cooling system, fluid systems and HVAC technology for target building). The NPI team role is to ensure practical implementation of this contribution. Apart from significant coordination, project management and technical efforts, this activity involves research and development of in-situ experimental methods and technologies combining neutron diffraction, imaging and other methods for characterization of engineering materials. A large number of external scientists have been working specifically on this topic on part time contracts, allowing them to bring expertise from other teams specialized in materials research to this project.

#### *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. NPI competencies and capacities in the field of fast neutron generators were 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. With the support of EU and national projects, the NPI contributed to SPIRAL2 with some in-kind deliveries to experimental equipment (experimental chambers, detectors).

#### *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 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 infrastructure center CANAM. 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, EU funds and consequent implementation of the open access regime since 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 for IFMIF, irradiation of biological samples for estimating DNA radiation damage, and research on fluorescent nanodiamonds production methods.

#### *TR-24 cyclotron*

In 2015 the new cyclotron TR-24 from the Canadian company ACSI was commissioned which represents a significant upgrade of the home experimental base. Cyclotron provides proton beams with energies from 18 MeV to 24 MeV a current up to 300  $\mu\text{A}$ . The range of energies, high currents of accelerated particles and generation of secondary neutron fluxes of very high intensity opened up the possibility to perform a variety of physical experiments and applications including preparation of a wide range of radionuclides for radiopharmaceutical research. Combination of two cyclotrons enables almost non-stop ability to provide beams for research.

#### *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 and radiation tests of materials and electronics. Data with relevance for accelerator-driven neutron sources and activation of high-power accelerator components and materials for fusion technology have been acquired. Neutron hardness test of microelectronics for ATLAS@LHC upgrade has also been an important application. Brand new high power neutron source based on  $^7\text{Li}(p,n)$  reaction is being developed and commissioned at the new cyclotron TR-24. This source will be one of the strongest sources of fast neutrons in fusion energy region in the world.

#### *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 experiments 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. Important methodological development concerning improvement of standardization procedures in INAA has been achieved.

Within the evaluated period, next significant upgrade of the CANAM instrumental base has started – namely the project of implementation of the Accelerator Mass Spectrometry. The project includes construction of a new building above the former Van de Graaff office building and purchasing of the new accelerator Milea from the Swiss producer IonPlus. This project with the total budget of about 383 mil CZK represents the biggest investment in NPI instrumental base since its foundation. At the end of the year 2019, the accelerator has been in production by the IonPlus company and the project was at 50% complete.

### **Other NPI experimental facilities**

#### *Laboratories of the Department of Radiopharmaceuticals*

In radiopharmaceutical laboratories research related to nuclear data measurement, target processing, radionuclides separation, quality control and labelled compounds with potential medical use is performed. Nuclear data measurement covers excitation functions relevant for both radionuclides production and cyclotron beam monitoring. Production of radionuclides of high specific activity covers both special radionuclides for physical experiments (e.g. calibration sources) and novel medical radionuclides. Medical radionuclides are either provided to other institutions or used in-house for manufacturing of labelled compounds that can be tested by standard QC methods up to cell culture experiments.

#### *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 external 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, paleoenvironmental research or wildlife crime. Environmental research concerning tritium and <sup>14</sup>C activities in the surroundings of nuclear power plants has been conducted.

## Research activity and characterisation of the main scientific results

At low energies the underlying fundamental theory of the strong interactions (QCD) is manifested in a model-independent way in the dynamics of lightest pseudo-Nambu-Goldstone bosons: the pseudoscalar pions, kaons and eta mesons. Supplemented by nucleons (and lightest strange baryons) these hadronic degrees of freedom serve as common tool for description of hadronic systems and processes near threshold in terms of the chiral perturbation theory (ChPT). It provides, in particular, a necessary input for description of (hyper)nuclei: two and three-baryon potentials. Appearance of the novel reliable “fundamental” interactions and important improvements of various few- and many-body techniques revived our hopes of understanding of enormous wealth of hadronic and nuclear phenomena within some common unifying framework. Some integral parts of this effort, namely studying wide range of nuclear and hypernuclear systems, their interactions with external hadronic and electroweak probes, which involve also understanding of related hadronic subsystems, are systematically developed also at our DTP.

Beyond the low energy regime hadronic dynamics is still not fully understood. For processes involving higher meson or baryon resonances, for meson productions or for interactions with energetic external particles one has to develop or overtake phenomenological QCD-motivated models. The models are then tested also in nuclear systems, from few hadron systems up to corresponding processes in infinite nuclear medium.

Theoretical nuclear and particle physics were always in lively contact with other fields, especially with solid state physics. Number of common general techniques emerged, in particular approaches based on symmetries of considered systems and on effective definition and description of relevant degrees of freedom. Most interesting and elaborate theoretical formulations become topics of rigorous scrutiny by mathematical physicists. The vital group of mathematical physicists is a strong integral part of our Department.

The research in mathematical physics follows several different directions such as models of specific physical systems, analysis of mathematical methods and techniques useful for the former purpose, as well as investigation of conceptual aspects of the theory. In the considered period, the first item included, for instance, problems coming from solid state physics like Dirac materials, transport in semiconductor wire networks, or gap engineering in metamaterials. On the mathematics side it was the shape optimization, spectral properties associated with complex potentials, or new approaches to the exact solvability. Finally, on the conceptual side, attention was paid to the ways in which non-self-adjoint, in particular PT-symmetric, operators can be used in quantum theory and other parts of physics. Needless to say, there are numerous overlaps between the indicated topics as well as relations to the problems on which the other groups in the Department work, in the true spirit of unity of theoretical physics.

In what follows we briefly present and comment results achieved at our Department in the last five years. Most of them were obtained together with our collaborators from elsewhere, given a limited space of this report we cannot explicitly mention them, so let us acknowledge their contributions and thank them for their help just by this note.

### STRUCTURE OF NUCLEI AND HYPERNUCLEI

*With reliable fundamental two-baryon and three-baryon interactions one is obliged to offer descriptions of various (hyper)nuclear systems. Several attempts towards this goal have been made also at our DTP.*

We built a comprehensive theoretical framework capable of a first-principles description of nuclear structure and reactions of light and medium-mass nuclei. To this aim, we endowed ab

initio symmetry-adapted no-core shell model (SA-NCSM) framework with the following newly developed many-body techniques:

- 1) Calculation of matrix elements of a realistic nuclear potential using  $Sp(3,R)$  symmetry-adapted basis (*Phys. Rev. Lett.* 124 (2020) 042501);
- 2) Calculation of nuclear densities, essential for the determination of nuclear spectroscopic properties and for studying nuclear reactions in the framework of SA-NCSM/RGM method (*Prog. Part. Nucl. Phys.* 89 (2016) 101; *Comp. Phys. Comm.* 207 (2016) 202);
- 3) Many-body perturbation theory based importance-truncation procedure in  $SU(3)$  symmetry-adapted basis (*Acta Physica Polonica B* 50 (2019));
- 4) Efficient methods for generating the  $SU(3)$ -coupled basis for medium mass nuclei (*Int. J. High Perform. Comp. Appl.* 33 (2019) 522; *Comp. Phys. Com.* 244(2019) 442). The above techniques were implemented for parallel computing architectures. This was instrumental in obtaining the U.S. NSF PRAC allocation award for our large-scale studies of medium-mass nuclei at the BlueWaters supercomputer.

We further developed the equation of motion phonon method (EMPM), applicable throughout a whole nuclear chart. In this method a set of equations is formulated and solved iteratively to generate an orthonormal basis of multiphonon states. In principle, the method does not rely on any free parameters, and is only limited by the necessity to truncate the multiphonon basis in which the nuclear Hamiltonian is solved. Recently we applied the EMPM on doubly-magic heavy  $^{208}\text{Pb}$  (*Phys. Rev. C* 92 (2015) 054315), neutron-rich open-shell  $^{20}\text{O}$  (*Phys. Rev. C* 93 (2016) 044314), and odd-even  $^{17}\text{O}$ ,  $^{17}\text{F}$  (*Phys. Rev. C* 94 (2016) 061301; *Phys. Rev. C* 95 (2017) 034327) nuclei. Within EMPM we also studied the role of correlations on the description of nuclear ground state properties (*Phys. Rev. C* 95 (2017) 024306). Further, we developed the proton-neutron- $\Lambda$  formulation of Hartree-Fock method and the nucleon- $\Lambda$  Tamm-Dancoff approximation. These methods implemented with three-body baryonic forces were applied in calculations of selected hypernuclei (*Phys. Scr.* 94 (2019) 014006).

We have formulated the ab initio no-core shell model (NCSM) methodology for nuclear systems with strangeness (*Phys. Rev. C* 97 (2018) 064315). For the first time, we have performed reliable systematic calculations of single- $\Lambda$  s- and p-shell hypernuclei, using realistic interaction models, such as those derived from ChPT. We performed hypernuclear NCSM calculations of the charge symmetry breaking (CSB) in  $\Lambda$ -nucleon interactions (*Phys. Rev. Lett.* 116 (2016) 122501; *Nucl. Phys. A* 954 (2016) 161). We demonstrated, for the first time, that the observed value of CSB can be reproduced by employing realistic interaction models supplemented by a CSB vertex derived from the  $\Lambda$ - $\Sigma$  mixing mechanism.

We applied the hypernuclear ab initio NCSM technique to the study of the topical question of the hypertriton half-life puzzle. We derived the potential for the  $\Lambda N \rightarrow NN$  weak interaction within the effective field theory formalism up to next-to-leading order (*Nucl. Phys. A* 954 (2016) 213). We have, for the first time, evaluated the effects of pionic final-state interactions and the importance of hyperon admixtures (currently being prepared for publication in *Phys. Rev. Lett.*).

We performed the first comprehensive calculations of light  $\Lambda\Lambda$  hypernuclei within a pionless effective field theory, aiming at a hot issue of the onset of binding in strangeness  $S=-2$  baryonic sector. We found that the  $\Lambda\Lambda n$  and  $\Lambda\Lambda nn$  systems are unbound,  $^4_{\Lambda\Lambda}\text{H}$  is on the verge of binding, and  $^5_{\Lambda\Lambda}\text{H}$  and  $^5_{\Lambda\Lambda}\text{He}$  are robustly bound (*Phys. Lett. B* 797 (2019) 134893). The measurement of  $A=5$   $\Lambda\Lambda$  hypernuclei is a subject of the J-PARC P75 proposal.

The spectrum of hypernuclear three-body systems composed of  $\Lambda$  and two nucleons is the subject of an ongoing experimental campaign. We have thus utilized baryonic effective field theory at leading order, constrained to reproduce the available low energy light hypernuclear data, to study the nature of the three-body hypernuclear states. Using the complex scaling

method and the inverse analytic continuation in the coupling constant method we found the existence of a virtual state in the  $\Lambda p(3/2^+)$  channel and a resonance in the  $\Lambda nn(1/2^+)$  channel (*arXiv:2003.08636 [nucl-th], subm. Phys. Lett. B*). Further, we studied application of leading order pionless effective field theory in a description of p-shell systems (*arXiv:2003.09862 [nucl-th]*). We found that the theory at leading order is not able to sustain p-shell bound states. This might imply that current formulation of the theory should be reconsidered in order to extend its range of applicability beyond s-shell.

We disproved the recent hypothesis of absolutely stable strange hadronic matter composed solely of  $\Lambda(1405)$  hyperons. The binding energy per baryon in  $\Lambda(1405)$  many-body systems was found to saturate, leaving these systems unstable against strong interaction decay (*Phys. Lett. B* 785 (2018) 90).

## HADRONIC INTERACTIONS

*Several interesting hadronic systems, both near threshold and at higher energies, have been topics of our attention.*

We performed a comparative analysis (*Nucl. Phys. A*954 (2016) 17) of the available NLO chiral models of the antikaon-nucleon interaction at low energies and explored their pole contents. The various approaches lead to very different predictions for the  $K^-p$  amplitude extrapolated to subthreshold energies as well as for the  $K^-n$  amplitude. The origin of the poles generated by the models was traced to a zero coupling limit, in which the inter-channel couplings are switched off. This paper appeared essential for on-going theoretical studies of kaonic atoms and  $K^-$ -nuclear quasi-bound states.

We studied the meson-baryon interaction in the  $S=-1$  sector, aiming at an improved determination of the next-to-leading order (NLO) terms of the chiral  $SU(3)$ . In our interaction model we have taken into account experimental data of processes that are especially sensitive to higher orders of the Lagrangian and also included explicit resonant contributions and additional isospin filtering reactions (*Phys. Rev. C*99 (2019) 035211).

We employed the state-of-the-art chirally inspired  $K^-N$  interaction models in the derivation of  $K^-$  optical potentials. These potentials need to be supplemented by a term representing  $K^-$  multi-nucleon interactions in order to fit kaonic atom data. Our calculations revealed the decisive effect of antikaon multinucleon interactions on the antikaon absorption in the nuclear medium. The calculated  $K^-$  nuclear states have huge widths, which makes their identification in experiment unlikely (*Phys. Lett. B*770 (2017) 342; *Phys. Rev. C*96 (2017) 015205). Recently, we have developed a microscopic model for  $K^-NN$  absorption in nuclear matter using chirally motivated  $K^-N$  amplitudes. After considering medium modifications of the amplitudes, we reproduced the ratio of  $\Lambda p/\Sigma^0 p$  production measured by the AMADEUS collaboration (*Phys. Rev. C*101 (2020) 035204).

We performed the first exact few-body calculation of the 1s level shift and width of the kaonic deuterium. Coulomb interaction was directly included into the Faddeev-type equations together with the strong interactions (*Phys. Lett. B*744 (2015) 105-108). We also performed the first Faddeev-type AGS calculation of the antiK-antiK-N three-body system and predicted existence of a quasi-bound state. The position and width of the state could correspond to the experimentally observed  $\Xi(1950)$  state (*Phys. Rev. C*92 (2015) 044001).

We developed a coupled-channel separable potential approach to  $\eta N$  and  $\eta' N$  interactions using a chiral-symmetric interaction kernel (*Nucl. Phys. A*992 (2019) 121630). The s-wave  $\pi N$  amplitudes and  $\pi^-p$  induced total cross sections were reproduced satisfactorily in a broad interval of energies. An explicit inclusion of the  $\eta_0$  meson leads to a more attractive  $\eta N$ . Within our model, the  $\eta' N$  diagonal coupling is large enough to generate an  $\eta' N$  bound state but the

inter-channel dynamics moves the respective pole far from physical region making the  $\eta'$ N interaction repulsive at energies around the channel threshold.

We studied the possibility of finding a hidden-charm strange pentaquark, as an  $S=-1$  partner of  $P_c(4450)$  observed at LHCb, in the decay of the  $\Lambda_b \rightarrow J/\psi \eta \Lambda$ . We observed that a resonance signal in the  $J/\psi \Lambda$  invariant mass spectrum is clearly seen. The exciting discovery of new  $\Omega_c^0$  states at LHCb triggered our interest in the study of the interaction of low-lying pseudoscalar mesons with ground-state baryons in the  $C=+1$ ,  $S=-2$ ,  $I=0$  sector. We found two structures with masses and widths similar to the experimental  $\Omega_c^0(3050)$  and  $\Omega_c^0(3090)$  values.

In view of the forthcoming experiments at FAIR aiming at exploring interactions of antiprotons with nucleons and nuclear matter, we performed first fully self-consistent calculations of anti-p nuclear bound states using RMF optical potentials consistent with anti-p-atom data (*Nucl. Phys. A945 (2016) 197*) as well as potentials derived from the 2009 version of the Paris anti-NN potential. We found that the Paris potential yields anti-p binding energies and widths very close to the values obtained by the RMF potentials (*Nucl. Phys. A969 (2018) 45*).

We used the previously constructed multichannel pion-pion scattering amplitude, that possesses a proper analytical continuation on the Riemann sheets, to account for the final state interaction (FSI) in decays of heavy mesons (*Phys. Rev. D91 (2015) 037901*; *Phys. Rev. D92 (2015) 036002*; *Phys. Rev. D97 (2018) 014009*). We have shown that the two-peak structure in the two-pion energetic spectrum can be explained as an effect of coupled channels in the FSI. Utilizing the dispersion relations constrained by crossing symmetry (Roy-like equation) we analysed the previously constructed unitary pion-pion amplitudes in S-, P-, D-, and F waves (*Phys. Rev. D94 (2016) 116013*). These new amplitudes are mutually consistent, fulfil the crossing symmetry condition imposed by the dispersion relations and describe well the experimental data. The improved amplitudes can be used to account for the final-state interactions in the analysis of heavy-meson decays or of the two-pion photoproduction process, like in our first attempt to analyse meson resonances in forward two-pion photoproduction (*Phys. Lett. B789 (2019) 287*). We achieved a satisfactory agreement with experimental data from CLAS in Jefferson Laboratory.

## WEAK AND ELECTROMAGNETIC INTERACTIONS

*We provide theoretical analysis for several international experimental collaborations on electroproduction of strangeness. Descriptions of nuclear electroweak interactions have long tradition at our DTP.*

We have constructed single-channel amplitudes for photo- (*Phys. Rev. C93 (2016) 025204*) and electroproduction (*Phys. Rev. C97 (2018) 025202*) of kaons on the proton, based on an effective hadron Lagrangian and utilizing the consistent formalism for description the higher spin ( $3/2$  and  $5/2$ ) baryon resonances. These amplitudes were fitted to the latest experimental data and can be used as an input in calculations of the cross sections in production of hypernuclei. Recently we have constructed a new hybrid Regge-plus-resonance model for photoproduction of kaons on the proton based on the Regge formalism replenished with exchanges of nucleon resonances in the s-channel (*Phys. Rev. C100 (2019) 035202*). In the model we adopted a novel method on restoring gauge invariance by Haberzettl et al. The model satisfactorily describes the data in the resonance region as well as above this region. It can be also used as an input in hypernucleus calculations in DWIA.

We took an active role in physical analysis of the cross sections in electroproduction of hypernuclei obtained in experiments at Jefferson Laboratory (*Phys. Rev. C91 (2015) 034308*; *Phys. Rev. C99 (2019) 054309*). We have updated our previous DWIA calculations of the hypernucleus cross sections. In the second (archival) paper we provide a consistent and comprehensive description of the data obtained for the targets  $^9\text{Be}$ ,  $^{12}\text{C}$ , and  $^{16}\text{O}$  together with discussion of the data on the elementary production. We also provided a theoretical support in



analysis of data on the electroproduction of kaons off the proton from the MAMI facility in Mainz. We are included in the list of A1 Collaboration in Institut für Kernphysik in Mainz (*Eur. Phys. J. A*53 (2017) 198).

We pursued our studies of the double-charge exchange reaction (analogous to a neutrinoless double beta decay) in massive white dwarfs (*Nucl. Phys. A*937 (2015) 17). Our calculations confirm that this reaction can affect the energy balance in these compact objects, but further investigations are necessary to confirm this finding for more realistic model of the star and to identify a clean experimental signal which would confirm its rate and (ideally) provide some information on neutrino masses.

## FIELD THEORETICAL METHODS

*In general terms the elementary particle physics deals with relativistic quantum systems in which the number of constituents during the interaction substantially changes. The appropriate tool for the description of such physics is the quantum field theory (QFTh).*

Some examples of current experimental interest, an important measure of relevance of the related theoretical research, are: (1) The proton-proton or nucleus-nucleus collisions at the LHC energies; (2) Transition form-factors of the colorless hadrons formed by the strong-coupling QCD from the colored quarks and the colored gluons; (3) Decays of the elementary particles produced at the LHC, including the recently discovered Higgs boson. Below we described three of our activities, closely related to these topics. Their common feature is that they are all the heuristic, non-systematic methods of QFTh at strong coupling which are not under rigorous theoretical control.

The correlation structures of multi-particle states created in high energy collisions are often studied in the framework of the clan concept introduced to interpret negative binomial distribution (NBD) occurring in different reactions over a wide range of physical variables. The clan structure of multiplicity distributions of charged particles produced in proton-proton collisions at the LHC energies was analysed (*Eur.Phys.J.C*78 (2018) 816) using weighted superposition of three NBDs. It was argued that there is strong evidence of the third component in the multiplicity frequencies which make up the data measured by the ATLAS Collaboration up to the energy  $\sqrt{s} = 13$  TeV. The appealing observation is natural increase of the average number of clans in the high- $n$  (semihard) component with the energy  $\sqrt{s}$ , which is in sharp contrast with two-NBD parameterizations of the measured distributions. In new approaches to the description of systems of increasing complexity, entropy emerges as an important quantity. A specific form of entropy of constituent configurations has direct relation to the z-scaling (*Theor.Math.Phys.*184 (2015) 1350, *Int. J. Mod. Phys. A*32 (2017) 1750029, *EPJ Web of Conferences* 204 (2019) 06001), observed in numerous analyses of the transverse momentum spectra of different particles produced in high energy collisions of hadrons and nuclei. The scaling is a manifestation of the self-similarity of hadron interactions at the constituent level and reflects fractal structure of the colliding objects as well as the general features of fragmentation processes expressed by the corresponding fractal dimensions. Due to the locality and fractal self-similarity of hadron interactions, there should exist (*Int. J. Mod. Phys. A*33 (2018) 1850057) a symmetry parameterized at any scale by the elements from the space of momentum fractions. Using the maximal entropy principle and the z-scaling scheme, a conservation of a new quantity was found. We argue that the conservation law should reflect the symmetry of transformation of one fractal structure of hadron constituents into another one at all scales. It was shown that the conserved quantity is proportional to the respective fractal dimensions and represents a simple function of the corresponding momentum fractions. Based on statistical ideas and entropy considerations it was demonstrated that the fractal dimensions possess quantum character.

Understanding of exclusive hadron form factors at a level of their colored constituents represents longstanding challenge of the Standard Model as a nonperturbative QFTh. The

pion electromagnetic form factor and the pion transition form factor (sometimes called pion off-shell anomaly) play crucial role in this respect. In the manuscript (*Phys. Rev. D* **102** (2020) 014049) the  $\gamma\gamma \rightarrow \pi$  transition form factor  $G(q^2)$  was computed in the entire domain of spacelike and time-like momenta using a quantum field theory continuum approach. The analytical continuation of the function  $G(q^2)$  was based on the utilization of the Gauge Technique with the entry of QCD Green's functions determined from Minkowski space solution of QCD Dyson-Schwinger equations. The transition form factor is deeply related with the phenomena of dynamical chiral symmetry breaking, which is a striking feature of low energy QCD. Using similar approximations of a QCD model, which is the truncated system of QCD quantum equation of motion for Green's functions (the Dyson-Schwinger equations) the hadronic vacuum polarization function  $\Pi_h$  for two light flavors is computed on the entire domain of spacelike and time-like momenta (*Few Body Syst.* **61** (2020) 23). The analytical continuation of the function  $\Pi_h$  is based on the Gauge Technique with the entry of QCD Green's functions determined from generalized quark spectral functions. For the first time, the light quarks (up and down) spectral functions are extracted from the solution of the gap equation for the quark propagator.

Glorious discovery of the Higgs boson, considered originally as the source of all elementary particle masses soon turned into frustration: It leaves the neutrinos massless, it does not offer any candidate for dark matter, and it leaves the lepton and quark masses theoretically arbitrary. An alternative to the weakly coupled Higgs sector of the SM which is under complete theoretical control is to postulate a new strong dynamics in which the Higgs particle is composite. The attempts are numerous, and the price is high: Like in QCD there are no systematic analytic tools for strong coupling. Unlike the vector-like QCD which can be dealt with numerically on the lattice the strong dynamics pretending to generate the calculable fermion masses must be chiral, and the known lattice methods do not apply.

In ([arXiv:1606.03292](#)) we have suggested to replace the Higgs sector of the SM by gauging properly the flavor (family, generation, horizontal)  $SU(3)_f$  symmetry with the huge ( $>10^{10}$  GeV) scale  $\Lambda$ . At strong coupling the resulting quantum flavor dynamics (QFD) generates: (1) Three Majorana masses  $M_R$  of order  $\Lambda$  of the right-handed neutrinos necessarily added to the SM fermion sector for anomaly freedom. (2) Three Dirac masses  $m_f$  exponentially small with respect to  $\Lambda$ , same for all SM fermion species in family  $f$ . (3) The composite SM-like Higgs boson  $h$  with mass of order  $\Sigma m_f$ , the effective Fermi scale. (4) Two new composite Higgs-like bosons  $h_3$  and  $h_8$  with masses at Fermi scale. In ([arXiv:1704.07172](#)) we have demonstrated that the model ([arXiv:1606.03292](#)) is a decent field-theory seesaw model of neutrino masses. We have illustrated phenomenologically ([arXiv:1708.08333](#)) that the model ([arXiv:1606.03292](#)) has the potential of describing the fermion mass splitting within families in terms of the known weak hypercharges. In ([arXiv:1903.10194](#)) we have suggested to extend the calculation of the fermion mass splitting in terms of the known fermion electric charges in the new Ball-Chiu electromagnetic vertex following from the Ward-Takahashi identity.

## QUANTUM THEORY ON GRAPHS AND WAVEGUIDES

*Confining a quantum particle to a configuration space of nontrivial geometry and/or topology induces an effective interaction coming from the confinement. In the period in question, new effects in such systems were discovered.*

Concerning quantum graphs, the most important results are the demonstration of Cantor type spectra in magnetic chain graphs (*J. Phys. A* **50** (2017) 165201), the discovery of graphs exhibiting the Bethe-Sommerfeld property (*J. Phys. A* **50** (2017) 455201) and of the vertex coupling leading to topologically induced transport properties (*Phys. Lett.* **382** (2018) 283; *J. Phys. A: Math. Theor.* **51** (2018) 285301; *J. Math. Phys.* **60** (2019) 122101; *Phys. Lett. A* **384** (2020) 126390). Wide classes of graphs without a lower bound on edge lengths including fractal structures were analyzed (*Ann. H. Poincaré* **19** (2018) 3457), local perturbations of

magnetic chains (*J. Phys. A* 48 (2015) 125302; *Ann. H. Poincaré* 18 (2017) 929) and properties of resonances on graphs were investigated (*J. Math. Phys.* 58 (2017) 042101).

As for quantum waveguides, a geometrically induced magnetic transport of Iwatsuka type in quantum layers was found (*J. Math. Phys.* 59 (2018) 042105), further results concerned spectral properties of waveguides with boundary consisting of parts with different boundary conditions (*Rep. Math. Phys.* 81 (2018) 213), gap engineering method in Neumann waveguides with periodic  $\delta'$  traps (*J. Phys. A: Math. Theor.* 48 (2015) 315301), metamaterial models (*J. Math. Phys. Anal. Geom.* 14 (2018) 270; *Asympt. Anal.* 110 (2018) 83), as well as bound states in magnetic wedges (*Rep. Math. Phys.* 82 (2018) 161) and non-selfadjoint waveguide models (*Proc. Amer. Math. Soc.* 145 (2017) 1231).

## SCHRÖDINGER AND DIRAC OPERATORS

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

For leaky quantum structures new asymptotic expansions with respect to the coupling strength and interaction support geometry were derived (*J. Spectr. Theory.* 5 (2015) 697; *J. Phys. A* 48 (2015) 495301; *Rep. Math. Phys.* 77 (2016) 1; *Asympt. Anal.* 97 (2016) 1; *J. Math. Phys.* 59 (2018) 013051), further results concerned properties of singular interactions (*Comm. PDE* 41 (2016) 999; *J. Math. Phys.* 57 (2016) 022101; *J. Math. Phys.* 57 (2016) 022104, *J. Math. Phys.* 57 (2016) 041507; *Ann. Henri Poincaré* 18 (2017) 1305; *Lett. Math. Phys.* 108 (2018) 2153; *Proc. Roy. Soc. Edinburgh* 149 (2019) 1663), their approximations by regular potentials (*Math. Nachr.* 290 (2017) 1215) or the Landau level splitting they cause (*Rev. Math. Phys.* 52 (2020) 2050010).

Schrödinger operators: several modifications of Smilansky-Solomyak model exhibiting abrupt spectral transition as well as intriguing resonance properties were proposed and analysed (*J. Phys. A* 49 (2016) 165302; *Rep. Math. Phys.* 80 (2017) 177; *Phys. Lett. A* 381 (2017) 756; *J. Phys. A* 50 (2017) 485203; *Phys. Lett. A* 382 (2018) 1207), and moreover, semiclassical bounds for magnetic bottles (*Rev. Math. Phys.* 28 (2016) 1650002) were derived.

Singular Dirac operators: spectral and scattering of such operators with the interaction supported on surfaces, both of electrostatic (*J. Math. Pures Appl.* 111 (2018) 47) and Lorentz scalar (*Quant. Stud.: Math. Found.* 6 (2019) 295) types were analyzed, including their relation to the bag models. Furthermore, spectra of two-dimensional Dirac operators in regions modeling quantum dots were analyzed (*Math. Phys. Anal. Geom.* 22 (2019) 13).

We also addressed questions of spectral optimization: new inequalities of the isoperimetric type and other spectral optimization results were found for Schrödinger and Dirac operators with singular interactions (*Lett. Math. Phys.* 107 (2017) 717; *Appl. Anal.* 98 (2019) 8; *J. Phys. A: Math. Theor.* 52 (2019) 405302).

## OPTIMAL SHAPES IN PHYSICS AND RELATED PROBLEMS

*The interplay between the spectrum of differential operators coming from quantum as well as classical physics and the geometry of underlying manifolds.*

Our group significantly contributed to resolving the celebrated conjecture of Baret's from 1977 stating that the disk maximizes the principal frequency of any membrane of fixed area with elastically supported edges. We disproved the conjecture (*Adv. Math.* 280 (2015) 322) and showed that it holds under the perimeter constraint (*Adv. Calc. Var.* 10 (2017) 357). We established unbounded versions of the conjecture for the exteriors of bounded sets (*J. Convex Anal.* 25 (2018) 319; *Potential Analysis* (2019)) which have applications for quantum nanostructures with attractive hollow defects. We also contributed to the Payne's nodal-line

conjecture (*J. Differential Equations* (2015)), Alexandrov's conjecture (*Tohoku Math. J.* 67 (2015) 405) and optimality of the Poincare-Wirtinger type inequality (*Atti Accad. Naz. Lincei Rend. Lincei Mat. Appl.* 27 (2016) 443).

New results were derived for special geometries. We established effective Hamiltonians in thin structures subject to magnetic fields (*J. Geom. Anal.* 25 (2015) 2546). We quantified the geometric effect of global twisting on transport properties of quantum (quasi-)particles in curved nanostructures by means of the mathematical concept of Hardy inequalities (*Lett. Math. Phys.* 109 (2015) 1473). As a completely new effect we showed that there is no transport in quantum waveguides with asymptotically diverging twisting (*Appl. Math. Lett.* 46 (2015) 7). The conceptual analogy between geometric and magnetic effects were quantified for the heat flow in (*Comm. PDEs* 41 (2016) 1056; *Portugal. Math.* 73 (2016) 91).

## UNCONVENTIONAL MATHEMATICAL TOOLS

*The advent of artificial materials in optics and mesoscopic physics as well as the new concept of quantum theory with observables represented by non-self-adjoint operators lead to challenging mathematical problems which cannot be tackled by standard tools.*

We proposed giving the mathematical concept of the pseudospectrum a central role in non-Hermitian quantum mechanics (*J. Math. Phys.* 56 (2015) 103513). We introduced a new classification of boundary conditions for non-self-adjoint graphs (*Trans. Amer. Math. Soc.* 367 (2015) 2921). We explained striking properties of a stochastic system by applying of quantum theory (*Math. Z.* 284 (2016) 877). Finally, we quantified the effect of tunneling by considering coalescing heterostructures modeled by Dirac-measure potentials imposed on two parallel hypersurfaces (*J. Math. Anal. Appl.* 446 (2017) 1328).

We are proud of the significant contribution of our group to the hot research topic of Schrödinger operators with complex potentials. We introduced a new model of a globally distributed discontinuous potential and demonstrated its unusual spectral properties (*J. Spectr. Theory* 7 (2017) 659). We proved the Agmon estimate for eigenfunctions despite the unconventional setting of potentials whose real part is not necessarily bounded from below (*Israel J. Math.* 221 (2017) 779). We developed the method of multipliers to establish the total absence of eigenvalues in the case of complex fields (*J. Spectr. Theory* 8 (2018) 575).

## CONSTRUCTIONS OF NOVEL EXACTLY SOLVABLE QUANTUM MODELS

*Realistic quantum systems are usually complicated, described by numerical techniques. Often, their qualitative features are much better revealed via simplified, solvable models.*

In (*Phys. Rev. A* 96 (2017) 012127) we showed that even via simplified models a fully realistic picture of reality may be obtained admitting, typically, the continuous (i.e., scattering-responsible) part in the spectrum. We found a model exhibiting a serendipitous advantage of being based on a Sturmian-coupling reinterpretation of the eigenvalues. The resulting rearrangement of Schrödinger equation made some phenomenological features of the system described analytically, in terms of continued fractions.

The concept of quasi-exactly solvable (QES) Schrödinger equations was generalized (*Phys. Lett. A* 380 (2016) 1414). The discovery was motivated by two paradoxes. Firstly, the sextic polynomial oscillators are known to be QES while the apparently simpler, phenomenologically more important quartic ones are not. Secondly, mathematical assumptions of different forms seemed to apply in the one- and more-dimensional systems. The resolution of both paradoxes has been found in a unifying idea of cutting of the domain of coordinates followed by the trick of the central matching of the elementary solutions on subdomains. In this way the existing QES class of models has been extended significantly.

## NEW ALTERNATIVE ABSTRACT FORMULATIONS OF QUANTUM THEORY USING NON-HERMITIAN OBSERVABLES AND HAMILTONIANS

*From textbooks we know that there exist multiple alternative, phenomenologically more or less equivalent formulations of classical mechanics, each one being adapted to various particular, model-dependent needs of an optimal and efficient applicability. In quantum physics such a tendency only appeared very recently, but they are becoming increasingly interesting and influential. These approaches are developed also intensively in the DTP, building abstract bridges between the mathematically oriented physics of theoretical predictions and a complementary area of their experimental confirmations.*

The research revisiting the foundations of quantum theory originated from an overlap between nuclear physics and mathematical physics. In our group the first climax of these efforts came in 2015 when several members of our team co-edited and co-authored the book („*Non-selfadjoint Operators in Quantum Physics: Mathematical Aspects*“, J. Wiley&Sons). Subsequently, our study of innovative formulations of quantum theory continued in a symbiosis of heuristic and rigorous methods. We complemented the existing, Bender-inspired Schrödinger-picture theory of closed quantum systems by its natural Heisenberg-picture analogue (*Phys. Lett. A379 (2015) 2013*). Another, still more general non-stationary formulation of quantum theory representing the Dirac alias interaction picture in its non-Hermitian extension was published in (*Ann. Phys. (NY) (2017) 162*).

In a collaboration initiated by an Algerian university in Constantine a resolution was offered to several paradoxes which emerged in the field. A guarantee of consistency has been shown to require an ad hoc upgrade of inner product. We proved, in (*Phys. Rev. A95 (2017) 042122*), that whenever we are given more than one candidate for an observable, such an upgrade need not exist in general.

The above-cited new forms of quantum theory proved efficient in applications. Thus, using elementary linear-algebraic methods, non-Hermitian difference-operator models were constructed admitting the Kato's exceptional points (EP) of orders 4 and 5 (*Phys. Rev. A98 (2018) 032109*).

Distinct areas of applicability were conjectured in *quantum* mechanics of non-Hermitian systems and in *classical* systems (e.g., coupled waveguides). An arbitrary perturbation of an exceptional-point-related unperturbed Hamiltonian was considered in (*Phys. Rev. A100 (2019) 032124*). It was proved that the spectrum remains real inside certain explicitly specified corridors of stability in which, self-consistently, the perturbations remain small when measured in the physical Hilbert space. The result can be read as a disproof of the recent conjectures of the detection of instabilities using the pseudospectra calculated in an auxiliary, unphysical Hilbert space.

## DIRAC MATERIALS

*In a large family of condensed matter systems, collective excitation of free electrons can be described by Dirac equation. The emergent relativistic behavior of the quasi-particles stays behind many remarkable properties of these materials.*

We employ both the rigorous qualitative spectral analysis as well as specific supersymmetric methods for investigation of systems described by low-dimensional Dirac Hamiltonians that appear in description of Dirac materials.

Supersymmetric transformation in quantum mechanics allows construction of the new exactly solvable models from the known ones. In the context of 1D Dirac equation, the supersymmetric transformation can alter the magnetic field or the mass term of the new model, however, it cannot change the electric field. This is quite a limiting factor in construction of the exactly

solvable models with new configurations of the electrostatic field. We proposed the way how to alter the electrostatic term of the new system with the use of a specific unitary transformation while keeping its exact solvability in (*Phys. Rev. D*91 (2015) 045039).

In the qualitative spectral analysis, it is possible to get valuable information on the spectral properties of the considered systems without the need to solve their stationary equations. Extending our previous results, we showed on the rigorous basis that specific energy bands induced by external magnetic field can be attributed to existence of the wave packets that are dispersionless in perpendicular direction to the axis of translation symmetry (*Ann. Phys.* 378 (2017) 171). These results were further developed in (*Ann. Phys.* 395 (2018) 219) where confinement by realistic magnetic fields was discussed. We proposed a simple device for fine-tuning transport properties of magnetic wave guide by changes of the currents in the bundle of wires that lies in the proximity of the graphene sheet.

### **PT-SYMMETRIC OPTICAL SYSTEMS**

*The way to the common ground of classical optics and quantum mechanics is paved by the paraxial approximation which turns the Maxwell equations for electric or magnetic field into the equation of Schrödinger type. The intersection between the two seemingly distant areas of physics has proven to be exceedingly fruitful.*

Paraxial approximation turns the Maxwell equations for electric or magnetic field into the equation of Schrödinger type. It makes it possible to use concepts and results of PT-symmetric quantum mechanics in optics. In this context, complex potentials correspond to the complex refractive index simulates gain and loss of light in the system. Supersymmetric quantum mechanics can be used effectively for construction of these systems. We considered construction of effectively one-dimensional systems with asymptotically periodic and real refraction index that possessed a complex, PT-symmetric periodicity defect (*Phys. Rev. A*92 (2015) 023839). We showed that the defect can give rise to a localized solutions (eigenvectors) of the Schrödinger equation whose eigenvalues (“energies”) are in correlation with the decay rate of the periodicity defect. We extended these results (*Phys. Rev. A*99 (2019) 053812) by employing the time-dependent supersymmetric transformations. It allowed us to consider truly two-dimensional systems with two-dimensional (non-separable) fluctuations of the complex refractive index. We focused on existence of the localized solutions that are specific for the new settings. We discussed number of physically relevant examples where the complex fluctuations of the refractive index form wave guides or the so called light dots.

## Research activity and characterisation of the main scientific results

### A) PHYSICS ANALYSES IN ALICE AND STAR EXPERIMENTS

The common goal of physics analyses carried out by our teams at STAR and ALICE is to investigate modification of jet- and heavy-flavor-quark production by the medium, created in ultra-relativistic nucleus-nucleus collisions. The observed modification can be then used to characterize properties of the produced hot and dense strongly interacting matter.

Experiments have shown that the QGP created in a laboratory behaves like a liquid with specific shear viscosity over entropy density ratio close to the minimum allowed by the laws of physics. An important set of probes of this fascinating state of matter arise from hard scattering of quarks and gluons that generate “jets” of particles emerging at large angles to the beam direction. These jets are produced in the process of parton showering when a highly virtual parton fragments. Jet production is well understood in proton-proton collisions and can be calculated accurately using the fundamental theory of the strong interaction, QCD. Such processes also occur in a very early stage of the nucleus-nucleus collision, at the time scales comparable to the QGP formation. In ultra-relativistic nucleus-nucleus collisions, jet fragmentation gets modified by interaction with the hot and dense medium. Such interactions result in changes to jet production rates and internal structure, known as “jet quenching”. These medium-induced modifications are observable experimentally and are calculable theoretically, using tools based in QCD. Jet measurements in nucleus-nucleus collisions thus represent a rigorous experimental tool which allows us to study properties of the QGP in unique and well-controlled ways.

#### 1. Studies of jet properties in ALICE

Studies of jet properties in the ALICE experiment undertaken by the team members cover all collision systems measured at the LHC, p+p, p+Pb and Pb+Pb as well as exploration of various observables described in more detail below.

Our first jet measurement in ALICE, was in fact carried in the previous evaluation period and the results were published early 2015 in the paper *Abelev et al. (ALICE), Charged jet cross sections and properties in proton-proton collisions at  $\sqrt{s} = 7$  TeV, Phys. Rev. D 91 (2015) 112012*. Ph.D. student M. Vajzer and his co-supervisor J. Bielčíková were among principal authors of the paper, where they contributed with the measurement of absolutely normalized charged jet cross section for several resolution parameters  $R = 0.2 - 0.6$  and their relative ratios as a measure of jet collimation together with comparisons to various MC generators. The other principal authors of the paper were O. Busch (Univ. of Heidelberg), S. Prasad (Bose Institute Kolkata/Wayne State Univ.) and C. Pruneau (Wayne State Univ.), who performed jet fragmentation and basic jet shape studies. M. Vajzer defended successfully his Ph.D. thesis at the CTU Prague in 2015.

Analysis of jets in heavy-ion collisions is complicated by the fact that a large fraction of reconstructed jets origins from an accidental combination of soft particles from the underlying event. In ALICE, we elaborated experimental observables which allow for subtraction of this complex background using a well-controlled, data-driven approach. Our method utilizes coincidence measurement of jets and high- $p_T$  hadrons which are nearly back to back in azimuth. This approach was used in the paper *Adam et al. (ALICE), Measurement of jet quenching with semi-inclusive hadron-jet distributions in central Pb–Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV, JHEP 09 (2015) 170* to assess the jet quenching effects in Pb+Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV and to search for possible quasi-particle composition of the QGP. Four principal authors of the paper were L. Cunqueiro (CERN), R. Ma (LBNL, USA), P. Jacobs (LBNL, USA) and F. Křížek. F. Křížek contributed with the analysis of the p+p reference. He presented results of the paper in a plenary talk on behalf of the ALICE collaboration at the Strangeness in Quark Matter conference in 2015.

In the next paper, *Acharya et al. (ALICE), Constraints on jet quenching in p-Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV measured by the event-activity dependence of semi-inclusive hadron-jet, Phys.Lett. B 783 (2018) 95*, F. Křížek together with P. Jacobs (LBNL, USA) utilized the same analysis technique to set a stringent upper limit on parton energy loss in a smaller p+Pb collision system. This measurement is important in the context of the discussion whether the QGP can be formed also in smaller collision systems. Recently it has been found that final states of p+Pb or high-multiplicity p+p collisions at the LHC exhibit the same kind of collective behavior that are believed to be experimental signatures of the QGP. Our paper shows that the size of the jet quenching effect in p+Pb collisions is compatible with zero. Results of this analysis were presented by F. Křížek at the Quark Matter 2017 conference.

In 2019, F. Křížek together with P. Jacobs were principal authors of the ALICE preliminary results on h+jet correlation measurements in high-multiplicity (HM) and minimum bias (MB) pp collisions at  $\sqrt{s} = 13$  TeV. The ALICE MB and HM triggers are based on a signal measured by the forward VZERO scintillator arrays which cover roughly the pseudorapidity between 3 and 5 units. Events selected with the HM trigger have 5-9 times larger VZERO signal when compared to MB and they constitute 0.1% of the MB cross section. Hadron-jet correlations measured in HM events exhibit a significant acoplanarity and suppression of back to back correlations with respect to MB. The observed effect is however probably not caused by the jet quenching since it is qualitatively reproduced by the PYTHIA event generator. Since autumn 2019, F. Křížek supervises a new MSc. student A. Kotliarov from Tomsk Polytechnic University in Russia whose task is to find a source of the observed phenomenon using PYTHIA simulations.

F. Křížek was also active in preparation of inputs for the *CERN Yellow Report: Monographs 7 (2019)*, which discusses an outlook for the future LHC Run 3 and Run 4 physics opportunities for high-density QCD with heavy-ion and proton beams. Together with P. Jacobs he contributed to the sessions *Jets and parton energy loss* and *Emergence of hot and dense QCD matter in small systems* by performing estimates for the h+jet correlation observables.

Since 2017, Ph.D. student A. Isakov and his supervisor F. Křížek work on the analysis of inclusive  $p_T$  spectra of b-jets produced in p+Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV. This analysis is carried out in cooperation with former team member R. Vertési (Wigner Research Center for Physics, Hungary) and A. Sheikh (Department of Atomic Energy, India). The measurement extends the existing LHC data on b-jet cross section to lower  $p_T$  and will constitute an important reference for future Pb+Pb analysis, since it constrains size of cold nuclear matter effects. Our contribution to the analysis is essential and comprises estimates of b-jet purity, correction of raw spectra via unfolding, and estimates of various sources of systematic uncertainties. R. Vertési and A. Sheikh contribute with the necessary POWHEG simulations. The inclusive spectra were approved as ALICE preliminary in 2019 and were presented by A. Isakov as a talk at the ICNFP2019 conference and posters (Hard Probes 2017, EPS HEP 2019). At the end of 2019, we also started to work on the p+p reference with the ultimate goal to obtain the nuclear modification factor for inclusive b-jets in p+Pb collisions. The analysis will be finished in 2020 and it will be summarized in a paper.

Ph.D. student V. Kučera and MSc. student V. Pacík focused under supervision of J. Bielčíková on studies of strange particle production in jets and the underlying event in p+p, p+Pb and Pb+Pb collisions. Taking advantage of unprecedented particle identification capabilities of the ALICE detector, unrivalled by other LHC experiments, this study should bring important insights into baryon and meson production mechanisms in heavy-ion collisions. Already at RHIC energy, it was observed that baryon-to-meson ratios in heavy-ion collisions are enhanced relative to those in p+p collisions. In order to quantify whether the enhanced baryon-to-meson ratio is due to radial flow, parton coalescence and recombination in medium or some other effects, it is necessary to establish whether the enhanced ratios that are present in bulk



are also seen in jets and what are their values in small collision systems where no QGP is expected to be formed.

Our group together with X. Zhang and M. Ploskon (LBNL, USA), initiated studies of strange particles,  $\Lambda$  and  $K^0_S$ , produced in jets in p+p (7 TeV) and p+Pb (5.02 TeV) collisions. We found that  $\Lambda/K^0_S$  ratios associated with jets in p+Pb collisions are consistent with the ratio measured in p+p collisions and with the expectation of jets fragmenting in vacuum given by the PYTHIA Monte Carlo event generator. This means that any cold nuclear matter effects present in p+Pb collisions do not affect  $\Lambda$  and  $K^0_S$  production mechanisms in this system. J. Bielčíková, V. Kučera and V. Pacík together with X. Zhang and M. Ploskon are principal authors of the ALICE manuscript under an IRC review. Furthermore, V. Kučera and J. Bielčíková together with the Ph.D. student A. Zimmermann and O. Busch (Univ. of Heidelberg) performed also the analysis of strange particle production in Pb+Pb collisions. Particle identification techniques were consulted with the ALICE group at IPHC Strasbourg (France), where V. Kučera had his co-supervising institution in a framework of the Czech-French double-doctorate studies. Our study in Pb+Pb collisions revealed that the  $\Lambda/K^0_S$  ratio is significantly enhanced in bulk matter but the same ratio in jets when compared to our results from p+p and p+Pb collisions is within current uncertainties consistent with production in vacuum. The results from Pb+Pb collisions await publication after ALICE internal issues with MC efficiencies in 2010/2011 are centrally resolved. V. Kučera and J. Bielčíková will be primary authors of this publication on behalf of the ALICE Collaboration. We note that both V. Pacík and V. Kučera successfully defended their theses and V. Kučera was awarded with the prestigious ALICE Best Thesis prize in 2017. Last but not least, J. Bielčíková and F. Křížek were often members of Internal Review Committees (IRC) of ALICE papers and members of Analysis Review Committees (ARC) of the related analysis notes that concerned ALICE jet measurements. In this role they contributed to the paper writing process and helped to solidify analysis results. In 2015–2019, J. Bielčíková chaired the IRC of the papers with the ASEP numbers 0479646, 0479642, 0508838, 0445828, 0512065 and the paper *Reaction plane dependence of jet-hadron correlations in Pb-Pb collisions at  $\sqrt{s_{NN}} = 2.76$  TeV (not published yet)*.

F. Křížek was in IRC of the papers with the ASEP numbers 0496715 and 0508845 and the paper *Exploration of jet substructure using iterative declustering in pp and Pb-Pb collisions at LHC energies* which was accepted by Phys. Lett. B in January 2020. F. Křížek was in ARC of **1)** Y. Dang et al., *Measurement of the semi-inclusive hadron+jet distributions in Pb-Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV* (2019), **2)** H. Andrews and L. Cunqueiro, *Softdrop in pp and PbPb* (2018), **3)** J. Norman, *Measurement of the semi-inclusive hadron+jet distributions in Pb-Pb collisions at  $\sqrt{s_{NN}} = 5.02$  TeV* (2018), and **4)** S. Sakai, *Measurement of heavy-flavor jets via electrons from heavy-flavor hadron decays in p-Pb at  $\sqrt{s_{NN}} = 5.02$  TeV* (2018).

## 2. Di-hadron correlation studies in STAR

Di-hadron correlations are frequently used to study jet properties on a statistical basis and have a long tradition in our team. While in p+p and d+Au collisions at RHIC, the near-side jet-like peak is narrow in azimuth and pseudorapidity, in central Au+Au collisions at 200 GeV an additional structure narrow in azimuth but broad in pseudorapidity (*ridge*) is present. Studies at the LHC energy revealed that the ridge-like structures are also present at an order of magnitude higher collision energies in Pb+Pb collisions but surprisingly also in small collision systems (high-multiplicity p+p and p+Pb collisions).

In this evaluation period, J. Bielčíková in collaboration with C. Nattrass (University of Tennessee in Knoxville, USA) extended their systematic study of energy and system size dependence of near-side di-hadron correlations in d+Au, Cu+Cu and Au+Au collisions at 62 and 200 GeV (*Phys. Rev. C85 (2012) 014903*) that enabled determination of the jet-like correlations and the ridge properties at fixed densities with different collision geometry. In particular, they focused on correlations using strange particles ( $\Lambda$ ,  $K^0_S$ ) in d+Au, Cu+Cu and

Au+Au at the top RHIC energy of 200 GeV to look for trigger particle type dependence, which could be connected with in-medium modification of fragmentation, as well as associated particle type dependence, which could in turn help to understand particle composition of the near-side peak and hadronization mechanisms at play. J. Bielčiková and C. Nattrass as principal authors of the paper *Abelev et al. (STAR), Near-side azimuthal and pseudorapidity correlations using neutral strange baryons and mesons in d+Au, Cu+Cu and Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV*, *Phys. Rev. C* **94** (2016) 014910 analyzed near-side correlation functions using neutral strange particles ( $\Lambda$ ,  $K^0_S$ ), which can be identified up to high  $p_T$  by optimizing topological decay cuts. The jet-like  $\Lambda/K^0_S$  associated yield at intermediate  $p_T = 2\text{--}6$  GeV/c is within uncertainty consistent with that of inclusive particle production in p+p collisions, indicating that the jet-like correlation in heavy-ion collisions is dominantly produced by fragmentation and strange particle production through recombination is not significant in contrast to the role of recombination explaining the enhanced inclusive  $\Lambda/K^0_S$  ratios. Our observation at RHIC energy is thus compatible with our  $\Lambda/K^0_S$  ratio measurement in reconstructed jets in ALICE in Pb+Pb collisions discussed above. In contrast to h-h correlations, where we found the jet-like yield to be essentially independent of centrality, the strange particle triggered jet-like yields show some centrality dependence for  $K^0_S$  triggers indicating possible modification of fragmentation functions or particle production mechanisms in central Au+Au collisions at the top RHIC energy. There is also a hint of a particle species ordering observed - the jet-like yield from  $K^0_S$  triggered correlations is generally above that of h-h correlations and the jet-like yield from  $\Lambda$ -h is below that of the h-h correlations. This is clearly different from the particle-type ordering predicted by PYTHIA. These measurements provide motivation for future studies of strangeness production in jets and exploring in-medium modification of fragmentation at RHIC using the larger Au+Au data sets from Run 14 and Run 16.

### 3. Studies of jet properties in STAR

Measurements of medium-induced modifications of jets at RHIC are complementary to the measurements carried out at the LHC. Due to lower center of mass energy at RHIC, hard scatterings probe on average higher Bjorken  $x$  values of parton distribution functions which are quark dominated. At RHIC energies jet analyses are however challenged by a relatively small production rate of jets relative to the LHC, where jet production is copious. In the evaluation period, our Ph.D. student J. Rusňák and his supervisor J. Bielčiková in collaboration with P. Jacobs (LBNL, USA) have continued this challenging analysis of charged-particle jet properties in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV from Run11 (2011) data. The analysis applies a moderate low-momentum cut-off on leading hadron in a jet, while keeping a low-momentum constituent cut of 200 MeV/c. The analysis was finalized and the paper was reviewed by the STAR internal review committee (IRC) in 2019. After passing the collaboration review, which got delayed due to Covid-19 pandemic, the paper was submitted and accepted for publication in *Phys. Rev. C* (*arXiv:2006.00582*). J. Rusňák and J. Bielčiková are together with P. Jacobs the principal authors of this collaboration paper. J. Rusňák defended his Ph.D. thesis *Jet reconstruction in Au+Au collisions at RHIC* in 2017 and in 2018, he was awarded for his thesis the prestigious RHIC/AGS Thesis Award.

Our measurement constitutes the first measurement of fully corrected charged-particle jet cross sections in Au+Au collisions at RHIC and we used it to determine the corresponding nuclear modification factor  $R_{AA}$ . The jet  $p_T$  spectra, unfolded for detector effects and background fluctuations, were studied both as a function of collision centrality as well as jet resolution parameter  $R$  to quantify jet profile broadening in medium. The nuclear modification factor of charged-particle jets in central Au+Au collisions reveals a large suppression of jet production due to jet quenching and the amount of suppression is comparable to that at LHC energies. The results were also compared with state of the art model calculations (SCET, NLO pQCD, Hybrid Model, LBT).

In summer 2019, the work of J. Rusňák was taken up by a new Ph.D. student R. Líčeník who is supervised by J. Bielčíková. R. Líčeník started to work on inclusive full jet measurements in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV in STAR based on the Run 14 data including for the first time in Au+Au collisions also the information from the STAR Barrel Electromagnetic Calorimeter. R. Líčeník extracted raw  $p_T$  spectra and worked on a systematic study of hadronic correction. This analysis is expected to significantly extend the  $p_T$  reach of earlier measurements as it benefits from a high-statistics BEMC triggered sample. Our undergraduate students, V. Prozorova, G. Ponimatkin and M. Robotková, worked within their Bc. and MSc. projects on various aspects of jet shapes and jet substructure measurements including also implementation of Machine Learning techniques for tagging of heavy-flavor jets. All of them successfully defended their Bc. theses at CTU Prague and started to work on their MSc. projects.

J. Bielčíková was a member of God Parent Committees (GPC) of the STAR papers with the ASEP number 0448888, 0477479, and 0504071 that concerned further STAR jet measurements. In this role she contributed to the paper writing process and helped to solidify analysis results.

#### 4. Open heavy flavor measurements at STAR

The measurements of production of hadrons containing a charm or a beauty quark play a key role in the STAR and ALICE experimental programs. Heavy quarks are produced in the initial stage of a nucleus-nucleus collision, traverse through the dense nuclear medium and interact with the surrounding matter before they hadronize to particles measured in detectors. Production of heavy-flavor 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 hot, strongly interacting matter. Properties of the nuclear matter could be studied by systematic investigation of these effects on open-heavy-flavor hadrons (D and B mesons,  $\Lambda_c$ ) or jets with open heavy mesons. Our group can thus exploit synergy between our STAR and ALICE heavy-flavor programs. For successful reconstruction of heavy-flavor particles a precise secondary vertex detector is essential. In 2014, the STAR experiment installed the Heavy-Flavor Tracker (HFT) which was designed and built with active participation of our team in the two previous evaluation periods. In this evaluation period, we could harvest the invested efforts and start to analyze the experimental data.

One of the target goals of the HFT program was the first measurement of the open heavy-flavor baryon  $\Lambda_c$  in heavy-ion collisions. The measurement of  $\Lambda_c$  production in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV is crucial for understanding of charm quark thermalization, transport, and hadronization. In particular, the transverse momentum ( $p_T$ ) and centrality dependence of the  $\Lambda_c/D$  ratio sets important constraints on charm-quark coalescence in the hot and dense QCD medium. This analysis was carried out by X. Dong and his colleagues S. Radhakrishnan and G. Xie at LBNL and our Ph.D. student M. Šimko, who is supervised by J. Bielčík and co-supervised by J. Bielčíková. The fully corrected  $\Lambda_c/D$  ratio and its  $p_T$  and centrality dependence are consistent with those of particles containing only light quarks ( $p/\pi$  or  $\Lambda/K^0_S$ ) which points to a similar hadronization mechanism for u, d, s as well as c-quarks. The analysis is finished and the corresponding paper, of which M. Šimko is one of principal authors, was submitted in 2019 to PRL and published early 2020 as *Adam et al. (STAR), First measurement of  $\Lambda_c$  baryon production in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV, Phys. Rev. Lett. 124 (2020) 17, 172301*. Preliminary results from the analysis were also presented by M. Šimko e.g. at the EPS-HEP 2017 conference.

J. Vaněk, our next Ph.D. student in STAR supervised by J. Bielčík and co-supervised by J. Bielčíková, has been working since 2017 on the analysis of inclusive  $p_T$  spectra of charged D mesons in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV measured in 2016. In 2018 and 2019, J. Vaněk had a couple of three-month internships at LBNL during which he worked on the

charged D meson analysis together with X. Dong. Also this analysis exploits the excellent secondary vertex reconstruction capabilities of the HFT detector, which enables reconstruction of the three-particle decay channel of the charged D mesons with high significance. In 2018, the analysis of charged D meson nuclear modification factor in Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV was approved by the STAR collaboration as preliminary. The observed suppression of charged D meson production relative to p+p collisions is consistent with that of  $D^0$  mesons and is within uncertainties of the same magnitude as for light-flavor hadrons. J. Vaněk presented results of his analysis in talks at several high-ranking international conferences (Hot Quarks 2018, Quark Matter 2018, and Strangeness in Quark Matter 2019). Let us also note that R. Líčeník, a new Ph.D. student in our group and a former MSc. student at the CTU Prague, finalized within first months of his Ph.D. study charged D-meson production in Run 16 data which was his MSc. thesis project and presented the results at the EPS HEP 2019 conference. Besides quantifying energy loss of charm quarks via nuclear modification factor  $R_{AA}$  and studying baryon-to-meson ratios, it is also very important to study anisotropic flow of particles containing c-quarks and investigate to which extent heavier quarks participate in collective flow phenomena. In this study, which P. Federič started in 2018, we work on further improving open heavy-flavor hadron reconstruction efficiency in the Au+Au data samples taken with the HFT by using the Kalman filter. On this analysis we closely collaborate with prof. I. Kisel from FIAS Frankfurt and his group as well as with P. Chaloupka from CTU Prague. This novel approach significantly improves the significance of reconstructed D mesons especially at low  $p_T$ , and we have verified that the extracted anisotropic elliptic flow ( $v_2$ ) agrees with the published STAR results. Nevertheless, our approach leads to smaller uncertainties and allows for extension to low  $p_T$ . In general, the KF Particle will be extremely useful also for other PID studies in STAR (e.g.  $\Lambda_c$ ).

## 5. Upsilon production in STAR

Besides open heavy-flavor production, we also investigated quarkonium production in high-energy heavy-ion collisions as it is expected to be sensitive to the energy density and temperature of the created medium. Dissociation of different quarkonium states due to color screening is predicted to depend on their binding energies. Therefore, measuring yields of different quarkonium states may serve as a model-dependent measure of the temperature in the medium. Although traditionally studies of  $J/\psi$  production, a bound state of c and c-bar quarks, were proposed as the key observable for QGP observation, in the last decade bottomonium states are considered to be a cleaner probe of the medium. Pair recombination and co-mover absorption effects which complicate interpretation of  $J/\psi$  measurements are predicted to be negligible at RHIC energies although initial state effects may still play an important role. Taking advantage of U+U data  $\sqrt{s_{NN}} = 193$  GeV measured in STAR which have about 20% higher energy density and thus higher temperature than that in central Au+Au collisions at  $\sqrt{s_{NN}} = 200$  GeV, our postdoc R. Vertési performed analysis of  $Y$  production. He is the only principal author of the STAR publication *Adamczyk et al. (STAR),  $Y$  production in U+U collisions at  $\sqrt{s_{NN}} = 193$  GeV measured with the STAR experiment, Phys. Rev. C 94 (2016) 064904* which summarizes the measurement. The paper contains measurement of the  $Y(1S+2S+3S)$  as well as  $Y(1S)$  cross section in the di-electron decay channel. A significant suppression is observed in central U+U data for both  $Y(1S+2S+3S)$  as well as  $Y(1S)$  which consolidates and extends the previously observed  $R_{AA}$  trend with centrality in Au+Au collisions. The data from 0–60% central U+U collisions is consistent with a strong suppression of the  $Y(2S+3S)$  states, which has also been measured in STAR in Au+Au collisions. Comparison of the suppression patterns from Au+Au and U+U data to different models favors an internal-energy-based quark potential scenario.

## B) HARDWARE AND SOFTWARE ACTIVITIES IN ALICE AND STAR

### 1. Hardware activities ALICE

The ALICE group participates in the upgrade project of the ALICE ITS detector which is intended to be installed for the LHC Run 3 and Run 4. The design of this new vertex detector is based on CMOS Monolithic Active Pixel Sensors (MAPS) which allow for significant material budget reduction in the vicinity of the interaction diamond. The new ITS will improve efficiency of secondary vertex reconstruction of heavy-flavor hadron decays and will enable measurement of tracks with  $p_T$  as low as 50 MeV/c. The detector will have seven concentric layers of MAPS pixel sensors called ALPIDE. The radial displacement of the first layer from the LHC beam will be 22 mm only which poses stringent requirements on radiation hardness of the sensors. Throughout the operation, the innermost barrel sensors will have to sustain about 270 krad of Total Ionization Dose (TID) and  $10^{12}$  1MeV  $n_{eq}$  cm<sup>-2</sup> of Non-Ionizing Energy Loss (NIEL). Nevertheless, according to the project design report, the sensors have to keep their performance for radiation loads that are 10 times higher. In 2015–2018, we have used the NPI cyclotron to test radiation hardness of the ALPIDE sensors and their prototypes. For this purpose, we built a dedicated irradiation setup which allows for remote manipulation with the irradiated samples, for on-line monitoring of the beam intensity and for integration of the total ionization dose accumulated in the samples. The setup and its performance were described in *F. Křížek et al., Irradiation setup at the U-120M cyclotron facility, Nucl. Inst. Meth. Phys. Res. A 894 (2018) 87*, where we also demonstrated versatility of our apparatus on a measurement of Single Event Transient events in the SRAM-based XC3S200 FPGA from Xilinx. Final results from the radiation hardness tests were summarized in *V. Raskina and F. Křížek, Characterization of Highly Irradiated ALPIDE Silicon Sensors, Universe 5 (2019) 91*, where we show that ALPIDE sensors fulfill the required limits on radiation hardness.

S. Kushpil and A. Isakov were performing characterization of ALPIDE sensors using data from test beams that were carried out at CERN PS and they used them to validate simulations of ALPIDE response in the ALICE O2 software for Run 3. Results from these studies were published in *S. Kushpil et al., Recent Results from Beam Tests of the ALPIDE Pixel Chip for the Upgrade of the ALICE Inner Tracker, IEEE Trans. Nucl. Sci. 66 (2019) 2319* and presented by S. Kushpil at *2017 Nuclear Science Symposium and Medical Imaging Conference on Room-Temperature X- and Gamma-ray Detectors* and *2018 IEEE Nuclear Science Symposium and Medical Imaging Conference*.

Ph.D. student T. Vaňát and his supervisor J. Ferencei were the driving force of the ITS Readout Unit radiation hardness tests that were carried out at the NPI cyclotron facility. They are principal authors of the paper *K. M. Siewlewicz et al., Prototype readout electronics for the upgraded ALICE Inner Tracking System, JINST 12 (2017) C01008*. Data from the test beams that were measured at our NPI cyclotron facility were an important input to the *ITS Upgrade - Readout Electronics Production Readiness Review* held at CERN in April 2018 (<https://indico.cern.ch/event/698929/>).

Since 2019, F. Křížek, S. Kushpil, A. Isakov and V. Raskina actively participate in commissioning shifts of the new ITS and A. Isakov contributes to the development of quality control software for the new detector. In 2019, S. Kushpil reported the current status of the ITS commissioning at *12th International "Hiroshima" Symposium on the Development and Application of Semiconductor Tracking Detectors (HSTD12)*.

### 2. Hardware activities in STAR

Our STAR team contributed to Heavy Flavor Tracker (HFT) in past. After its installation in 2014, M. Šimko tested and developed parts of the slow simulator for the pixel sensors of the HFT in a close collaboration with the RNC group at LBNL (USA). This work included optimization of

parameters of the slow simulator and comparisons to data. The effort was later continued by a MSc. student J. Kvapil (FNSPE CTU) supervised by J. Bielčík and M. Šimko. The work was concluded in 2016.

The NPI STAR group together with CTU Prague is responsible for the Zero-Degree Calorimeter. In 2015–2019, M. Šimko acted as an on-call ZDC expert. This job included daily maintenance and calibration of the ZDC. At present, the work is continued by J. Vaněk, who joined the ZDC project in 2017. In 2018, M. Šimko and J. Vaněk performed a critical upgrade and testing of ZDC photomultipliers.

At the beginning of their Ph.D., doctoral students in STAR are required to contribute with service work to the STAR experiment. In 2017, J. Vaněk performed as his service task calibration of the electromagnetic barrel calorimeter (BEMC) for the Au+Au data at 54 GeV. We also encourage our undergraduate students to work in summer on various detector projects at BNL. In 2019, V. Prozorova and M. Robotková contributed to the new STAR Forward Calorimeter System (FCS) project. FCS will consist of a Spaghetti Electromagnetic Calorimeter (SPACal), followed by a lead and scintillator plate sampling Hadronic Calorimeter (HCal). For the Electromagnetic Calorimeter (ECal), the calorimeter from the PHENIX experiment will be used as it has the required energy resolution and constitutes a very cost-effective solution. V. Prozorova within her stay at BNL polished and painted HCal scintillating tiles and also helped with characterization of the Silicon Photomultipliers (SiPMs) for the ECal. M. Robotková within her stay at BNL studied calorimeter's response to muons in PYTHIA simulations of p+p collisions at 200 and 510 GeV.

### **3. Large Scale Computing Activities for ALICE**

Computing for ALICE is an integral part of the research activity of our team. In 2015-2019, we have been active in the ALICE Offline project and also in the Online-Offline (O2) Upgrade project, specifically in the WP8 (Control, Configuration & Monitoring) working group. We have one representative in the ALICE Software and Computing Board (D. Adamová) and also in the ALICE Computing Resource Board (D. Adamová). In particular, our team is responsible for processing and simulation of ALICE data in the Czech Republic. This is done at the pragueclg2 Tier-2 computing center, which is a part of the Worldwide LHC Computing Grid (WLCG) computing infrastructure. The amount of the computing and storage resources that has to be delivered into the ALICE Grid is stated by the ALICE Constitution and represents continuous work on providing and installing new hardware at our Tier-2 center. The smooth data processing and delivery of mandatory resources is closely controlled by the ALICE management. The pragueclg2 computing center is a part of the computing center of the Institute of Physics (IoP) of the CAS in Prague. At NPI we operate an additional storage server cluster which is used for ALICE data. Based on the grant and institutional funds of NPI and IoP, the computing and storage infrastructure is gradually upgraded. In December 2019, there were ~ 6000 CPUs and over 2 PB of disk storage available for the needs of ALICE in the CPU-sharing regime. These capacities are fully continuously utilized: the data processing of ALICE is ongoing also during the current technical break in the LHC operation, the Long Shutdown 2. Our job is to monitor progress of the data production and in case of a problem to 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 of software upgrades required for the proper operation of data production at the computing center. Furthermore, we have to ensure a regular supply of new hardware to meet increasing ALICE requirements. Between 2015 and 2019, about 21.5 million ALICE grid jobs were processed in the Czech Republic and 139.7 PB of data for processing were transferred/downloaded from the ALICE data cluster. The results of our work, as well as reports on ALICE production results and so-called status reports are regularly presented at international conferences and workshops, e.g. Annual ALICE Tier-1/Tier-2 Workshops.

Our MSc. student M. Adam, who is co-supervised by D. Adamová, in addition to his activities at the Prague Tier-2 center, worked on development of a Machine Learning based method for identification of improper behavior of computing servers in large clusters running large distributed applications. He collaborated with colleagues from CERN IT and the tool is currently being tested on the CERN MONIT infrastructure. M. Adam reported on this work at several international conferences on Computing for High Energy Physics including CHEP2016, CHEP2018, and CHEP2019.

#### 4. Large Scale Computing Activities for STAR

Our team also pursues continuously computing research for STAR. In the evaluated period, one Ph.D. student was active in this area. D. Makatun, who defended his Ph.D. thesis in 2018, was supervised by M. Šumbera and co-supervised by J. Lauret (STAR computing coordinator at BNL) and prof. H. Rudová (Masaryk University in Brno). In his thesis *Distributed data processing in High Energy Physics*, D. Makatun deals with and attacks the complex problem of efficient data movements on the network within a distributed environment. He developed a new job planner which takes into account capacity of processing sites and the bandwidth of mutual interconnecting links and based on that designs a strategy of data transport and job processing on such a distributed system. His planner achieves superior performance w.r.t. to common commercial planners. The results were presented at several high-ranking conferences in the field, 7th Multidisciplinary International Scheduling Conference (MISTA) in 2015, 17<sup>th</sup> International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT2016), 2016 IEEE Symposium on Computational Intelligence in Scheduling and Network Design, 22<sup>nd</sup> International Conference on Computing in High Energy and Nuclear Physics (CHEP2016) and were also published in *D. Makatun et al. Planning of distributed data production for High Energy and Nuclear Physics, Cluster Computing 21 (2018) 1949–1965*.

### C) PHENOMENOLOGY OF HEAVY-ION COLLISIONS

Theory and phenomenology topics which are pursued by members of our group are closely related to RHIC and LHC physics programs. In the framework of color-dipole approach, R. Pasechnik, M. Šumbera and their collaborators developed a theoretical apparatus describing production of Drell-Yan di-leptons and  $J/\psi$  mesons in p+p and p+A collisions at RHIC and at the LHC. This approach, which is relevant for the current and future measurements, does not have any free parameters unlike other approaches. Lepton pairs produced in a hard collision do not suffer from final state interactions and are therefore cleaner and more efficient probe to study nuclear effects than produced hadrons. We predict strong nuclear suppression at large  $p_T$ , rapidity or energy caused by effects of quantum coherence in combination with initial state effects. Lepton pair production allows elimination of effects of quantum coherence at large invariant masses of lepton pairs. A strong nuclear suppression at large  $p_T$  will then be a clear demonstration of pure initial state effects. Results were published in *E. Basso et al., Drell-Yan phenomenology in the color dipole picture revisited, Phys.Rev. D93 (2016), 034023*. In addition, they were presented on several international conferences and workshops (*EPS-HEP 2015*), *High- $p_T$  Physics in the RHIC-LHC Era* and *7th International Conference on Physics Opportunities at an Electron-Ion-Collider* in 2016, *QCD challenges in pp, pA and AA collisions at high energies* (2017), *International Workshop on Forward Physics and Forward Calorimeter Upgrade in ALICE* (2019).

In the paper *M. Krelina et al., “Spin rotation effects in diffractive electroproduction of heavy quarkonia”, Eur. Phys. J. C79 (2019) 154*, we presented for the first time a comprehensive study of the Melosh spin rotation effects in diffractive electroproduction of S-wave heavy quarkonia off a nucleon target. Within the color dipole approach we used 2 popular parametrizations of the dipole cross section and 2 potentials describing the interaction

between quark and antiquark entering in the Schroedinger equation based the formalism for determination of the quarkonia wave functions. A strong onset of spin rotation effects in 1S charmonium photoproduction was found which is neglected in present calculations of corresponding cross sections. For photoproduction of radially excited  $\psi(2S)$  these effects are even stronger leading to an increased photoproduction cross section by a factor of 2–3 depending on the photon energy. Finally, we predicted that the spin effects vanish gradually with photon virtuality following universality properties in production of different heavy quarkonia as a function of the hard scale.

In the paper *J. Cepila et al. "Theoretical uncertainties in exclusive electroproduction of S-wave heavy quarkonia", Eur. Phys. J. C79 (2019) 495* we revised the conventional description of  $J/\psi$  and  $\psi'$  photo- and electroproduction off a nucleon target in the color dipole picture and studied various sources of theoretical uncertainties. For this purpose, we tested the predictions using a bulk of available dipole parameterizations against the final HERA data. Specifically, we provided the detailed analysis of the energy and hard-scale dependences of these observables employing the comprehensive treatment of the quarkonia wave functions in the Schroedinger equation based approach for a set of available c-cbar interaction potentials and quantified the effect of Melosh spin rotation and an uncertainty due to charm quark mass variations.

In the paper *M. Krelina et al. "D-wave effects in diffractive electroproduction of heavy quarkonia from the photon-like  $V \rightarrow QQ\bar{q}$  transition", Eur. Phys. J. C80 (2020) 92* we presented for the first time the study of the Melosh spin rotation in production of S-wave states off a nucleon target assuming a similar structure of the virtual photon and vector meson transitions to  $QQ\bar{q}$ . We employed the color dipole Light-Front formulation based upon the radial wave function of heavy quarkonia computed in the  $QQ\bar{q}$  rest frame by solving the Schroedinger equation with two realistic interaction potentials. Adopting the photon-like Lorentz structure of the  $V \rightarrow QQ\bar{q}$  Light-Front wave function, we have found a significant reduction of the photoproduction cross section compared to experimental data due to the Melosh transformation. We have also analyzed the dependence of such a pronounced impact of spin effects on the photon energy and virtuality, as well as on the quarkonia mass. We have found their stronger onset in production of radially excited 2S and 3S states giving rise to a worse description of available data on the  $\psi(2S)$ -to- $J/\psi$  ratio of photoproduction cross sections.

Scope of research of R. Pasechnik is very broad and includes in addition study of QCD-gravity relations, theories with multiple Higgs bosons or physics of diffraction. Recently he has published on these topics 5 papers which are listed in our team publications. R. Pasechnik was also often giving talks at high-ranking physics conferences e.g. at XIII Quark Confinement and the hadron spectrum 2018, EPS HEP 2019 or ISMD 2019. In 2017, R. Pasechnik with M. Šumbera published an extensive, highly cited review paper *Phenomenological Review on Quark–Gluon Plasma: Concepts vs. Observations*, Universe 3 (2017), 7.

## **D) STUDY OF WEAK INTERACTIONS AT ISOLDE CERN**

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



The WITCH (Weak Interaction Trap for CHarged particles) facility consisting of a world-unique combination of 2 Penning traps and a retardation spectrometer allowed to trap radioactive nuclei and to form a cooled and scattering-free radioactive source, where the nuclei could decay at rest. Shape of energy spectrum of the recoiling nuclei is very sensitive to the character of the weak interaction. Its precise measurement enabled to search for a possible admixture of the scalar/tensor component. Results with the  $^{35}\text{Ar}$  isotope, sensitive to a possible admixture of the scalar interaction, were published in *P. Finlay et al., First high-statistics and high-resolution recoil-ion data from the WITCH retardation spectrometer, Eur. Phys. J. A 52 (2016) 206*. Since 2016 the experimental setup WITCH started to be modified to employ other experimental effect to probe the existence of scalar currents in the weak interactions via the study of  $\beta$ -delayed protons emitted in the decay of  $^{32}\text{Ar}$  - project WISArD (Weak-Interaction Studies with  $^{32}\text{Ar}$  Decay). High precision measurement of the kinematic effect on the protons emitted from the moving recoil nuclei after the  $\beta$ -decay of  $^{32}\text{Ar}$  carries information about  $\beta$ - $v_e$  correlations, which are different for a scalar current compared to the dominant vector current. Since 2014, D. Zákoucký and his ISOLDE collaborators work on a new method to study the same effect. They utilize the ISOLDE beam-line rebuilt to enable polarization of the incoming beam of radioactive ions with lasers (VITO project - Versatile Ion-polarized Techniques On-line). The aim here is to start measuring the angular asymmetries of  $\beta$ -particles emitted during the  $\beta$ -decays of spin oriented samples of selected sensitive isotopes, which includes also the development of new detector systems tailored for the envisioned physics tasks. The results from the period 2015–19 were published in total in 8 papers, e.g. *T. Porobic et al., Space-charge effects in Penning ion traps, Nucl.Instr.Meth. A785 (2015) 153*, *M. Stachura et al., Versatile Ion-polarized Techniques On-line (VITO) experiment at ISOLDE-CERN, Nucl.Instr.Meth.B 376 (2016) 369*, *M. Kowalska et al., New laser polarization line at the ISOLDE facility, Journal of Physics G, Nucl.Part.Phys. 44 (8) (2017)* or the *P. Finlay et al., Eur. Phys. J. A 52 (2016) 206*, already mentioned above. To the published papers D. Zákoucký contributed at the level of about 15%. His contribution consists in design, installation, and tuning of the experimental setups, adjustment of the setups before each experiment and in active participation in online and offline experiments. D. Zákoucký presented results of the WISArD experiment at the 57th International Winter Meeting on Nuclear Physics in 2019.

## Research activity and characterisation of the main scientific results

### Experimental study of hadron's properties in medium

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 present unique probe of the deep nuclear interior, which makes it possible to study a variety of otherwise inaccessible nuclear phenomena. Therefore, experimental program of RHIC group concentrates on the measurement of dilepton and strange particles yields in different combination of projectile and target.

### Hot and compressed nuclear matter (Au+Au and Ag+Ag experiments)

The RHIC group scientists participated during the evaluation period in the High Acceptance Di-Electron Spectrometer (HADES) international collaboration on the analysis of previous experiments, interpretation of measured data and paper writing. Particularly, senior P. Tlustý was member of writing committee of paper "*Probing dense baryon-rich matter with virtual photons*" which was published in prestigious journal *Nature Physics Volume 15, Issue 10, 1 October 2019, Pages 1040-1045*, recently. This paper was thoroughly discussed between members of collaboration including whole our group and it summarized all HADES dilepton results in general and results from Au+Au experiment in particular. The spectral distribution of the electron–positron pairs presented in paper is nearly exponential, providing evidence for a source of temperature in excess of 70 MeV with constituents, whose properties have been modified, thus reflecting peculiarities of strongly interacting QCD matter. Its bulk properties are similar to the dense matter formed in the final state of a neutron star merger, as apparent from recent multi-messenger observation. We observed in Au+Au central collisions the strong enhancement  $\sim 8x$  over properly scaled superposition of the dielectron sources measured in elementary pp and quasi-free np reactions, which is much more than enhancement  $\sim 3x$  reported by us in Ar+KCl collisions, see previous HADES paper based on results of our former Ph.D. student F.Krizek. 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  $A_{part}$ . In fact, at a given bombarding energy the excess scales  $Y_{excess} \propto A_{part}^{1.4}$ , i.e. much more strongly than the pion production does. 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.

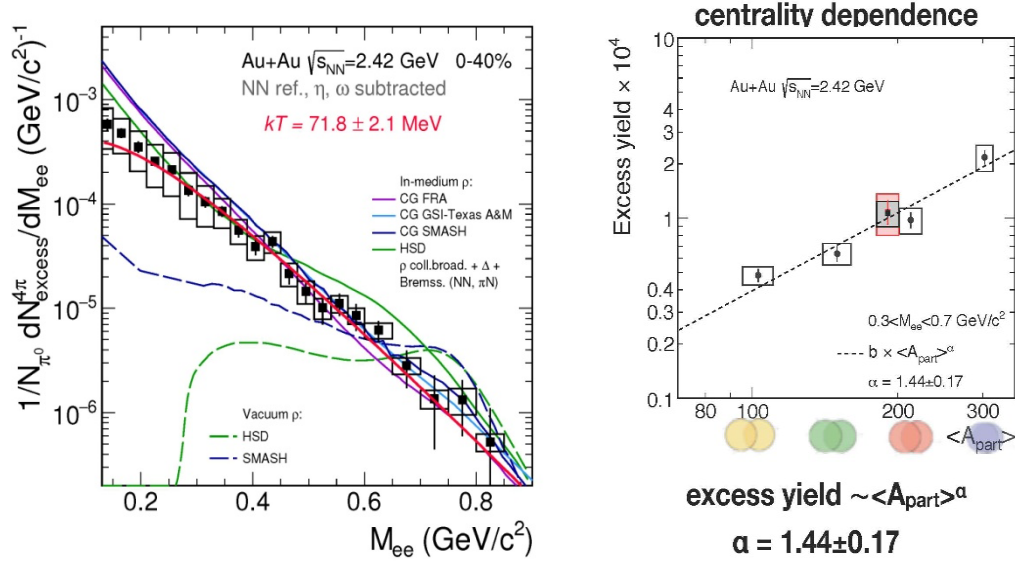


Fig. 1 Invariant mass spectra of electron positron pairs measured in Au+Au experiment (left) and excess yield as a function of number of participants (right).

Further, we presented data about strangeness yields in paper “*Deep sub-threshold  $\phi$  production in Au+Au collisions*”, *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics*, 778, pp. 403-407 (2018). It is the first simultaneous measurement of  $K^-$  and  $\phi$  mesons in central heavy-ion collisions below a kinetic beam energy of 10 AGeV. The  $\phi/K^-$  multiplicity ratio is found to be surprisingly high with a value of  $0.52 \pm 0.16$  and shows no dependence on the centrality of the collision. Consequently, the different slopes of the  $K^+$  and  $K^-$  transverse-mass spectra can be explained solely by feed-down from decay of  $\phi$  mesons, which substantially softens the spectra of  $K^-$  mesons. Hence, in contrast to the commonly adapted argumentation in literature, the different slopes do not necessarily imply diverging freeze-out temperatures of  $K^+$  and  $K^-$  mesons caused by different couplings to baryons. Our Ph.D. student L. Chlad participated in analysis and interpretation of data about production of strangeness from Au+Au experiment. Results of his analysis of Kaon's flow were presented in international conferences, like SQM2019 and QM2018, and final results are to be published soon. The obtained data had very high statistic which allows him to study the flow of Kaons in much more detail in comparison with previous studies. His results, in accordance with previous studies confirmed, that the flow of both charged and neutral kaons has the same magnitude and can be explained by introducing corresponding potential describing interaction of kaons with hadron medium. He plans to submit his Ph.D. thesis soon.

To summarize, our results indicated, that medium effects are important both in the case of vector mesons and in the strangeness production inside a collision zone.

To further clarify these findings, about fourteen billion Ag+Ag collisions at 1.58 AGeV have been recorded in March 2019 with an event rate of 14 kHz. Members of the Czech group have been present during the four-week beam time of Ag+Ag experiment and served as detectors experts (TOF, FW, ECAL), shift leaders (seniors) and DAQ experts. We prepared the calibration of the TOF and ECAL detectors including time-walk correction, performed analysis of embedded simulation data into experimental one with the aim to deduce on efficiency corrections. We also deduced from the data of FW the size of the collision zone (centrality of collision) and orientation of the reaction plane per event. The Ph.D. thesis of our student, A. Prozorov, will be based on the data obtained during Ag+Ag experiment. Series of corresponding publications on dilepton and strangeness production, particle spectra etc. can be expected soon.

### Cold nuclear matter (pion induced collisions)

We also participated in interpretation and analysis of data from proton induced reactions studied in experiments carried out before 2015. For example results on the production of the double-strange cascade hyperon  $\Xi^-$  were reported for collisions of p (3.5 GeV) + Nb, in paper “*Subthreshold  $\Xi^-$  Production in Collisions of p(3.5 GeV)+Nb*” *Phys.Rev.Lett.* 114 (2015) 212301. For the first time, subthreshold  $\Xi^-$  production was observed in proton-nucleus interactions. Assuming a  $\Xi^-$  phase-space distribution similar to that of  $\Lambda$  hyperons, the production probability amounts to  $P_{\Xi^-} = (2.0 \pm 0.4 \text{ (stat)} \pm 0.3 \text{ (norm)} \pm 0.6 \text{ (syst)}) \times 10^{-4}$  resulting in a  $\Xi^- / (\Lambda + \Sigma^0)$  ratio of  $P_{\Xi^-} / P_{\Lambda + \Sigma^0} = (1.2 \pm 0.3 \text{ (stat)} \pm 0.4 \text{ (syst)}) \times 10^{-2}$ . Available model predictions are significantly lower than the estimated  $\Xi^-$  yield. In another paper “*The  $\Lambda p$  interaction studied via femtoscopy in p + Nb reactions at  $\sqrt{s_{NN}}=3.18 \text{ GeV}$* ”, *Phys.Rev.* C94 (2016) no.2, 025201, comparing the experimental correlation function to model calculations, a source size for pp pairs of  $r_{0,pp}=2.02\pm0.01\text{(stat)}+0.11-0.12\text{(sys)}\text{fm}$  and a slightly smaller value for p $\Lambda$  pairs of  $r_{0,\Lambda p}=1.62\pm0.02\text{(stat)}+0.19-0.08\text{(sys)}\text{ fm}$  are extracted. Using the geometrical extent of the particle-emitting region, determined experimentally with pp correlations as reference together with a source function from a transport model, it was possible to study different sets of scattering parameters. The p $\Lambda$  correlation is proven to be sensitive to predicted scattering length values from chiral effective field theory. We demonstrate that the femtoscopy technique can be used as a valid alternative to the analysis of scattering data to study the hyperon-nucleon interaction. The paper “*Inclusive  $\Lambda$  production in proton-proton collisions at 3.5 GeV*” *Physical Review C*, 95 (1), art. no. 015207, (2017) is devoted to comparison of the experimental data to a data-based model for individual exclusive  $\Lambda$  production channels in the same reaction. The contributions of intermediate resonances such as  $\Sigma(1385)$ ,  $\Delta^{++}$ , or  $N^*$  are considered in detail. In particular, the result of a partial-wave analysis accounts for the abundant pK $+\Lambda$  final state. Model and data show a reasonable agreement at midrapidities, while a difference is found for larger rapidities. A total  $\Lambda$  production cross section in p+p collisions at  $s=3.18\text{GeV}$  of  $\sigma(p+p\rightarrow\Lambda+X)=207.3\pm1.3-7.3+6.0\text{(stat.)}\pm8.4\text{(syst.)}-0.5+0.4\text{(model.)}\mu\text{b}$  is found.

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. Secondary pion beam with rather broad distribution of momenta allowed during two experiments in 2014 excellent scanning of corresponding excitation functions of baryonic resonances 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 1 seconds, full spill duration was about 2.8 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 Hodoscope detector together with the diamond START detector were analysed by L. Chlad (our diploma student in 2014). 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 constraints 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 in 2014) and P. Ramos (our Ph.D. student). P. Ramos continued in the analysis of the data during his Ph.D. studies in period 2015-2019. Results of his analysis of dilepton's yield in pion-nucleon reaction were presented in international conferences, like QM2018 and FAIRNESS2016, and final results have to be published soon. He will submit finished Ph.D. thesis soon.

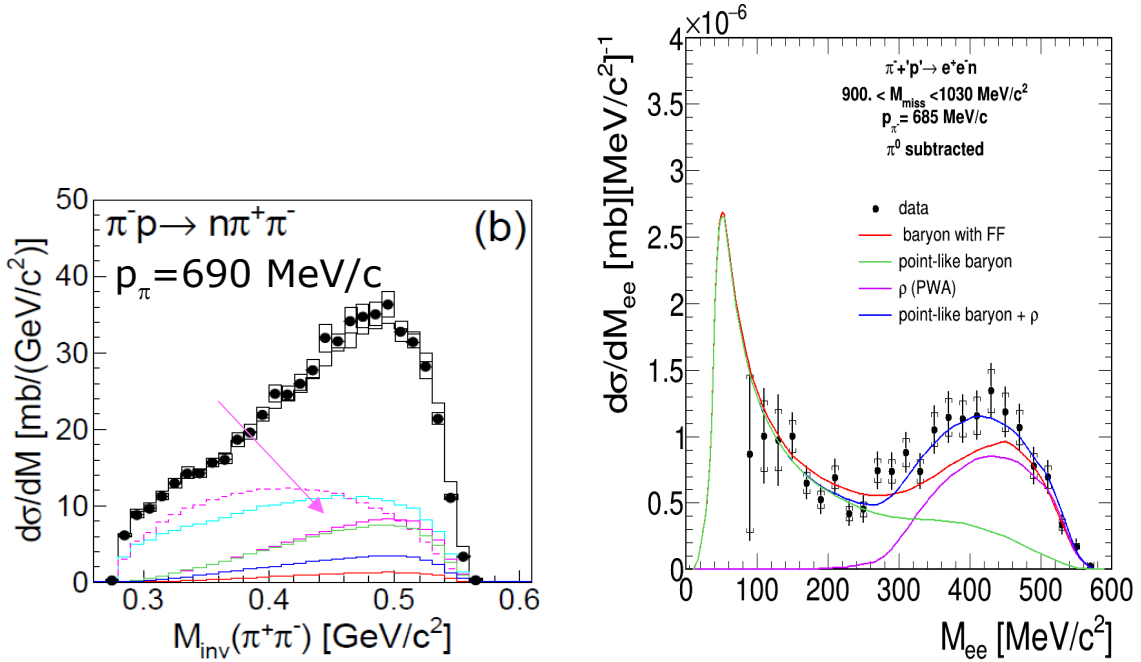


Fig. 2 The  $\pi^+\pi^-$  invariant mass spectrum from pion induced reactions on proton (left) and invariant mass spectra for electron positron pairs from pion induced reactions on proton (right).

### Upgrade of HADES experimental setup

In the past five years the HADES spectrometer was undergoing an extensive upgrade to be used at the FAIR project for experiments at energies up to 10 GeV per nucleon. Czech scientists were significantly contributing to this upgrade by design and built up of the Electromagnetic Calorimeter (ECAL). This project is lead by the Czech group. The ECAL will allow measurements of the direct decay of the eta and pion neutral 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 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.

Senior of our group P. Tlustý is a technical coordinator of the ECAL project since its beginning. In the previous period 2010 – 2014 all crucial parts of the calorimeter were developed and tested. The ECAL consists of 978 lead glass modules read out by two types of photomultipliers which were selected as the suitable ones (1.5" EMI9903KB photomultipliers from former

MIRAC experiment and new 3" photomultipliers Hamamatsu R6091). The ECAL stability monitoring and calibration is 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 was 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.

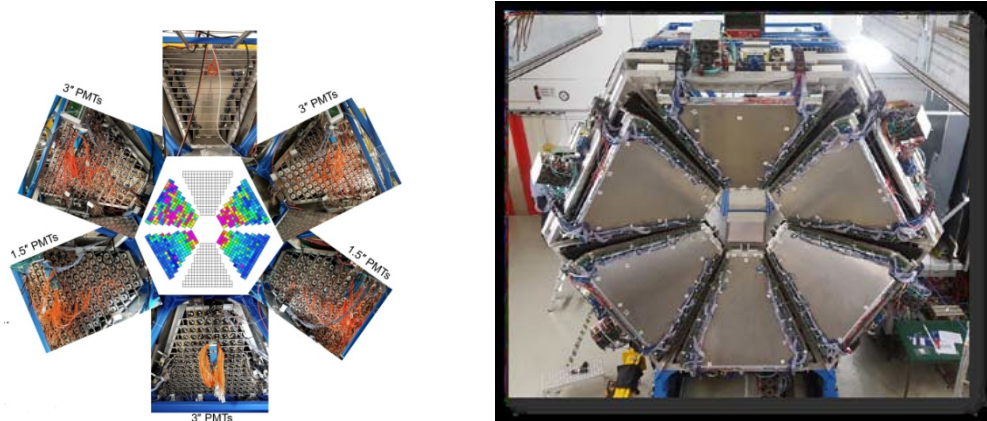


Fig. 3 Artistic collage of photos of six ECAL sectors in combination with figure from data acquisition (left) and photo of the whole ECAL detector frame with RPC detector in front of it (right).

Czech team with the help of our international partners started installation of ECAL in 2015. Four sectors out of six were installed and tested before first FAIR experiment carried out by HADES in March 2019. Remaining two sectors are now under installation to be finished soon before forthcoming next HADES experiment planned for 2021.

### **R&D for future CBM at FAIR(Darmstadt)**

Scientists from the RHIC group are also founding members of the Compressed Baryonic Matter (CBM) experiment as a successor project to the HADES. The CBM experiment is under preparation at FAIR 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. For details see our paper "*Challenges in QCD matter physics --The scientific programme of the Compressed Baryonic Matter experiment at FAIR*": CBM Collaboration in *European Physical Journal A*, 2017, 53(3),

The scientific team from NPI participated together with our Russian colleagues in the development of the PSD detector for measuring of the projectile fragments („Projectile Spectator Detector“) which will provide information on the reactions centrality and the reaction plane in forthcoming CBM experiments. Reaction plane reconstruction and particle flow were studied by simulations using various reaction models. These simulations were carried out by our Ph.D. student V. Mikhaylov. His 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, he 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.

Silicon PhotoMultipliers (SiPM) are used for the scintillator light readout at PSD. The main issue of SiPM application is their degradation due to high neutron fluence that can reach up to  $2 \times 10^{11} \text{ n}_{\text{eq}}/\text{cm}^2$  per year of the CBM experiment operation. Multiple irradiation tests of SiPMs were conducted at Řež cyclotron using quasi-monoenergetic and white-spectrum neutron sources and total fluence in the range of  $5 \times 10^{10} - 6 \times 10^{12} \text{ n}_{\text{eq}}/\text{cm}^2$ . Our Ph.D. student V. Mikhaylov supervised by senior V. Kushpil developed dedicated setup to measure Capacitance-Voltage (C-V), Current-Voltage (I-V), and Capacitance-Frequency (C-F) characteristics of SiPM 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.

Further, PSD single module response to proton beams was studied in the momentum range of 2 – 80 GeV/c. Module was consequently equipped with 3 batches of Hamamatsu SiPMs MPPC S12572-010P irradiated by  $2.5 \times 10^{11}$ ,  $1.6 \times 10^{12}$  and  $4.5 \times 10^{12} \text{ n}_{\text{eq}}/\text{cm}^2$ . These SiPMs were chosen for the superior radiation hardness and small pixel recovery time allowing PSD to operate at collision rates up to  $10^8$  ions/s. Their small  $10 \times 10 \text{ } \mu\text{m}^2$  pixel size not only increases the calorimeter dynamic range, but also is presumably related to the better radiation hardness. These results were presented by V. Mikhaylov on several conferences and CBM meetings and published in conference proceeding as well as in refereed journals, like V. Mikhaylov et al., *Radiation hardness of Silicon Photomultipliers for BM@FAIR, NA61@CERN and BM@N experiments, Nuclear Inst. and Methods in Physics Research, A 912 (2018) 241–244*. Based on these results V. Mikhaylov will submit his Ph.D. thesis soon.

Last, A. Kugler and our postdoc P. Chudoba coordinated design of supporting frame for PSD developed and built by our partners from Czech Technical University. It was delivered to FAIR site and passed Final Acceptance Test in September 2020.

### **R&D for future BM@N at NICA JINR (Dubna)**

Scientists from the RHIC group are also members of the Baryonic Matter at Nuclotron (BM@N) experiment at Joint Institute for Nuclear Research (JINR) Dubna, Russia. The BM@N experiment is under preparation at JINR to study the nuclear matter at extreme conditions with aim to detect hadrons originating in the nucleus-nucleus collisions at energies up to 4 GeV per nucleon. Hence BM@N will carry out studies of dense baryonic matter in the energy regime complementary both to HADES and future CBM. Further, this experiment will serve as a test bench for CBM, as it has to start operating with relativistic heavy ions from Nuclotron after 2021. The Czech group participates together with our Russian colleagues in R@D and built up of the Forward Hadron Calorimeter (FHCaI), which is analog of PSD designed for CBM mentioned above. Therefore, results obtained during development of PSD will be used also for development of FHCaI. Last, we are coordinating development of corresponding carbon beam pipe designed and built by our partners from Czech Technical University.



### Accelerator driven transmutation technologies

Spallation reactions as a perspective source of neutrons have been studied with an increased interest in the last decades. Corresponding studies carried out by our group, particularly senior V. Wagner and his Ph.D. students, 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 goal of the group of the “Accelerator driven transmutation technologies” is 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 (Russia). 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. The Czech team is concentrated on study of neutron field spatial and energy distribution as well as on detailed study of neutron induced reactions. We used activation detectors from Au, Al, Bi, In, Ta, and Y 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 used (n,xn) reactions were measured using quasi mono energetic neutron source based on Řež and Uppsala cyclotrons. Gained data were after the analysis published in series of papers (as example see “*Activation Measurements of Cross Sections for Ground and Isomeric States Production in Neutron Threshold Reactions on Y and Au*” in *Nuclear Science and Engineering* 198 (2018) 150-160 and included in the EXFOR database. A systematic analysis of experiments with assemblies of lead or uranium target and uranium blanket irradiated by relativistic beams with accelerators in JINR Dubna was published in a number of articles, as an example can be used “*Activation measurement of neutron production and transport in a thick lead target and a uranium blanket during 4 GeV deuteron irradiation*” in *NIM A908* (2018) 347-360.

### Neutrino mass measurement in tritium decay

With the evidence of massive neutrinos from oscillation experiments, one of the fundamental tasks of particle physics is the determination of the absolute mass scale of neutrinos. It has crucial implications for cosmology and particle physics. The objective of the KATRIN (Karlsruhe TRItium Neutrino experiment) is a direct model-independent determination of the neutrino mass via the measurement of the endpoint of the tritium beta decay spectrum. Currently, the upper limit of the neutrino mass is 2 eV/c<sup>2</sup>. The aim of KATRIN is to measure the neutrino mass with the sensitivity of 0.2 eV/c<sup>2</sup>.

### KATRIN and our electron spectroscopy group

The KATRIN complex with length of 70 m consists of rear section, windowless gaseous tritium source (WGTS), differential and cryogenic pumping section, electron pre-spectrometer (PS), electron main spectrometer (MS), monitoring spectrometer (MoS) and focal plane detector (FPD).

There exist five systematic effects whose uncertainties have the direct influence on the  $m_\nu^2$  value to be determined in the KATRIN experiment. Our activity in the KATRIN project is related to two of these systematic effects and to the calibration of the energy scale.



The first systematic effect is represented by an unrecognized instability of the analysing 20 kV high voltage (HV) at the MS. Additionally to the measurement of the HV by means of the two precision high voltage dividers and two voltmeters, the HV stability is monitored with the MoS. Any change of the position of the monoenergetic electrons line measured at MoS, indicates the instability of the HV. The second systematic effect is connected with the plasma charge and its fluctuation in the WGTS. The plasma electric potential influences the starting energy of the beta electrons produced in tritium decays. In order to investigate this disturbing effect, the gaseous source of monoenergetic electron has to be inserted into the WGTS. From the comparison of the spectra of monoenergetic electrons measured with and without tritium inside the WGTS, the information about the plasma behaviour is obtained.

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  $^{83}\text{Rb}$  into a suitable substrate. The daughter isotope  $^{83\text{m}}\text{Kr}$  ( $T_{1/2}=1.8$  h) emits monoenergetic K shell conversion electrons of the 32.2 keV transition, K-32 with energy of 17824 eV, that is conveniently close to the tritium endpoint energy of about 18575 eV. Our task was the reliable production of the vacuum evaporation and/or implanted sources with the stability of the K-32 electron energy at level of 3 ppm/month. Evidently, a similar  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  generator, emanating, on the contrary the  $^{83\text{m}}\text{Kr}$ , is suitable for application into the WGTS. Such a gaseous source of monoenergetic electrons provides information about plasma charge value (from shift of the conversion line energy) and its fluctuation (from broadening of the conversion line). Moreover, the KATRIN energy scale can be calibrated. For these purposes we suggested and developed the source based on deposition of the  $^{83}\text{Rb}$  into the zeolite beads. The sources are described in our presentation: *Sources of monoenergetic electrons from decay of  $^{83\text{m}}\text{Kr}$  for KATRIN, poster at the Int. Conf. On Neutrino Phys. Astrophys., Heidelberg, 4. – 9. June 2018.*

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

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 measured energy of the K-32 electrons from the sources is linearly dependent on the time but its change, a drift, is less than KATRIN limit of 3 ppm/month. In such a way the monitoring concept for the KATRIN was justified. Therefore, the Mainz electron spectrometer was transported to KIT and renovated with our hardware contribution in order to serve as the KATRIN MoS. Due to the strong competition on the ISOLDE ion beam time, the production of the implanted sources was relocated to the mass-separator of the Bonn University. 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 ( $^{83}\text{Rb}$  activity, activity distribution on the source surface, retention of daughter  $^{83\text{m}}\text{Kr}$  in source) before their installations into MoS were developed by us. The measurement showed the retention value of 90%. Using the  $^{83\text{m}}\text{Kr}$  transition energies of 32151.7(5) and 9405.8(3) eV, previously measured in our group, the precise energies of all groups of the  $^{83\text{m}}\text{Kr}$  conversion electrons observed in the decay of the  $^{83\text{m}}\text{Kr}$  can be determined, see: *Properties of  $^{83\text{m}}\text{Kr}$  conversion electrons and their use in the KATRIN experiment, 2018 JINST 13 T02012*. After the MoS was commissioned at the KIT, the measurement of the K-32 electron line energy stability with various sources, substrates ZnO and HOPG, has continued. The K-32 electron energy with HOPG substrate exhibits even slightly better energy stability in comparison with the Pt and the  $^{83\text{m}}\text{Kr}$  retention is close to 100%. Due to this in the next only the HOPG was used for the source productions. The 65 days measurement of the K-32 electron energy stability yielded for two sources a very favourable low drift of  $\sim 0.3$  ppm/month. In such a way the system MoS+electron source for the monitoring of the KATRIN HV become ready for the use. The MoS construction

and experiences gained during the K-32 electrons energy stability measurements were published see: *High-voltage monitoring with a solenoid retarding spectrometer at the KATRIN, 2014 JINST 9 P06022*. 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 substrate on the value and stability of the electron binding energies of atoms was studied and a row of papers were published. The most recent paper is: *Effects of the atomic environment on the electron binding energies in samarium, Jour. Elect. Spec. Rel. Phen. 207(2016)38*. Recently, we have published our knowledge on the properties of the electron sources in the review article: *Various applications of precision low-energy nuclear electron spectrometry in the KATRIN tritium neutrino project, Physic of Particle and Nuclei (2019) V50 No.6 p. 683*.

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

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 paper: *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 radon emanation will be safe for the application into the WGTS. The degree of  $^{83m}\text{Kr}$  release from the source based on zeolite type 5A was measured to be of about 80% when placed in the vacuum. 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, about four foreign institutions are using our zeolite sources in their research, mostly in neutrino mass and dark matter experiments. Moreover, we collaborated with Münster University on the method for the investigation of the noble gas flow in the circulation systems, see: *A novel  $^{83m}\text{Kr}$  tracer method for characterizing xenon gas and cryogenic distillation systems 2014 JINST 9 P10010*.

The generator for injection of the  $^{83m}\text{Kr}$  emanated from zeolite beads into the WGTS was designed according to the KIT Tritium lab (TLK) demands, completed and tested, see the article: *Gaseous  $^{83m}\text{Kr}$  generator for KATRIN, 2018 JINST 13 P04018*. After the test the apparatus was moved to TLK, see the figure 4 where the generator (packed in the second containment), cabinet with generator electronics and yellow container for the transport of the zeolite source are shown.

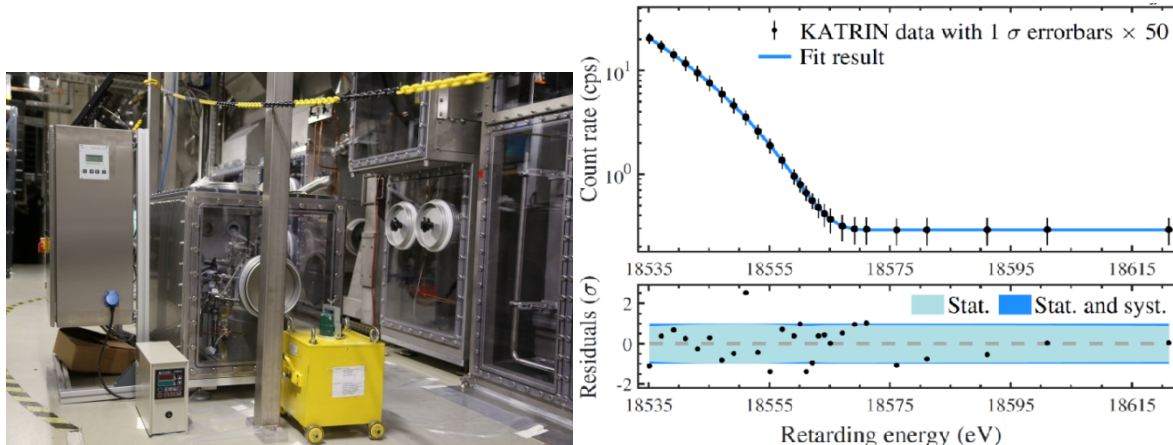


Fig. 4 Generator (packed in the second containment), cabinet with generator electronics and yellow container for the transport of the zeolite source in KIT (left), KATRIN electron spectrum (right).

### KATRIN: test measurement and first limit on the neutrino mass

In 2016 when the significant parts of the KATRIN complex were finished, the “KATRIN all” articles have begun to appear. Since 2017 we have started to participate in the KATRIN measurements runs. In this year the test of the whole electron beam line was accomplished using also the electrons from our zeolite source, see: *First Transmission of electrons and ions through the KATRIN beamline*, (2018) JINST 13 P04020 and *High-resolution spectroscopy of gaseous  $^{83\text{m}}\text{Kr}$  conversion electrons with the KATRIN experiment*, arXiv: 1903.06452v2, 18<sup>th</sup> Mar 2019. In the next article: *Calibration of high voltages at the ppm level by the difference of  $^{83\text{m}}\text{Kr}$  conversion electron lines at the KATRIN experiment*, Eur. Phys.J. C (2018) 78: 368, the calibration of the KATRIN precise high voltage divider by means of nuclear  $^{83\text{m}}\text{Kr}$  electron energy data was accomplished for the first time. On July 11<sup>th</sup>, 2018, the ceremony of launching the tritium  $\beta$ -spectrum measurement took place at KATRIN in KIT. The first scientific KATRIN run - KNM1 (Katrin Neutrino Mass 1) was realized in April-May in 2019. Within this 4-week measurement with the limited amount of tritium in WGTS (22%  $T_2$  of designed value) a new upper limit on neutrino mass of 1.1 eV was obtained being almost by factor of 2 better in comparison with the current value, see: *Improved upper limit on the neutrino mass from a direct kinematic method by KATRIN*, Phys. Rev. Let. 123 221802 (2019). This achievement becomes the objective of the numerous press releases and articles in popular physical and technical journals. The measured tritium  $\beta$ -spectrum is shown in the figure 4 – the error bars are enlarged by factor of 50. The accompanying systematic test with the tritium +  $^{83\text{m}}\text{Kr}$  present in the WGTS has shown that the influence of the plasma charge on deduced neutrino mass could be neglected in this initial stage of the experiment. The 2<sup>nd</sup> KATRIN campaign KNM2 was realized within September-November 2019. For this run a fresh zeolite source was provided by our team. The analysis of these new more precise data strongly indicates that the systematic correction indicated by gaseous  $^{83\text{m}}\text{Kr}$  measurement is unavoidable.

### Miscellaneous

We accomplished the extensive literature search and published two review articles about the direct methods for the neutrino mass determination, see e.g.: *Constraints on the active and sterile neutrino masses from beta ray spectra: past, present and future*, Open Phys. Jour. (2016), 3, 3-44. In 2016, the Ph.D. student M. Slezák, supervised by D. Vénos, defended his doctoral thesis *Monitoring of the energy scale in the KATRIN neutrino experiment*. In 2016 a TRISTAN (TRitium beta decay to search for Sterile Neutrino) group was established in frame of the KATRIN. The group develops multipixel silicon detector. For its tests the vacuum evaporated  $^{83}\text{Rb}$  sources are prepared by our team. Within the period 2015-2019 we have produced 15  $^{83}\text{Rb}$  zeolite sources from which six were delivered to our krypton generator at KATRIN. Further, we organized at the mass-separator of Bonn University the production of the 17 implanted sources for the MoS. Approximately five zeolite sources were provided for the calibrations of the dark matter experiments at the universities in Münster and Zürich.

## Research activity and characterisation of the main scientific results

### Radioanalytical methods

#### Methodological developments

Improvements and novel procedures continued to be developed in all stages of instrumental NAA and PAA (INAA and PAA, respectively), i.e., sample preparation, irradiation, calibration, gamma-ray spectrometry, and separations for radiochemical NAA (RNAA).

For determination of impurities in phosphoric acid by INAA, a novel, simple, and contamination-free procedure for the transformation of phosphoric acid into ammonium phosphate has been developed, which is based on isothermal distillation of ammonia vapours. Thus, the obstacle of banned irradiation of liquid acids in many nuclear reactors has been surmounted. Favourably low detection limits for more than 35 elements have been achieved and the accuracy of the results has been established by analysis of NIST SRM 1515 Apple Leaves (J. Kameník, H. Amsil, J. Kučera, J. Radioanal. Nucl. Chem. 304 (2015) 157–162, 70 % share, NPI workers underlined).

With regard to the decreasing availability of nuclear reactors for NAA worldwide, we tested an alternative neutron source – accelerator driven fast neutron source at the NPI cyclotron U120M – for low level determination of fluorine by INAA. We reported results for fluorine in several biological and environmental reference materials with the new procedure and compared them with those achieved by other methods in terms of limits of detection, accuracy and precision, where available (J. Kučera, M. Štefánik, P. Veselka, J. Radioanal. Nucl. Chem. 322 (2019) 1517–1523, 80 % share).

We have also contributed to modernization of parameters of microtron MT-25, which is used as a source of bremsstrahlung for PAA. The mean accelerated electron current, quality of the beam and irradiation fields, and long-run operation stability and reliability were improved. Moreover, an automated pneumatic transport system for rapid sample transport between the beam position and the detector was installed, which provides extension of the analytical range of PAA in the short time irradiation mode (P. Krist, Z. Horák, J. Mizera et al., J. Radioanal. Nucl. Chem. 304 (2015) 183–188, 50 % share). The improvements were exemplified by devising a new IPAA procedure for the determination of fluorine in environmental samples (I. Krausová, J. Mizera, Z. Řanda, et al., Nucl. Instrum. Methods Phys. Res. B 342 (2015) 82–86, 80 % share).

Our activities in  $k_0$ -standardization in INAA ( $k_0$ -INAA) continued by the use of an HPGe coaxial detector with extended energy range efficiency calibration. We showed that the use of the radionuclide  $^{56}\text{Co}$ , which emits abundant gamma-rays with energies up to 3451.2 keV, for calibration of the full energy peak efficiency,  $\epsilon$ , of a coaxial HPGe detector, in addition to the commonly employed set of activity standards ( $^{133}\text{Ba}$ ,  $^{241}\text{Am}$ ,  $^{152}\text{Eu}$ ,  $^{57}\text{Co}$ ,  $^{137}\text{Cs}$ ,  $^{88}\text{Y}$ ,  $^{65}\text{Zn}$ ), affects significantly the  $\epsilon$  values in the high energy region. This change resulted in substantial improvement of the accuracy of Ca determination by  $k_0$ -INAA via the  $^{49}\text{Ca}$  radionuclide, which emits predominantly the 3084 keV photons, as demonstrated by Ca results in NIST SRMs 1547 Peach Leaves, 1633b constituent elements in coal fly ash, and 2711 Montana II Soil (J. Kučera, M. Kubešová, O. Lebeda, J. Radioanal. Nucl. Chem. 315 (2018) 671–675, 80 % share).

INAA was used for determination of vanadium mass fraction in crystals of incipient ferroelectric strontium titanate and ferroelectric barium titanate. In order to improve vanadium limit of detection, discriminating gamma-ray spectrometry was used by inserting an absorption filter between the samples and an HPGe detector. The use of the absorption lead filter 6-mm thick

yielded improvement of the vanadium limit of detection by a factor of two (J. Kameník, K. Dragounová, J. Kučera et al., J. Radioanal. Nucl. Chem. 311 (2017) 1333–1338, 75 % share). In the field of RNAA, we reviewed our past achievements and reported new radiochemical separation procedures for determination of ultra-low levels of long-lived radionuclides  $^{232}\text{Th}$  and  $^{238}\text{U}$  in highly enriched  $^{82}\text{Se}$  (source) and in Cu, a component of detectors for SuperNEMO experiment aimed at detection of neutrinoless double  $\beta$ -decay. The above radionuclides form a significant part of background radiation, which must be reduced as much as possible to allow detection of the studied phenomenon, and therefore for assessment of radioactive contamination of construction materials used in SuperNEMO and similar deep underground experiments, the ultra-sensitive analytical methods, such as RNAA, are to be applied for the determination of the sources of background (J. Kučera, J. Kameník, P. P. Povinec, J. Radioanal. Nucl. Chem., 311 (2017) 1299–1307, 80 % share, P. P. Povinec, ..., J. Kameník, J. Kučera et al., J. Radioanal. Nucl. Chem., 318 (2018) 677–684, 15 % share). Our experience with atom counting of other long-lived radionuclides using INAA and RNAA, namely  $^{99}\text{Tc}$  and  $^{129}\text{I}$ , was reviewed and the results obtained were compared with those achieved by other methods, where available (J. Kučera, J. Kameník, P. P. Povinec et al. Proc. 5th Int. Conf. on Environmental Radioactivity ENVIRA 2019, 8–13 Sept. 2019, Prague, Czech Republic, pp. 46–49, share 85 %).

#### **Geo- and cosmochemical research**

NAA and PAA, particularly in their instrumental modes (INAA and IPAA, respectively), are indispensable tools in geo- and cosmochemical research. We have 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.

Geochemical characteristics and petrogenesis of phonolites and trachytic rocks from the České Středohoří Volcanic Complex, the Ohře Rift, Bohemian Massif were studied. We presented the first comprehensive dataset on phonolites and trachytic rocks from the Bohemian Massif and discussed origin of the whole subalkaline-alkaline volcanic suite, and modelled the assimilation-fractional crystallization processes. We provided geochemical characterization of the studied sample suite by INAA and IPAA and participated in interpretation of the analytical data (L. Ackerman, ..., Z. Řanda, ..., J. Frána et al., Lithos, 224/225 (2015), 256–271, share 20 %).

Radiolytic alteration due to the presence of uranium was studied in a Cenomanian amber-like fossil resin from Křižany in the North Bohemian Cretaceous uranium ore district. Structural changes observed in the amber involved increase in aromaticity due to dehydroaromatization of aliphatic cyclic hydrocarbons, loss of oxygen functional groups, an increase in the degree of polymerization, crosslinking of C-C bonds, formation of a three-dimensional hydrocarbon network in the bulk organic matrix, and carbonization of the organic matrix around the uraninite infill. We participated in geochemical characterization of the studied samples by INAA, interpretation of results, and preparation and revision of the manuscript (M. Havelcová, V. Machovič, J. Mizera, et al., J. Environ. Radioact. 158-159 (2016) 89–101, share 20%).

The Late Glacial sedimentary sequence of the Stará Jímka paleolake (Bohemian Forest, Czech Republic) was studied. The sequence contains a continuous horizon with the phonolitic Laacher See tephra (LST). This was probably the first finding of LST in the Bohemian Massif and in the Czech Republic. We participated in geochemical characterization of the studied samples by INAA, interpretation of results, and preparation and revision of the manuscript. (V. Procházka, J. Mizera, G. Kletetschka, et al., Int. J. Earth Sci. 108 (2019) 357–378).

Studies of tektites, natural glasses produced from impact on large asteroids, belong to our long-lasting interests. In this field, a study was devoted to formation of moldavites based on chemistry of tertiary sediments in the surroundings of the Ries impact structure. The study provided complete analyses (including elements not reported in literature so far) for a set of sediments from the surroundings of the Ries impact structure. Comparison of their chemical compositions with that of moldavites confirmed dominance of the Miocene Upper Freshwater Molasse in the source material of moldavites. Additional minor components (incombustible residues of organic matter, soils) may have been present in much smaller proportions. We participated in sampling and geochemical characterization of the studied samples by INAA and IPAA, interpretation of the analytical and literature data, and preparation and revision of the manuscript (K. Žák, ..., Z. Řanda, J. Mizera, ..., J. Kameník et al., *Geochim. Cosmochim. Acta* 179 (2016) 287–311, share 35 %).

Further we investigated the behavior of osmium and other siderophile elements during impacts, namely with special insight on the Ries impact structure and central European tektites. Evidence was provided for a complex behavior of Os and other highly siderophile elements (HSE) during a hyper-velocity impact which formed the Ries structure and central European tektites - moldavites. The processes involve evaporative loss of HSE from the overheated tektite melt, mixing of target-derived and impactor-derived HSE vapor phases, and early high-temperature condensation of a part of the mixed vapor phase back to silicate melt. Addition of meteoritic material could be observed. This was found by geochemical characterization of the studied samples by INAA and IPAA and by interpretation of the analytical data (L. Ackerman, ..., J. Mizera, Z. Řanda, *Geochim. Cosmochim. Acta* 210 (2017) 59–70, share 25 %).

Australasian tektites (AAT) represent the largest group of tektites and their strewn field covers one sixth of the Earth's surface. A parent crater for AAT is still unknown. Based on geochemical and isotopic compositions of AAT and their potential source materials, the study has impeached the universally accepted hypothesis of a crater location in Indochina and suggested a new location in deserts of NW China. The new hypothesis altered the current view of formation and transport of impact ejecta. We designed the entire concept of the study, carried out geochemical characterization of the studied samples by INAA and IPAA, interpreted the analytical and literature data, and prepared the manuscript (J. Mizera, Z. Řanda, J. Kameník, *Earth Sci. Reviews* 154 (2016) 123–137, share 100 %).

The  $^{10}\text{Be}$  content in AAT and its geographic controls was discussed in terms of the AAT potential source materials. This is a continuation of argue about interpretation of  $^{10}\text{Be}$  content in AAT and presentation of an alternate interpretation based on an original hypothesis of the origin of AAT from deserts of Northwest China proposed by the author and his team (J. Mizera, *Geology* 47 (2019) 459–459, share 100 %).

In studying irghizites, tektite-like ejecta from the Zhamanshin crater, Kazakhstan, chromium and oxygen isotopes were used to identify the impactor and impact-plume processes for the Zhamanshin astrobleme. The impactor was identified as carbonaceous (CI-like) chondrite. The observed  $^{17}\text{O}$  depletion in irghizites relative to the terrestrial range has been ascribed to partial isotope exchange with atmospheric oxygen following material ejection (T. Magna, ..., J. Mizera, Z. Řanda, *Nature Commun.* 8 (2017) 227, share 20 %).

In addition to tektites, analysis of meteorites belongs to our favourite tasks. Using INAA, we also found new data on the concentrations of 43 major and trace elements in the Slovakian meteorites Uhrovec, Veľké Borové (Nagy-Borove), Rumanová, Košice and in the popular Chelyabinsk meteorite. The results were in good agreement with the mean data for an average ordinary chondrite of the respective class and with the data obtained by the same and/or different methods published earlier (J. Kaizer, J. Kučera, J. Kameník et al., *J. Radioanal. Nucl. Chem.* 311 (2017) 2085–2096, share 40 %).

### Geomycology

Mushrooms are known for their fundamental importance in the biosphere, involving 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 (their sporocarps or fruit-bodies). In contrast to other teams in the world, which mainly analyze the most common edible mushroom species, Jan Borovička is also a renowned mycologist who can find and identify also unusual or even rare mushroom 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 mushrooms), with the exception of Hg and Pb. Therefore, we have been able to identify various effective mushroom accumulators, especially species accumulating Ag, As, Cl, Cu and Zn.

The main task of the NPI CAS in the joint projects with other teams thus represents identification and selection of the most interesting mushrooms species suitable for speciation studies. At the University of Chemistry and Technology (team led by prof. P. Kotrba), the chemical form of accumulated metals (Ag, Cd, Cu, Zn) is studied together with the molecular aspects behind the accumulation of these elements. At the Institute of Microbiology CAS (team led by assoc. prof. J. Jansa), 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. Jan Borovička is also employed at the Institute of Geology CAS, where other useful methods are available, especially ICPSFMS and TIMS. Most of our studies were based on close co-operation with other teams and in some papers, possibilities of INAA and ICP-MS were also compared. At the University of Graz (team led by assoc. prof. W. Goessler), arsenic species are identified in mushrooms samples selected by the NPI CAS team (for details, see below).

In our research papers, we mostly reported results from the joint studies with the abovementioned institutes. In a study where two our Ph.D. students were involved (J. Cejpková, ..., Z. Řanda, I. Synková, J. Borovička, Environ. Pollution 218 (2016) 176–185, share 65 %) we focused on terrace element accumulation in ectomycorrhizae (mutual organs of plants and symbiotic fungi) and we also attempted to quantify the fungal biomass in these organs using qRT-PCR method with specific primers. In a focus on the genus *Cortinarius*, subg. *Phlegmacium*, we published two studies where i) *Cortinarius prodigiosus* was described as new species for science and characterized in terms of trace element composition (J. Borovička et al., Mycological Progress 14 (2015) 29, share 15 %) and ii) systematic position and taxonomy of *Cortinarius coalescens* was clarified and this species was characterized in terms of trace element composition and arsenic speciation (J. Borovička, ..., J. Kameník et al., Mycological Progress 16 (2017) 927–939, share 25 %).

In addition to the studies within the frame of the joint project with the University of Graz, we recognized *Cyanoboletus pulverulentus* as hyperaccumulator of arsenic. Furthermore, high concentrations of dimethylarsinic acid in this fungus may be carcinogenic and this mushrooms should therefore not be further recommended as edible fungus (S. Braeuer, ..., J. Kameník, ..., J. Borovička Food Chemistry 242 (2018) 225–231, share 35 %). A highly interesting and unusual speciation of As was further reported in deer truffles – *Elaphomyces* spp. (S. Braeuer, J. Borovička, W. Goessler, Anal. Bioanal. Chem. 410 (2018) 2283–2290, share 35 %) which are widely consumed by wild boars.

Our long-term interest in Ag hyperaccumulation in *Amanita strobiliformis* resulted in a study where we attempted to identify soil pool from which Ag is accumulated by this fungus. This was conducted by use of Pb isotopic fingerprinting and qRT-PCR with specific primers (J.

Borovička, ..., J. Kameník et al., Sci. Total Environ. 694 (2019) 133679, share 25%). According to the results, the topsoil layer of circa 12 cm depth likely represents the main source of metallic elements accumulated in *A. strobiliformis*.

### Environmental research

INAA of local soil, coal, water, and crops from the village of Awdarda in the North Gondar, Ethiopia, where the residents suffer from various disabilities, was performed in an attempt to elucidate the existing health problems. More than forty elements were determined in the samples analyzed. Comparison of our results with literature values indicates highly elevated contents of terrigenous elements in Awdarda cereals, possibly due to contamination by excavation and indoor combustion of local coal-bearing sediments. Impact was discussed of the elevated aluminium and the rare earth elements levels in crops on the health problems (T. A. Bitewlign, ..., J. Mizera et al., J. Radioanal. Nucl. Chem. 311 (2017) 2047–2059, share 75 %).

Our previous studies concerning the use of RNAA for determination of toxic elements in environmental samples continued by assay of mercury in soils formerly contaminated by different processes from two sites in the Czech Republic. The total mercury (T-Hg) was determined by RNAA, while other species, such as elemental mercury ( $\text{Hg}^0$ ), methylmercury ( $\text{MeHg}^+$ ), phenylmercury ( $\text{PhHg}^+$ ), and gaseous elemental mercury (GEM) were determined by a variety of other methods. The first sampling site was in the surroundings of a former  $\text{PhHgCl}$ -based fungicide processing plant (where the production stopped at the end of the 1980's) next to Příbram (central Bohemia). Highly elevated Hg contents in soil were still observed there, reaching T-Hg values  $>13 \text{ mg kg}^{-1}$ . The second sampling site was an abandoned mining area named Jedová hora Hill near Hořovice (central Bohemia), where cinnabar ( $\text{HgS}$ ) was occasionally mined as by-product of Fe ores hematite and siderite. Although mining activities were stopped there in 1857, very high contents of T-Hg are still found at this site, up to  $144 \text{ mg kg}^{-1}$ . In most cases we found a statistically significant correlation between T-Hg and  $\text{Hg}^0$  values regardless of the pollution source (J. Sysalová, J. Kučera, ..., J. Kameník, Sci. Total. Environ. 584–585 (2017) 1032–1039, share 30 %).

Within a joint development and research project with the Scientific and Technological Research Council of Turkey (TÜBİTAK) we performed two environmental studies using  $k_0$ -INAA. One concerned elemental characterization of lignite from The Afşin-Elbistan lignite deposit, which is used in two nearby located lignite-fired power plants. The main emphasis was to determine the potentially hazardous elements, such as As, Cd, Co, Cr, Mn, Ni, S, Sb, U, but we found in total 39 elements. Our results indicate the need for regular environmental pollution monitoring around the Kışlaköy mine and the Afşin-Elbistan power plants concerning both immisions from the mines, power plants, and waste piles and leakages from the waste piles (M. Kubešová, ..., I. Krausová, J. Kučera, J. Radioanal. Nucl. Chem. 308 (2016) 1055–1062, share 50 %). Second one concerned the use of  $k_0$ -INAA of plant tissues and soils for biomonitoring in urban areas in Istanbul. The aim of this study was to determine the elemental concentrations of plant tissues and soils collected in Istanbul to evaluate the possible use of selected tree species, *Carpinus betulus* L., *Quercus petraea* (Mattuschka) Liebl., *Tilia argentea* Desf. ex DC., as biomonitors. The concentrations of 26 elements were determined. Generally, the element concentrations in samples from urban areas were found to be higher than those of control area. *Tilia argentea* Desf. ex DC. was found to be an effective biomonitor for As, Br, Ca, Cl, Cr, Fe, Hf, K, Sb, Sc, Sr, and Th (A. N. Esen, M. Kubešová, S. Hacıyakupoglu, J. Kučera, J. Radioanal. Nucl. Chem. 309 (2016) 373–382, share 60 %).

Another study dealt with the possible contamination of the river Mara from a spill from a tailing dam and leachate at the North Mara gold mine (NMGM) in Tanzania. Using INAA and EDXRF we analysed twenty samples of lungfish (*Protopterus aethiopicus*) and catfish (*Clarias mossambicus*) from the river Mara collected from two sites downstream and upstream from



the seepage. The sampling sites were 70 km apart. Results for 16 elements were obtained in both fish species using both analytical methods, namely for the following elements Na, Cl, K, Ca, Sc, Cr, Mn, Fe, Co, Ni, Cu, Zn, Se, Br, Rb and Sr. Significantly higher concentrations ( $p \leq 0.05$ ) of Cr, Ni, Cu, and Se in one of the species taken downstream than in those taken upstream indicated contamination of the river Mara caused by the mining activities. Lungfish appeared to be a better indicator of elemental contamination than catfish (N. K. Mohamed, A. V. R. Ntarisa, I. N. Makundi, J. Kučera, J. Radioanal. Nucl. Chem. 309 (2016) 421–427, share 40 %).

### Agriculture and nutrition

In continuation of our co-operation with researchers of the Nuclear and Technological Institute, Sacavém, Technical University of Lisbon, and National Institute of Biological Resources, Elvas, Portugal, we focused on the ability of bread and durum wheat to accumulate selenium (Se) via a soil-addition procedure at sowing time. Total Se in mature-grain samples was determined by neutron activation analysis (cyclic and RNAA). Results show that Se-supplementation at the top rate ( $100 \text{ g Se ha}^{-1}$ ) 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 (C. Galinha, ..., M. Fikrlé, J. Kučera et al., J. Radioanal. Nucl. Chem. 304 (2015) 139–143, share 25 %).

An IPAA method of non-destructive determination of nitrogen was developed and optimized. The method utilizes measurement of the annihilation gamma line at 511 keV from the short-lived photoactivation product  $^{13}\text{N}$ , corrected for interference contributions from other positron emitting nuclides. In cooperation with the University of Chemistry and Technology, Prague, the method was applied for nitrogen assay in malting barleys and compared with the standard Dumas method (I. Krausová, J. Mizera, P. Dostálek, Z. Řanda, J. Inst. Brew. 124 (2018) 4–8, share 80%). In cooperation with the Czech University of Life Sciences in Prague, the method was applied for nitrogen assay in winter wheat from various crops grown organically or conventionally. Results compared well to those obtained by the Kjeldahl method. A positive impact of conventional agriculture on higher crude protein content in grain was found (M. Mádlíková, I. Krausová, J. Mizera, et al., J. Radioanal. Nucl. Chem. 317 (2018) 479–486, share 50 %).

### Cultural heritage

Activities of a Danish-Czech consortium aimed at elucidation of the possible reasons of death of the famous astronomer Tycho Brahe continued. After exclusion of a murder scenario due to mercury poisoning in our previous work, we studied other elements in Brahe's remains, namely in hair and bone samples. The samples were analysed by several analytical techniques, among them by INAA and RNAA by our team. In segmented hair samples, concentrations of Fe, As, Ag and Au at the tips exceeded values for the contemporary population; however, they decreased towards the hair bulbs, similarly to Hg, indicating that recent exposure was discontinued ~2 months prior to Brahe's death. Possible sources of the elements Fe, As, Ag and Au could be alchemical activities or medicines, which he could have either manufactured or self-administered. On the other hand, the concentrations of these elements were relatively low, which makes it unlikely that the exposure could have caused any acute health problems. Analyses of bones revealed signs of long-term exposure to Au, while many other elements were within expected ranges. Histopathological examination of bone sections yielded no signs of severe bone metabolic disorders. Thus, the study did not provide any conclusive evidence about the reason of Brahe's death, which yet remains unexplained (J. Kučera, K. L. Rasmussen, J. Kameník et al., Archaeometry 59 (2017) 918–933, share 30 %).

The determination of long-lived radionuclides, namely  $^{41}\text{K}$ ,  $^{232}\text{Th}$  and  $^{238}\text{U}$ , in construction materials for archaeometric purposes is needed for thermoluminescence (TL) dating of various materials, because their age can be assessed only with an appropriate evaluation of the natural

annual dose. In this work, the determination of the above radionuclides in brick samples was performed by XRF, gamma-ray spectrometry, and by NAA. Results obtained by the last technique by our team were considered as “reference values” (H. Bártová, J. Kučera, L. Musílek et al., Radiat. Physics Chemistry 140 (2017) 161–166 (share 25 %)).

Total nitrogen content was determined by IPAA to reveal the matrix composition of the bracelet from the late Bronze Age found in the site (hill fort) Soví Skály in Karlovy Vary – Drahovice (Drahovice cadastre, Czech Republic) from the collections of the Museum Karlovy Vary, Czech Republic. Its exact age was determined by radiocarbon dating (I. Krausová, J. Tajer, I. Světlík, D. Chvátíl, Nucl. Instrum. Meth. in Phys. Res. B 448 (2019) 26–30, share 60 %).

Analysis of historical artefacts from Egypt is extremely specific, because only samples from old excavations deposited in European museums are usually available. Therefore, an assemblage of ancient Egyptian metalwork was studied using a wide range of available archaeometallurgical methods, such as mass spectrometry for isotopic analysis, and INAA and XRF analyses for elemental characterization. Rather surprising findings are discussed (J. Kmošek, M. Odler, M. Fikrle, Y. V. Kochergina, Archaeological Science 96 (2018) 191–207, share 20 %).

In cooperation with various Czech archaeological institutions, both INAA and XRF, but predominantly the latter technique, were used for elemental characterization of metal historical artefacts, especially large sets of coins connected to the Czech state (M. Fikrle, Prague, National Museum, 2018, pp. 63 – 84, share 100 %), but also Roman coins (M. Fikrle and J. Militký, in Coins of the Roman Republic. The National Museum, Prague, 2018, pp. 30–35, share 50 %), Greek coins - represented by the ancient coins of Bactria (M. Fikrle and J. Militký, in Sylloge Nummorum Graecorum. Czech Republic. Volume I. The National Museum, Prague. Part 10. Baktria and India (Early Baktria, Graeco-Baktrian and Indo-Greek Coins, Imitations, Indo-Scythians)., Prague, National Museum, 2019, pp. 14–21 share 50 %) and a large set of Hungarian ducats.

#### Material research and reference materials

Using INAA with both short- and long-time irradiations, we determined up to 38 elements in polymers used in cable safety systems for new nuclear power plants (NPP) generation and for the Large Hadron Collider (LHC). For LHC cables, halogen-free composition is required. The INAA assay of halogens can be accomplished in a shorter time than achievable by alternative analytical methods. (J. Kučera, M. Cabalka, J. Ferencei et al., J. Radioanal. Nucl. Chem. 309 (2016) 1341–1348, share 65 %).

Samples of graphite from a RBMK-1500 reactor at the Ignalina Nuclear Power Plant, Lithuania from different construction elements (stack, sleeve, and bushing) were analyzed by INAA and other methods. The experimentally obtained RBMK-1500 graphite impurity values in different graphite constructions were compared with other measurements and new limits of the possible maximal concentrations of nuclear RBMK graphite impurity concentrations were obtained (R. Plukienė, ..., J. Kučera et al., Radiocarbon 60 (2018) 1861–1870, share 15 %).

In cooperation with several Czech institutions and one from Australia, we used our experience with neutron irradiation of various samples to design and test an easily scalable method for rapid irradiation of nanodiamonds by  $\alpha$  particles ( $^4\text{He}^{2+}$ ) and  $^7\text{Li}^+$  ions formed homogeneously in situ by the  $^{10}_5\text{B} + ^1_0\text{n} = ^4_2\text{He} + ^7_3\text{Li} + \gamma$  nuclear reaction. We produced 70 g of fluorescent nanodiamonds in an approximately 30-minute irradiation session, as well as fluorescent silicon carbide nanoparticles. Our method thus increased current preparative yields by a factor of  $10^2$ – $10^3$ . We envision that our technique will increase the production of ion-irradiated nanoparticles, facilitating their use in various applications (J. Havlík, ..., J. Štursa, J. Kučera et al., Nature Commun. (2018) 9:4467, share 20 %).

In cooperation with the King Abdullah University of Science and Technology, Saudi Arabia (KAUST), we assayed six carbon materials with potential application in research and development of battery electrodes for mass fractions of more than 40 elements by INAA and ion-beam methods. The results indicated the methods potential for characterization of materials with very low content of impurities (carbon black) as well as those with relatively high content of certain transition metals (e.g., single walled carbon nanotubes, SWCNT). Our results are being used for benchmarking of analytical procedures, namely ICP-OES, currently under development at KAUST (J. Kameník, ..., J. Kučera, V. Havránek, J. Radioanal. Nucl. Chem. 318 (2018) 2463–2472, share 60 %).

The favourable features of NAA and its property of being the primary measurement method predetermine this method for certification of element contents in reference materials of chemical composition. Therefore, in cooperation with the Australian Nuclear Science and Technology Organisation, the U.S. National Institute of Standards and Technology, the Nuclear Energy Center for Agriculture, University of São Paulo and the National Research Council Canada (NRCC), we used INAA with both relative and  $k_0$ -standardization to determine element mass fractions in single-wall carbon nanotube certified reference material (CRM) SWCNT-1. Results obtained were in agreement with NRCC certified values for Fe, Co, Ni, and Mo and provided mass fraction values for 13 additional elements, namely, Na, Mg, Al, K, Ca, Ti, V, Cr, Mn, Br, La, W, and Au (J. Kučera, ..., M. Kubešová et al., Anal. Chem. 87 (2015) 3699–3705, share 30 %).

Similarly, favourable properties of IPAA were employed for the non-destructive assay of oxygen in titanium in certification campaigns of ERM®-EB090a and ERM®-EB090b prepared at the EC JRC Geel (The certification of the mass fractions of C, H, N and O in the certified reference materials ERM®-EB090a and ERM®-EB090b: under preparation).

Iodine homogeneity in NIST SRM SRM 1548a Typical Diet was improved by cryogenic grinding as proved by analyses carried out by INAA and RNAA (J. Kučera, J. Kameník, Accred. Qual. Assurance 20 (2015) 189–194).

We also regularly (each year) participated in interlaboratory comparisons organized by the International Atomic Energy Agency (IAEA), Vienna aimed at the performance evaluation of elemental characterization of botanical and environmental samples for laboratories using mostly nuclear analytical techniques. Our team has always been ranked among the top performing laboratories.

### **Radionuclides in the environment**

In collaboration with University of Hawaii, an autonomous monitor of submarine groundwater discharges was developed and deployed on the sea. The device was based on a scintillation gamma ray spectrometer that was able to record changes of short-lived daughter products of  $^{222}\text{Rn}$ . The device was equipped with an embedded PC and a battery pack charged by solar panels placed on buoy top. The work included development of automatic routines for evaluation of recorded gamma ray spectra for quantification of long-term trends of discharges (H. Dulai, J. Kameník et al., J. Radioanal. Nucl. Chem. 307 (2016) 1865–1870, 40% share).

In cooperation with the National Radiation Protection Institute, the Nuclear Power Plant (NPP) Temelín and the NPP Dukovany, determination of  $^{14}\text{C}$  was employed to measure the radionuclide in samples of liquid discharges from NPP, because no such data are reported in the literature. For this purpose, a novel methodology has been developed (I. Světlík, ..., T. Kořínková, P. Šimek, et al., J. Environ. Radioact., 177 (2017) 256–260 share 80%; M. Fejgl, I. Světlík et al., J. Nucl. Radioanal. Chem., 318 (2018) 2263–2271, share 30 %).

Elevated levels of organically bound tritium in the vicinity of Mohelno reservoir, which receives outlet cooling waters from the Dukovany NPP, were determined and reviewed, because no such measurements were reported in the past (P. Šimek, T. Kořínková, I. Světlík, ..., L. Tomášková et al., J. Env. Radioact., 166 (2017) 83–90, share 75%, T. Kořínková, I. Světlík, ..., P. Šimek, et al., J. Radioanal. Nucl. Chem., 307(2016) 2295–2299, share 85%).

Other studies on measurement of radionuclides in the environment can also be mentioned (P.P. Povinec, I. Světlík, ....., J. Kučera et al., J. Radioanal. Nucl. Chem. 307 (2015) 2295–2299, share 15%; P. P. Povinec, ..., I. Světlík et al., Radiocarbon 57 (2015) 355–362, share 15%).

### **Radiocarbon dating in archaeological research**

Old cave paintings made by charcoal were recently found in the Kateřinská cave in the Moravian karst. The carbon particles were sampled from the cave walls in such a way that the paintings were not significantly damaged. After the necessary treatment the sampled carbon was subjected to radiocarbon dating using accelerator mass spectrometry in cooperation with the Institute for Nuclear Research of the Hungarian Academy of Sciences. The age of the paintings turned out to be 4450–4230 years BP, which means that the paintings are the oldest ones found in the territory of the Czech Republic (P. Zajíček, M. Golec, I. Světlík, Vesmír 98 (2019) 588–591 (in Czech), share 45 %; M. Golec,... I. Světlík, K. Pachnerová Brabcová, Z. Ovšonková, Radiocarbon, in press, share 60%).

Accelerator Mass Spectrometry allows very accurate measurements of  $^{14}\text{C}$ . Due to fluctuations of the radiocarbon calibration curve, the resulting calibrated time intervals vary from decades up to centuries. We prepared a curve of time-resolution for the radiocarbon dating method. We found time intervals with substantially better time resolution compared to the surrounding parts of the calibration curve including several intervals providing resolution below 50 years for the last 3 ka (I. Světlík, ..., K. Pachnerová Brabcová, V. Brychová, ..., P. Šimek, Radiocarbon 61 (2019) 1729-1740, share 55 %).

The dating of samples originating from the time interval 1650 – 1950 AD is difficult, due to the environmental  $^{14}\text{C}$  activity oscillations during this period, which results several possible intervals of the sample age. On the basis of radiocarbon dating in combination with archaeological and anthropological context, it could be concluded that the found skeletal remains were most likely of soldiers who died in the provisional military hospital as a result of injury or infection after the Battle of Austerlitz in 1805. An alternative hypothesis, that they are the remains of soldiers who died in the Battle of Hradec Králové in 1866, was excluded by radiocarbon dating (K. Vymazalová, ....., I. Světlík I, K. Pachnerová Brabcová, V. Brychová. Stud. Geoph. et Geodaetica (2020) 64:143-152, share 45%).

Other archaeological studies using radiocarbon dating method were published in Czech journals, but they are recorded in WoS (M. Chytráček, ..., I. Světlík, Památky Archeologické 110 (2019) 59–172; M. Dobeš,..., I. Světlík, Archeologické Rozhledy 70 (2018) 507–525, share 15%; Bravermanová, ..., I. Světlík, Archeologické Rozhledy 70 (2018) 260–293, share 15%).

### **Radiocarbon dating using bomb peak**

Radiocarbon dating of skeletal remains in routine forensic medical practice using the  $^{14}\text{C}$  bomb peak has been improved. In order to suppress the ambiguity of the  $^{14}\text{C}$  bomb peak, we proposed using a combination of  $^{14}\text{C}$  activities in tissues with shorter and longer turnover time and proposed for correct interpretation (P. Handlos, I. Světlík, ..., V. Brychová, N. Megisová et al., Radiocarbon 60 (2018)1017–1028, share 85 %).

### **Radiocarbon analysis and dating in geology**

Using petrographic, geochemical and dating methods using several isotopes we provided evidence that the carbonate cave wall deposits in the Chlupáčova sluj cave represent the oldest calcareous tufa in the Bohemian Karst having precipitated between 620-120 ka. We also reconstructed the evolution of the cave in terms of geology starting from an early hypogene stage to a shallow subsurface cave influenced by descending meteoric waters. This general genetic model can serve as a paradigm to explain the evolution of other caves not only in the Bohemian Karst (V. Suchý, ..., I. Světlík et al., Sediment. Geol. 385 (2019) 110–125, share 65 %).

In another study, Palaeo-thermal and coalification history of Permo-Carboniferous sedimentary basins of Central and Western Bohemia, Czech Republic were studied using Apatite Fission Track Analysis and other methods (V. Suchý et al., Bull. Geosci. 94(2019) 201-219, share 70 %).

### **RAMSES project**

The project application was elaborated and after its approval and receiving the award, tenders were organized for the construction of new premises and of a new accelerator. Introductory experiments on sample preparation were performed using the NPI existing facilities. Model experiments were also performed on sample sputtering with the use of an ion source at the linear accelerator Tandetron of NPI.

## Research activity and characterisation of the main scientific results

In the past period, two research infrastructure projects have substantially influenced the team: CANAM and SPIRAL2-CZ.

While we continued our research activities, thanks to this support, we were able to number of developments in FNG (Fast Neutron Generators), we strengthened the collaboration with other NPI departments (Department of radiopharmaceuticals and department of Accelerators), we managed to connect the INFN LNS and GANIL/SPIRAL2 collaborations in the nuclear astrophysics and entered the newly commissioned SPIRAL2/NFS laboratory with the first prepared experiment.

The local technical developments in NPI:

- design and construction of a new neutron collimator (in a close collaboration with the cyclotron group)
- experimental setup and new state-of-the-art on-line neutron detection and acquisition systems
- new reaction chamber dedicated for (neutron, charged particle) reaction
- four HPGe detector system for (neutron, gamma) reactions
- high-power neutron generator based on Be on TR-24 cyclotron is in construction
- buncher for extended TOF measurements using neutron beams is in construction
- Be and Li generator's neutron fields were characterized in detail and are used for high-quality cross-section measurements. (measurement and integral validation of nuclear data, fast neutron activation analysis).

Hereby we present several (three) results per year, that may be not the most cited or impacted publications, but they best characterize the work of the team.

*Characteristic results per year:*

### 2015

#### Improvement of the high-accuracy $^{17}\text{O}(\text{p},\alpha)^{14}\text{N}$ reaction-rate measurement via the Trojan Horse method for application to $^{17}\text{O}$ nucleosynthesis

The  $^{17}\text{O}(\text{p},\alpha)^{14}\text{N}$  and  $^{17}\text{O}(\text{p},\gamma)^{18}\text{F}$  reactions are of paramount importance for the nucleosynthesis in a number of stellar sites, including red giants (RGs), asymptotic giant branch (AGB) stars, massive stars, and classical novae. In particular, they govern the destruction of  $^{17}\text{O}$  and the formation of the short-lived radioisotope  $^{18}\text{F}$ , which is of special interest for  $\gamma$ -ray astronomy. At temperatures typical of the above-mentioned astrophysical scenario,  $T=0.01\text{--}0.1$  GK for RG, AGB, and massive stars and  $T=0.1\text{--}0.4$  GK for a classical nova explosion, the  $^{17}\text{O}(\text{p},\alpha)^{14}\text{N}$  reaction cross section is dominated by two resonances: one at about  $E_{\text{cmR}}=65$  keV above the  $^{18}\text{F}$  proton threshold energy, corresponding to the  $EX=5.673$  MeV level in  $^{18}\text{F}$ , and another one at  $E_{\text{cmR}}=183$  keV ( $EX=5.786$  MeV). We report on the indirect study of the  $^{17}\text{O}(\text{p},\alpha)^{14}\text{N}$  reaction via the Trojan Horse method by applying the approach recently developed for extracting the strength of narrow resonance at ultralow energies. The mean value of the strengths obtained in the two measurements was calculated and compared with the direct data available in literature. This value was used as input parameter for reaction-rate determination and its comparison with the result of the direct measurement is also discussed in the light of the electron screening effect.

Our team members worked on the experiment during planning, preparation and measurement stages and also added to formulation of the results (Phys. Rev. C 91 (2015) 065803).

### **Accurate measurement of the $^{23}\text{Na(d,p)}^{24}\text{Na}$ cross section in the 1.7–20 MeV energy range**

The  $^{23}\text{Na(d,p)}^{24}\text{Na}$  cross sections were measured in two complementary experiments using a cyclotron and a variant low-energy energy LINAC, effectively covering the 1.7–19.8 MeV energy range. The present results allow one to use the  $^{23}\text{Na(d,p)}^{24}\text{Na}$  process as a standard monitoring cross section in future measurements of deuteron reactions.

The measurement was done in cooperation with SOREQ, Izrael. Our team has prepared the experimental setup and conducted the experiment together with partners. The analysis was done by partner team, our team also contributed during the interpretation and formulation of results (Nucl. Instrum. Methods Phys. Res. B362 (2015) 29).

### **Nuclear structure studies of $^{24}\text{F}$**

The structure of the  $^{24}\text{F}$  nucleus has been studied at GANIL using the  $\beta$  decay of  $^{24}\text{O}$  and the in-beam  $\gamma$ -ray spectroscopy from the fragmentation of  $^{27,28}\text{Na}$ ,  $^{25,26}\text{Ne}$  and  $^{29,30}\text{Mg}$  nuclei. Combining these complementary experimental techniques, the level scheme of  $^{24}\text{F}$  has been constructed up to 3.6 MeV by means of particle- $\gamma$  and particle- $\gamma\gamma$  coincidence relations. Experimental results are compared to shell-model calculations using the standard USDA and USDB interactions as well as ab initio valence-space Hamiltonians calculated from the in-medium similarity renormalization group based on chiral two- and three-nucleon forces. Both methods reproduce the measured level spacings well, and this close agreement allows unidentified spins and parities to be consistently assigned.

This experimental work represents the continuation of the previous campaign of measurements of exotic nuclei with the GANIL team, where a team member was on postdoc. The contribution was in experiment preparation and the measurement itself plus contribution during the formulation of results (Phys. Rev. C 92 (2015) 014327).

## **2016**

### **Au, Bi, Co and Nb cross-section measured by quasimonoenergetic neutrons from $p + ^7\text{Li}$ reaction in the energy range of 18–36 MeV**

Accelerator Driven Systems and fusion are two possible means of energy production in future. Both systems operate with a substantially different neutron spectrum than the well-known neutron spectrum from modern reactors. Activation foils are one of the possibilities how to determine and monitor the energy distribution and spatial flux of such neutron spectrum. Such methodology requires a good knowledge of the neutron cross-sections in the energy range above the standard 20 MeV limit of the today's reactor physics. The measurements of the neutron cross-sections are a complex task, especially in the energy range above 20 MeV, where there are no known monoenergetic neutron sources. In recent years, NPI has been working on a program for the measuring and analysis of neutron activation cross-sections above 20MeV for reactions which were selected for these purposes at accelerator driven facilities such as the International Fusion Material Irradiation Facility (IFMIF). The activation cross sections were obtained for  $^{197}\text{Au}(n,2-4n)$ ,  $^{209}\text{Bi}(n,3-5n)$ , and  $^{59}\text{Co}(n,x)$ ,  $^{93}\text{Nb}(n,x)$  reactions. In respect to our previously published cross-sections, a better accuracy was obtained mainly due to new experimental data on the neutron spectra measured by the Time-Of-Flight method, the measurement of the  $^7\text{Be}$  production in the lithium target, and the revision of the gamma intensities used in the analysis. The measured data were compared with the EAF-2010 and IRDFF cross-section data libraries. Several useful conclusions for future versions of these libraries can be extracted from these comparisons.

This experiment was completely the result of the team. It was one of the first experiments, where the new generation of experimentalists in the group took the responsibility (Nuclear Physics A 953 (2016) 139–157).

### **An above-barrier narrow resonance in $^{15}\text{F}$**

Nuclear properties on drip line play important role in BBN and rp-processes. The radioactive beam with a thick target – allowed to study resonances in  $^{15}\text{F}$  in  $^{14}\text{O}(p,p)$  reaction. Spin 1/2 was determined for the very narrow resonance (36 keV) observed at high energy (4.8 MeV). The structure of this narrow above-barrier state in a nucleus located two neutrons beyond the proton drip line was investigated using the Gamow Shell Model in the coupled channel representation with a  $^{12}\text{C}$  core and three valence protons. It is found that it is an almost pure wave function of two quasi-bound protons in the  $2s\ 1/2$  shell. Analysis shows that  $1p$  decay is suppressed and two-proton emission takes place.

The team has contributed in experiment preparation, experiment supervision and in work on formulation of the results. The follow-up of this experiment was conducted later in 2019, where the spokesperson was from our team (Physics Letters. B 758 (2016) 26-31).

### **Deuteron-induced reactions on Ni isotopes up to 60 MeV**

Deuteron – being the loosely bound state of proton and neutron – has a complex behaviour in nuclear reactions. Partially, it breaks-up and proton and neutron interact with the target independently. The correct description of these reactions with construction materials is important for the development of future energy generation technologies. One of the important materials is nickel, used in alloys and for coating of metallic surfaces. Experimental measurement was on U-120M cyclotron in NPI, on CANAM research infrastructure. Deuteron beam irradiated Ni foils, that were analysed by gamma spectroscopy methods. Analysis was done with a combination of several nuclear reaction models, from direct reactions to statistical models. Production of  $^{55,56,57,58,58m,60}\text{Co}$ ,  $^{57,65}\text{Ni}$  and  $^{60,61,64}\text{Cu}$  isotopes was observed and described, production of  $^{65}\text{Ni}$  and  $^{58m}\text{Co}$  was measured for the first time. Experimental measurements were compared with libraries EAF and TENDL and it shows the importance of the proper treatment of the reactions and inclusion of direct processes. The results will help to develop more precise and correct global libraries of the reaction cross sections.

The experimental part and data analysis were conducted by the team in NPI. The theoretical interpretation was done by colleagues from IFIN-HH, Bucharest. We have collaborated on formulations of results (Phys. Rev. C 94 (2016) 014606).

## **2017**

### **New improved indirect measurement of the $^{19}\text{F}(p,\alpha)^{16}\text{O}$ reaction at energies of astrophysical relevance**

Fluorine abundance determination is of great importance in stellar physics to understand s-elements production and mixing processes in asymptotic giant branch (AGB) stars. Up to now, theoretical models overproduce F abundances in AGB stars with respect to the observed values. In particular, the  $^{19}\text{F}(p,\alpha)^{16}\text{O}$  reaction is the main destruction channel of fluorine at the bottom of the convective envelope in AGB stars, an H-rich environment where it can experience temperatures high enough. In this measurement – performed by Trojan Horse Method (THM) – characteristics of (mainly) three lowest resonances were determined and analysed by R-matrix method. The thorough analysis revealed discrepancies between 10-30% in reaction rates for relevant temperatures.

Team members participated on preparation of the experiment, measurement, on-line analysis. They also contributed to formulation of results (The Astrophysical Journal, 845 (1) (2017)).

### **Assessing the near threshold cross section of the $^{17}\text{O}(n,\alpha)^{14}\text{C}$ reaction by means of the Trojan horse method**

The study of the  $^{17}\text{O}(n,\alpha)^{14}\text{C}$  reaction has been performed by means of the Trojan horse method (THM) applied to the quasifree  $^2\text{H}(^{17}\text{O},\alpha)^{14}\text{C}^1\text{H}$  reaction induced at a beam energy of 43.5 MeV. The THM allowed us to study the 8121-keV  $^{18}\text{O}$  resonant level, for which the



previous THM investigation pointed out the ability of the method to overcome the centrifugal barrier suppression effects in the entrance channel. Here, in view of the developments of the method for resonant reactions, the detailed analysis of the performed experiment will be discussed, focusing on the extraction of the 8121-keV resonance strength for which no information is present in scientific literature. Moreover, the experimental results clearly show the excitation of the subthreshold level centered at -6 keV in the center-of-mass system, which is fundamental to determine the  $^{17}\text{O}(n,\alpha)^{14}\text{C}$  reaction rate of astrophysical interest. Finally, a new recommended reaction rate is presented for future astrophysical application. The team participated on preparation of the experiment, running the experiment and the on-line analysis. Contributed to the formulation of the results (Phys. Rev. C 95 (2017) 025807).

#### **Neutron spectrum determination of d(20)+Be source reaction by the dosimetry foils method**

The experiments for neutron field investigation from the deuteron bombardment of thick beryllium target at 20 MeV were performed at the NPI. For the neutron spectrum measurement of the d(20)+Be source reaction, the dosimetry foils activation method was utilized. Obtained high-flux white neutron field from the d(20)+Be source is useful for the intensive irradiation experiments and cross-section data validation.

This is the work of the team in NPI. The team has introduced the high-quality methods for characterization of neutron spectra (Radiation Physics and Chemistry, 140 (2017) 466-470).

### **2018**

#### **Consistent account of deuteron-induced reactions on $^{nat}\text{Cr}$ up to 60 MeV**

Reaction databases used in industry and applied research are based mainly on equilibrium and pre-equilibrium processes calculations. Experimental discrepancies for Cr isotopes observed in NPI in CANAM accelerator centre were described by direct processes as break-up and stripping. It was shown that these processes play an important role for all energies and reactions of deuterons with nuclei around energies of Coulomb barrier are to a large extent driven by direct processes.

The experimental part and data analysis were conducted by the team in NPI. The theoretical interpretation was done by colleagues from IFIN-HH, Bucharest. We have collaborated on formulations of results (Phys. Rev. C 98 (2018) 034606).

#### **The intensities of $\gamma$ -rays from the decay of $^{196\text{m}2}\text{Au}$**

Due to their purity, gold foils are used as monitoring standard for neutrons. Gold foils were irradiated in NPI CAS. Isomers of radioactive isotope  $^{196}\text{Au}$  were produced and measured. Intensities of gamma transitions were measured with a larger accuracy and uncertainties were reduced (factor of several). This potentially means a reduction of uncertainties for future applications and measurements with neutrons.

The uncertainties and contradictions in data were identified by the team during previous measurements and the dedicated experiment was performed by the team in NPI (Applied Radiation and Isotopes, 141 (2018) 5-9).

#### **Investigation of the elastic and inelastic scattering of $^3\text{He}$ from $^9\text{Be}$ in the energy range 30–60 MeV**

Nucleus of  $^9\text{Be}$  is an example of a so-called Borromean system, where the nucleus is formed from 3 components (2x alpha and one neutron). In NPI, centre of accelerators CANAM, we have measured the cross-sections for the elastic and inelastic scattering populating excited states in  $^9\text{Be}$  using  $^3\text{He}$  beams. The experimental results were analysed using the Woods–Saxon optical model, double-folding potentials and the coupled-channel method. The analysis shows that the excited state (5/2-) of  $^9\text{Be}$  is strongly deformed ( $\beta=0.8$ ).

Our team prepared and conducted the experiment NPI with our JINR Dubna colleagues. Dubna team has worked on interpretation of the results. Our team contributed also to formulation of the results (International Journal of Modern Physics E, 27 (10) (2018) 1850089).

**2019**

**Cross-section measurement of the cosmologically relevant  ${}^7\text{Be}(n, \alpha){}^4\text{He}$  reaction over a broad energy range in a single experiment**

Studying interactions of radioactive ions with neutrons is particularly demanding. The case of the  ${}^7\text{Be}$  destruction induced by the  $(n, \alpha)$  reaction is investigated at the energies typical of the primordial nucleosynthesis by means of the Trojan Horse Method applied to the  ${}^2\text{H}({}^7\text{Be}, \alpha, \alpha)p$  quasi-free reaction. The  ${}^7\text{Be}(n, \alpha){}^4\text{He}$  cross-section has been measured down to cosmological energies. The deduced reaction rate has the impact on big bang nucleosynthesis and on the lithium problem.

The team has contributed to the preparation and running of the experiment and to the formulation of the results (Astrophysical Journal 879 (2019) 23).

**Neutron field study of  $p(24) + \text{Be}$  source reaction using the multi-foil activation technique**

The  $p(24) + \text{Be}$  neutron producing reaction was investigated at the NPI using the 24 MeV proton beam on thick beryllium target. Neutron field in close target-to-sample distance was determined employing the activation foils method; set of ten activation foils (Al, Au, Fe, Ni, Y, Ti, In, Co, Nb, Lu) was utilized. Neutron spectrum reconstruction from reaction rates obtained by means of gamma-ray spectroscopy was performed using the modified version of SAND-II unfolding code and relevant activation cross-sections from the EAF-2010 nuclear database. Determined neutron energy spectra were validated against the Monte Carlo MCNPX predictions. Developed  $p(24) + \text{Be}$  neutron field up to 22 MeV represents a useful tool for validation of cross-sections in energy range relevant to fusion neutrons ( $\geq 12$  MeV), intensive irradiation experiments, and radiation hardness study of materials.

This work was done by team in NPI. This is a continuation of application of high-quality neutron field determination (Fusion Engineering and Design, 146 (2019) 2053-2056).

**The determination of the astrophysical S-factor of the direct  ${}^{18}\text{O}(p, \gamma){}^{19}\text{F}$  capture by the ANC method**

The depletion of  ${}^{18}\text{O}$  via the  $(p, \gamma)$  capture competes with the  $(p, \alpha)$  capture during the CNO cycles in AGB stars. While the  $(p, \alpha)$  capture is dominant, the  $(p, \gamma)$  can play an important role in mixing stages of the AGB star evolution. We determined the astrophysical S-factor of the direct part of the  ${}^{18}\text{O}(p, \gamma){}^{19}\text{F}$  capture by the indirect method ANC and the direct contribution to the  ${}^{18}\text{O}(p, \gamma){}^{19}\text{F}$  capture process and it was compared with the older mutually different results.

This experimental work was done in NPI by the team, including analysis and interpretation of data and formulation of results with the important contribution to experimental part from INFN LNS and T A&MU (European Physical Journal A 55, 114 (2019) 12801-8).

Moreover, our team has started a novel, multidisciplinary research in material damage connected with irradiation. The methods and knowledge base used require efforts and competences of different teams:

*Verification of the theory of primary radiation damage by comparison with experimental data*

Understanding of radiation damage in a solid is important for development of advanced material technologies, namely, for space application, electron microscopy, semiconductor processing, fission and nuclear fusion. Many properties of materials including mechanical

properties are governed by the presence and behavior of lattice defects. Hence, the study of the radiation-induced defects is an important task combining two fields: radiation physics and solid state physics. The paper presents new knowledge on primary defect formation in the main materials for advanced fission and nuclear fusion reactors, bcc tungsten (W) and bcc iron (Fe). The objective of this work is to compare the new experimental data of neutron- and proton-induced defects in W and Fe using well-established method of positron-annihilation lifetime-spectroscopy (PALS) in combination with the literature data with models of radiation damage. It is shown that experimental data for neutron- and proton-irradiated Fe are better described by arc-dpa model than NRT-dpa model. Whereas experimental data for neutron- and proton-irradiated W are between the NRT-dpa and arc-dpa predictions. The obtained results shed new light on the formation of the primary radiation defects in materials and indicate the need for further development of the theory of radiation damage in a solid (O. V. Ogorodnikova, M. Majerle, V. V. Gann, J. Cízek, P. Hruska, S. Simakov, M. Stefanik, V. Zach, Journal of Nuclear Materials 525 (2019) 22-31).

Our team members have participated in other highly impacted publications. We did not present them as the typical work of the team, as the topic or/and the collaboration did not quite represent the team program. Nevertheless, the contribution in the form of the introduction of the data acquisition system that was built from scratch in our team was important for the success of the experiments.

The experiment DIRAC concentrated on the observation of pi-K and pi-pi atoms in CERN PS accelerator. Statistically significant number of 350 and 436 atoms respectively was observed. The very long lifetime of the 2p state of pi-pi atom was observed - in the order of  $10^{-11}$  – and was found not contradicting the theoretical predictions.

- |                                 |                 |            |
|---------------------------------|-----------------|------------|
| - Physical Review Letters. 2016 | 117(11) 112001. | (IF 9.227) |
| - Physical Review Letters. 2019 | 122(8) 082003.  | (IF 9.227) |
| - Physical Review D. 2017       | 96(5) 052002.   | (IF 4.368) |

## Research activity and characterization of the main scientific results

### **Introduction**

Additionally to our research in 2015-2017 new research fields were growing quickly in 2017-2019 namely in deposited nanostructures, 3D structures in surface layers etc. were realized using existing and newly established facilities for such as - PIXE channelling, complex ion beam implantation instrument enabling precise ion implantation parametr control, heating and cooling sample stage with mass spectrometry in situ device, ion microbeam instrument with rotational stage and morphology studies with Scanning Transmission Ion Microscopy (STIM) in 3D using circle of detectors and comprehensive 3D analysis using PIXE, RBS, Proton Elastic Scattering Analysis (PESA).

We installed two laser sources for optical ellipsometry, optical characterization of materials as well as laser modification of surfaces. Small deposition laboratory (chemical vapour and magnetron sputtering deposition, annealing furnace, spin coating device etc.) and analytical laboratory mainly for optical, electrical and sensing properties characterization.

Beside the infrastructure and equipment upgrades and extensions, corresponding attention is paid also to compliance of the in-house research with the direction of international top research. Following the strategy to study actual and top-science topics, the main scientific activities are discussed on internal seminars and meetings of the groups:

- a) The results achieved in the last period (usually 2 months) are presented and discussed, and it is decided whether to complete them or prepare a draft of an article.
- b) The current state of technology (devices, methodology) and the need to refill the systems with consumed materials or to replace defective parts are discussed.

From discussions about ongoing experiments, achieved results, state of technology and other topics, the groups suggest how to continue (or end) the study of the issue, and creates an idea, how to use the acquired knowledge and skills in other areas that can be explored by the technologies available to the team. This makes a proposal to extend (or transfer) scientific activity also to other issues.

The main areas of the LT and MRNIB scientific activity in which the groups have been involved are listed below, including several recent publications with brief descriptions of some of them.

### **Ion implantation, defect accumulation study in ZnO, Si and GaN**

[ASEP (ID 479677), ASEP (ID 484877), ASEP (ID 493527), ASEP (ID 497100), ASEP (ID 497102), ASEP (ID 511855)]

Ion modification and structural study was provided in Si and diamond to follow ion implantation/irradiation usability for doping, nanostructuring and optical properties tuning as well as in ZnO, GaN crystalline materials to discover potential usage of hexagonal crystal nonpolar facets for optical application. Fundamental processes of damage accumulation, band gap engineering, defect migration and thermal stability mainly in attractive GaN, ZnO semiconductors are still not understood. Crystals were implanted with Er, Gd and Au ions with broad energy range 200 keV up to 5 MeV to follow the distinct radiation damage connected to differing ion masses and their chemical nature in various facets (in case ZnO, GaN in polar and non-polar crystal surfaces), distinct damage accumulation depending on prevailing electronic or nuclear ion stopping mechanism. The lower damage grow in (11-20) in Zn and Ga-sublattices was observed compared to other orientations connected to preserved ion channelling phenomena in this orientation detected by RBS-channelling analysis see Fig. 1. Contrary O-sublattice disorder created in non-polar facets (11-20) and (10-10) was identified with Raman spectroscopy. XRD analysis discovered compressive strain around stacking faults in polar (0001) facets contrary expansive one was identified in non-polar orientations. Er, Gd exhibited preferably substitutional or Zn/Gd shadowed position being less thermally stable in m-plane and c-plane facets. Au exhibited preferably interstitial positioning with tendency to create ZnO

defect clusters containing Au as was followed with TEM. Monte Carlo simulations of ion channelling phenomena were provided using FLUX code in various facets taking into account relative damage in Zn or Ga sub-lattice taken from RBS-channelling experiments showing agreement with the experimentally observed effect of narrowing channels in ion implanted crystals in various facets. It turns out that by targeted defect formation it is possible to change the optical luminescence in individual orientations, strongly suppress exciton luminescence and shift the luminescence in the yellow region to other wavelengths.

Si crystals implanted with Kr, Ag, Au ions of energies 0,4 – 5 MeV exhibited various defects which strongly influences ion-beam channelling phenomena. He ion channelling in the ion-implanted Si structures was studied showing narrowing of channels correlated to the number of produced vacancies in MC simulations. The damage depth profiles were extracted showing the density of gradually displaced atoms as a function of ion fluence and ion mass. Nanostructured surface morphology modification has been detected for lower energies.

Diamond is proposed as an extraordinary material usable in optics and photonics. DFT simulations of Er dopant in diamond were provided and Er doped diamond crystal samples were prepared by ion implantation. The prepared Er-doped diamond samples annealed in a vacuum revealed clear luminescence, where the (110) cut sample has the highest luminescence. The reported results are the first demonstration of the Er luminescence in the single crystal diamond structure for the near-infrared spectral region.

We started with complex MC simulation of ion channelling and back-scattering maps which can be using FLUX code directly comparable to the experimental data and used for the advanced structural analysis based on RBS/C enabling deep insight into radiation defect accumulation in crystals Fig. 2.

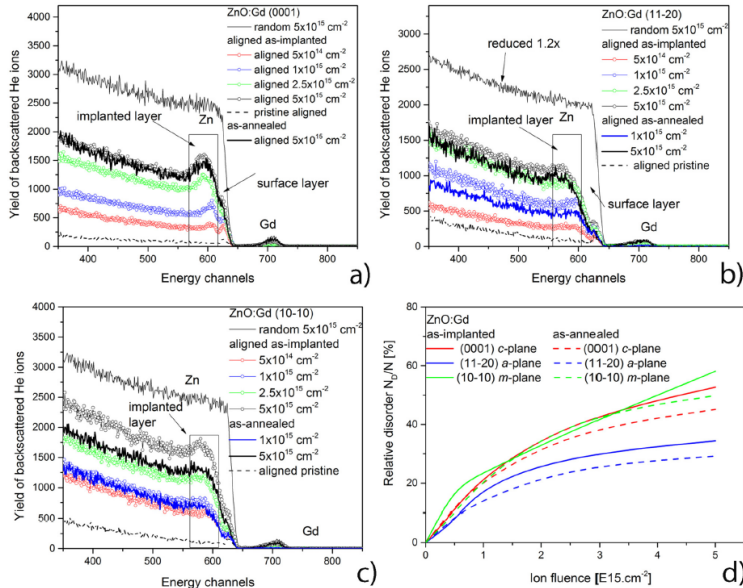


Fig. 1 RBS-C analysis of ZnO as-implanted samples with Gd ions at various fluences ranging in c-plane (0001) ZnO in (a), a-plane 11-20) ZnO in (b), and m-plane ZnO (10-10) in (c). The relative disorder induced in Zn-sublattice analyzed by RBS-C in as-implanted and as-annealed samples as a function of Gd ion implantation fluence in c-plane (0001) ZnO, a-plane ZnO (11-20), and m-plane (10-10) ZnO is depicted in (d).

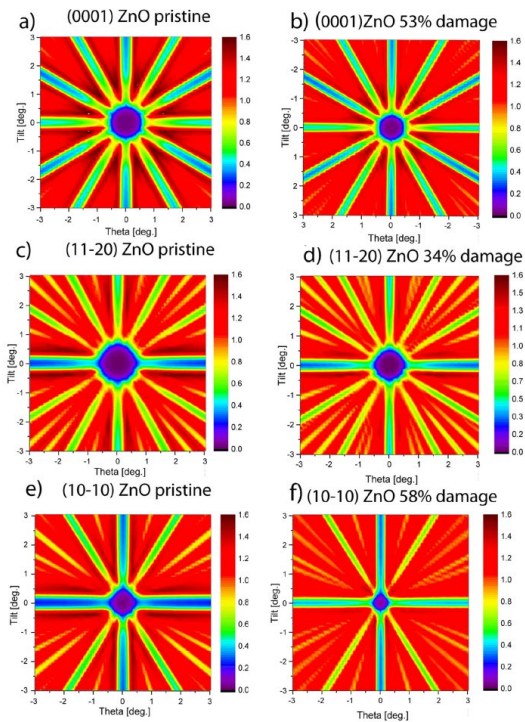


Fig. 2 FLUX simulation of the backscattering yield of He 2 MeV-ions from various ZnO orientations—2D maps with colour scaling of He backscattered ion intensity.

The results are documented with chosen impacted journal publications (some of them in journals SCT, PCCP, Vacuum, Applied Surface Science, Micromachines, Optical Materials have impact factor about 3 - 5 and are in Q1 or Q2 in branches - solid state matter, chemical engineering, surface and coatings films and associated fields). We added also associated publications in other journals [ ASEP (ID 520868), ASEP (ID 508842), ASEP (ID 504789), ASEP (ID 519076), ASEP (ID 519076), ASEP (ID 464366), ASEP (ID 465018)].

## **2D materials (graphene oxide, graphene, MoS<sub>2</sub> modification), defect engineering, functional properties development and microdevice lithography synthetization in graphene oxide and polymers/metal/composites**

[ASEP (ID 443062), ASEP (ID 445113), ASEP (ID 454106), ASEP (ID 463672), ASEP (ID 475667), ASEP (ID 492112), ASEP (ID 502236), ASEP (ID 503136)]

Graphene is a two-dimensional allotropic modification of carbon and has exceptional properties of chemical, electrical, mechanical and optical. During the preparation (several chemical methods were used) there may be contamination of a number of elements, heteroatoms, metals and other impurities, which results in undesirable changes in the properties of graphene. In samples of graphene by several chemical processes we are systematically studied the contents elements of nuclear analytical methods (RBS, ERDA, and PIXE PIGE) to evaluate the degree of contamination and determine the most appropriate method of chemical preparation. For preparation were used two different oxides graphene whose reduction gives the desired graphene, ERDA was used as a unique analytical method for monitoring the content of hydrogen and deuterium. Deuterium was used as a tracing element monitoring hydrogenation during graphite oxide reduction and graphene synthetization.

The ion microbeam was used to generate microstructures with the ion beam writing process, wherein the ion beam, on radiation-sensitive materials, produces microstructures that have significant optical and electrical properties. The ion microbeam precision and applicability for high resolution lithography was investigated and improved with focus on heavy ion focusing being rare for applications. An efficient mask-less production of patterns in insulating foils of graphene-oxide was carried out under impact of ion beams delivered by the Ion Micro Beam system at the Tandetron Laboratory. Graphene-



oxide (GO) matrix has been exposed to controlled ion fluences with the aim of inducing deoxygenation and enhancement of the electrical conductivity in selected areas of the exposed samples. The compositional changes in the exposed areas of the GO were investigated by IBA methods, electron microscopy, and correlated with the electrical properties measured by a standard 2-point probe technique. The control of the size, morphology, structural defects and oxygen groups in GO were correlated to the performance of the GO. Graphene oxide (GO) is an electrical insulator as most of the carbon atoms in this material are sp<sup>3</sup>-hybridized. Its physical, optical and chemical properties depend on the type and degree of reduction process. Contrary graphene layers would be intentionally modified to get semiconductor or insulator behavior. Various high energy ion beams (H, He, C, Si, Au) were used to alter the electrical properties and structural morphology in GO, rGO and graphene which elemental composition, internal structure and electrical, optical properties were also investigated. The different mass of ions leads to the significantly different electronic and nuclear stopping ratios and thus a difference in ion beam induced defects. The used ion irradiation leads to defect production in graphene structures whose density increases with increasing ion fluence significant decrease of graphene conductivity and is significantly more pronounced for heavier gold ions.

Ion lithography was successfully used for microstructuring in graphene oxide see Figure 3, where super-micro-capacitor in GO is depicted. Most interesting examples of ion beam microstructuring in various materials as channels created with focused ion beam of He ions in PMMA polymer are shown in Figure 3 as they are visualized with STIM microscopy using proton beam. Optical grating prepared in PYREX glass using carbon focused ion beam with changing of fluence to create Gaussian profile is shown in Figure 3 as was visualized with AFM. The ion microbeam can be used to generate microstructures with the ion beam writing process, wherein the ion beam, on radiation-sensitive materials, produces microstructures that have significant optical and electrical properties. The ion microbeam precision and applicability for high resolution lithography was investigated and improved with focus on heavy ion focusing being rare for applications.

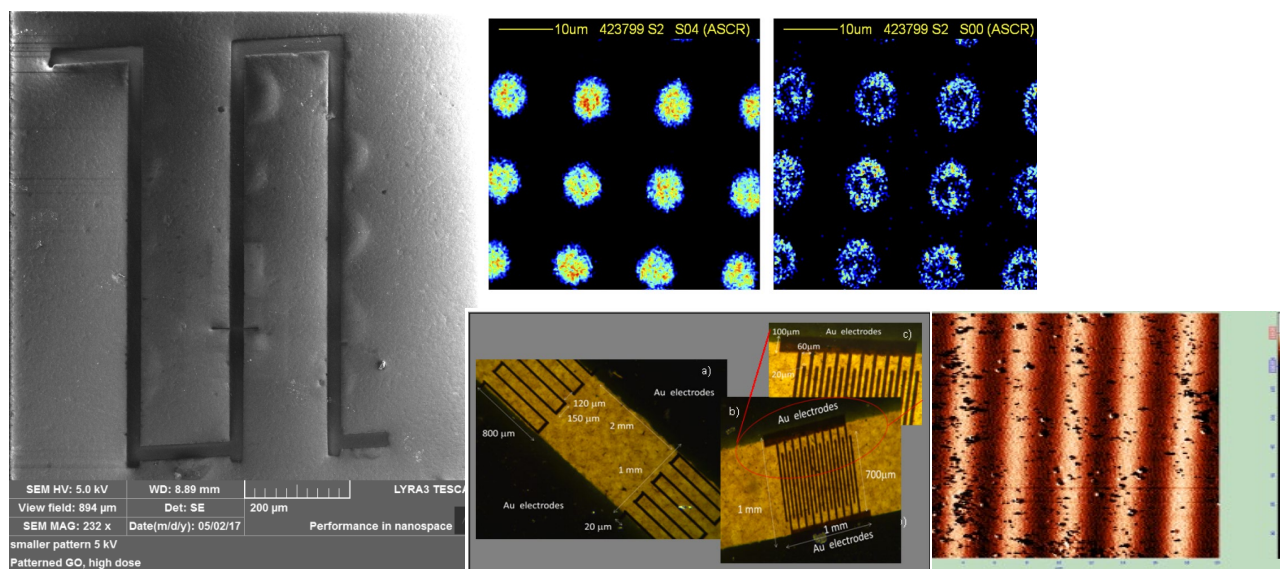


Fig. 3 SEM image of the micro-patterns written in PDMS using C ion microbeam at Tandatron accelerator at ion fluence  $10^{13}$ - $10^{14}$  ions/cm<sup>2</sup> is presented on the left. STIM visualization of micro patterning of PMMA polymer prepared with ion microstructuring using focused H<sup>+</sup> ion beam with energy 2 MeV in PMMA - right up and optical microstructures in PYREX glass prepared by microbeam- right bottom. Super-micro-capacitors prepared by ion beam lithography in grafene oxide - optical images (4x magnification) of two capacitors connected in parallel a) a large view of a capacitor b), a detail of the capacitor c) all written in graphene oxide (GO) – on the bottom right.

### **MoS<sub>2</sub> surface structure tailoring for hydrogen evolution reaction**

[ASEP (ID 517489)]

MoS<sub>2</sub> can be prepared in a monoatomic layer and thus has considerable potential for the hydrogen producing electrocatalytic reaction - the promising cleanest energy source. Catalytic properties of 2D materials, incl. MoS<sub>2</sub> can be modified directly by changing the electron structure of the surface and creating defects. The method of targeted defects (vacancies of sulfur or their clumps) due to energy transfer by ballistic processes (low ion energy), eventually by ionization and minority ballistic processes (high ion energy) is not investigated precisely, there are only simulations. We reported the influence of ion bombardment (S, Se and Te ions) with medium ion energy (400 keV) as well as (He, Au, Si) ions at high energy 1.8 MeV and various ion fluences on the electro-catalytic properties as well as hydrogen and other light element surface uptake in ion beam modified surfaces of MoS<sub>2</sub>. Our results showed that upon irradiation, sulphur vacancies were created. Upon exposure to ambient atmosphere, sulphur vacancies were partially replaced by oxygen, which led to surface oxidation. Nevertheless, samples irradiated using the higher ion fluences have generally showed enhanced catalytic hydrogen enhanced reaction (HER) performance in comparison with untreated MoS<sub>2</sub> crystals. Furthermore, we have also demonstrated that ion irradiation/implantation can serve as a tool for doping of MoS<sub>2</sub> crystals with Se and Te which can also influence the HER performance. Rutherford Back-Scattering spectrometry (RBS) and Elastic Recoil Detection Analysis (ERDA) were used for elemental analysis, including hydrogen surface depth profiling, of the modified MoS<sub>2</sub> samples. Electrical resistivity after Si and Au irradiation increased for the lowest ion fluence and subsequently decreases with increasing ion fluence being higher for the irradiated samples compared to the pristine one which is in accordance with HER catalytic activity.

### **Polymer irradiation/degradation studies**

[ASEP (ID 443404), ASEP (ID 454106)]

The fundamental studies of swift heavy ion energy losses and straggling were provided simultaneously with the modelling of ion solid interaction and validation of the present semi-empirical models. The information is irreplaceable in dosimetry, microelectronics and application on ion detector instrumentation. Simultaneously was realized the study of the optical, mechanical, electrical, compositional and structural changes of the materials irradiated by the swift heavy ions. Comprehensive study of heavy energetic ion energy stopping and polymer degradation under the ion beams was provided, where the crucial role of polymer back-bone complexity was discovered as well as new original unique experimental stopping powers of ions in various compounds were obtained newly added in the world-wide used empirical database, e.g. [https://www-nds.iaea.org/stopping/stopping\\_timg.html](https://www-nds.iaea.org/stopping/stopping_timg.html).

### **Laser assisted ion generation and laser generated plasma investigation**

We realized investigation of laser based multicharged energetic ion production in plasma, laser-generated plasma investigation and application of laser-generated plasma on surface tailoring, nanostructuring and multi-charged and multi-energetic ion implantation into various materials. The results are documented with additional and relevant impacted journal publications [ASEP (ID 458644), ASEP (ID 474564), ASEP (ID 482518), ASEP (ID 505696)].

### **Synthesis and characterization of thin hybrid films**

This activity has been developed in the team for a long time and has brought a number of interesting and valued publications. Some of the team members began to address this issue as one of the first in the world [ASEP (ID 466601)].

The paper reports on a comprehensive study related to solubility of Co in a mixture of Co and C<sub>60</sub> fullerenes. The evolution of Co<sub>x</sub>C<sub>60</sub> was analyzed for a wide range of Co concentration (0 < x < 50). The results showed that the structure and properties (e.g., magnetization) of Co<sub>x</sub>C<sub>60</sub> are dependent on the parameter x, and on exposure to air. The synthesized hybrid structure exhibits interesting properties that can be used in a variety of applications (e.g., in hybrid batteries).



The NPI's contribution to the study can be assessed to at least 75 percent. In NPI, thin layers of hybrid composites were synthesized and analyzed using AFM and IBA methods, in the partner organization (FI CAS) analysis of hybrid films were performed using Raman spectroscopy and XRD method. In NPI all data were evaluated and the text of the manuscript prepared [ASEP (ID 477480)].

The paper reports on a magnetic effect in air-exposed  $\text{Co}_x\text{C}_{60}$  nanocomposites. To verify the influence of air, magnetization of the film at low temperatures was tested. For  $\text{Co}_x\text{C}_{60}$  exposed to air in the field cooling regime, a vertical shift of the hysteresis loops was observed. The shift is caused by uncompensated magnetic moment induced by exchange coupling of the Co spins at the Co/CoO interface. The discovered effect implies a possible application of  $\text{Co}_x\text{C}_{60}$  composites in sensors and catalysis.

The NPI's contribution to the study can be assessed to at least 70 percent. In NPI, thin layers of hybrid composites were synthesized and analyzed using AFM and IBA methods, in the partner organization (FI CAS) analysis of hybrid films were performed using other techniques (HRTEM, SQUID). The data were evaluated in NPI, where also a manuscript was formulated [ASEP (ID 488726)].

Driving by interplay between plasmonic and magnetic effects in organic composite semiconductors is a challenging task with a huge potential for practical applications. The paper reports on evidence of a quantum plasmons that can be excited in the self-assembled  $\text{Co}_x\text{C}_{60}$  nanocomposite films for various stoichiometric parameters  $x$ . For plasmon-induced conditions, it is possible to propose a Rashba-like spin splitting effect that suggests valuable sources for spin polarization.

The NPI's contribution to the study can be assessed to about 70 percent. In NPI, thin layers of hybrid composites were synthesized and analyzed using AFM and IBA methods, in the partner organization (FI CAS) analysis of hybrid films were performed using other techniques (TEM, SQUID, ES). The data were evaluated in NPI, where also a manuscript was prepared [ASEP (ID 506052)].

Controllable access to the hybrid plasmonic nanostructures offers a tempting set of electronic excitations, which proper handling promises valuable applications. The paper reports on the remarkable plasmonic properties of the  $\text{Au}_x\text{C}_{60}$  hybrid nanostructures. The obtained results point at the self-assembled  $\text{Au}_x\text{C}_{60}$  nanocomposites representing promising plasmonic materials with potential for application in nanoplasmonics, nanoelectronics, and nanomedicine.

The NPI's contribution to the study can be assessed to about 70 percent. In NPI, thin layers of hybrid composites were synthesized and analyzed using AFM and IBA methods, in the partner organization (FI CAS) analysis of hybrid films were performed using other techniques (TEM, EDX, EELS, SE). In NPI was processed the measured data and prepared a manuscript.

### **Application of hybrid films in tissue engineering**

It has been shown that hybrid materials using fullerenes and titanium have interesting applications in tissue engineering. In collaboration with specialists - biologists, many experiments were carried out with promising results [ASEP (ID 444386)].

The work deals with the possible use of hybrid interfaces in tissue engineering. In this work, thin films created by co-deposition of fullerenes ( $\text{C}_{60}$ ) and titanium in various stoichiometric ratios was tested for the first time. The results showed that both fresh and aged  $\text{C}_{60}/\text{Ti}$  composites are suitable for adhesion and growth of human bone cells and can be considered as promising materials in bone tissue engineering. The article has a very positive response in the tissue engineering community.

The work was carried out gradually at two academic workplaces - NPI and IoP CAS. At NPI, the method of simultaneous deposition was used to prepare thin hybrid layers  $\text{C}_{60}/\text{Ti}$  with the required structural parameters, research on growth and quality of human cells on hybrid layers was carried out at the Institute of Physiology (IPHYS). The NPI's contribution to the study was 50 percent.

### **Study of etched ion tracks in polymers**

The research team has been dealing with the issue of nuclear tracks for a long time, some older members since joining the NPIs. It is an issue which, although studied for decades, is still not well understood and, in addition, it appears that nuclear tracks in a form of micro- or nano-pores have unusually high applicability in many areas (biology, medicine, electronics, catalysis, energy storage, etc.). Therefore, this issue is still very topical [ASEP (ID 458220)].

A model describing radial structure of latent tracks produced by energetic ions in polymers was created. The model is based on the assumption that the composition of latent pathways is the result of chemical reactions of transient degradation products formed by the ion passage. This model allows describing the process of pore formation during chemical etching. The work is important for experts who prepare pores of various shapes in polymers for practical applications (e.g., for biosensors).

The study was carried out at NPI, ion irradiation of polymers was carried out at the JINR Dubna. The NPI's contribution to the study (creation of theoretical model, chemical etching and characterization of the pore shapes) was at least 70 percent.

### **Synthesis and modification of thin metal films for gas sensors**

This topic is relatively new, the team deals with it within one of the grant projects. Given the possibilities provided to the team by the technology of thin film preparation, developed in the team, and by deep knowledge of the problems of one of the team members (acquired during the preparation of the dissertation), it was possible to develop this issue [ASEP (ID 464874)].

The paper reports on fabrication of CuO films for gas sensor application. In the study, the CuO thin films were prepared by ion beam sputtering followed by thermal annealing in air. It was found that CuO can be synthesized only at elevated annealing temperatures. The sensing was successful for H<sub>2</sub> and CH<sub>3</sub>OH gases. Thus, the study showed that with a relatively simple way it is possible to prepare thin films that are suitable for sensing of certain gases that need to be monitored.

Preparation and characterization of CuO thin films with required parameters (thickness, stoichiometry, sheet resistance) was performed in NPI, sensing study for hydrogen and methane was carried out at the University of Chemistry and Technology (NPI also participated in the experiment). The data were evaluated in NPI, where also the text of manuscript was prepared. The NPI's contribution to the study can be assessed as at least 75 percent.

### **Study of distribution of light elements in advance materials by NDP technique**

The team developed a special method for neutron depth profiling (NDP) of elements in materials that is unique within the EU (the new NDP devices exists at TU Garching, which the team helped implement, and at TU Eindhoven). This methodology makes it possible to perform non-destructive analyses of the depth (and spatial) distribution of some light elements (Li, B, N, Cl etc.) that cannot be analyzed by other methods. NDP is therefore requested in a number of areas where it is essential to determine the distribution of relevant elements (isotopes) in the thin layers of the studied materials. In cooperation with other teams in the CR and abroad, hundreds of analyses were performed, mainly regarding Li and B (technologically very important elements) in various systems (nanodiamonds, Li ion batteries, etc.) [ASEP (ID 477395)].

The paper reports on the electronic entanglement between superconducting and ferromagnetic states observed in hydrogenated boron-doped nanodiamond films. In the study was found anomalous magnetic and electrical transport properties that indicate a precursor phase, in which spin fluctuations intervene as a result of the interplay between the two antagonistic states. The observed effects bring attention to the potential applications in magnetoelectronics, spintronics, and magnetic field sensing. In the NPI, a study of boron distribution in the nanodiamond films was conducted using the neutron depth profiling method (NDP). NDP is the only one technique that can measure the spatial profiling of boron in solids nondestructively using a thermal neutron beam (in NPI prepared by a mirror neutronguide at the LVR-15 reactor). Synthesis of boron-doped nanodiamonds and other analyses

were performed in other laboratories. The NPI's contribution to the study can be assessed to about 15 percent [ASEP (ID 523929)].

In the experiment (joint with the team from RIKEN), Li-ion diffusion in a thin all-solid lithium-ion battery (ASSLiB) was studied using the NDP nuclear analytical technique. It has been found that the Li distribution depends on the state of charge of the battery. Only about one-third of the total Li ions in ASSLiB can move between the electrodes during charging / discharging processes. It has been also shown that the lateral distribution of Li is not homogeneous, which means that the position of Li might be affected by structural defects that arise in the battery during charging or discharging.

The thin ASSLiB battery was produced by RF sputtering in RIKEN, the NDP study, evaluation and an article preparation was carried out in NPI. The NPI's contribution to the study can be assessed to about 75 percent.

### **Study of thermal neutron cross sections of the light radioactive isotopes**

As a part of the neutron spectroscopy activity, the team also focused on measuring cross-sections of nuclear reactions of thermal neutrons with light radioactive nuclei (such as  $^7\text{Be}$ ), which are of great interest to astrophysics. These experiments are very technologically demanding, especially because they are working with highly radioactive targets [ASEP (ID 501154)].

In the work, a cross-section of the  $^7\text{Be}(n,p)$  reaction with thermal neutrons (that plays an important role in the primordial nucleosynthesis) was measured. The cross section was studied by several groups only with various conclusions. A new experiment was performed in NPI Rez, the obtained result is in agreement with some earlier studies, but other studies are significantly different. Because of high  $^7\text{Be}$  target radioactivity, all measurements are, unfortunately, subjected to large errors.

In the NPI Rez, a main experiment was carried out using the thermal neutron beam at LVR15 research reaktor. In NPI were also processed measured data and prepared a manuscript. In PSI Villigen and ILL Grenoble was prepared  $^7\text{Be}$  sample (produced radioactive  $^7\text{Be}$  nuclei, which were then implanted into a thin Al foil). The NPI's contribution to the study can be assessed to about 75 percent.

### **Research with/for industrial partners**

The very important is common instrumental development realized with industrial partners in the frame of the ion beam instrumentation development.

We collaborated with the industrial companies in the development of:

- the precise mechanical devices for sample positioning and of the sophisticated automated mechanical instrumentation implemented in vacuum beam target chambers (PZP Komplet, SKS, Opava, Czech Republic, SEVEN Lanškroun s r.o., Czech Republic),
- the complex solution for ion beam line vacuum system operating under the software control with self-regulating and safety options (Vakuum Praha, Prague, Czech Republic),
- the innovative and newly proposed instrumentation for thin layer coating deposition under the various conditions including plasma discharge deposition including the plasma cleaning, multilayer deposition (HVM Plasma, Prague, Czech Republic).

-

Based on the contracts we provided the ion beam analytical services for industrial partners:

- UJP a. s., Prague, Czech Republic- the study and characterization of corrosion processes in Zr alloys devoted for nuclear fuel coating materials,
- Bosch a.s., Prague, Czech Republic, compositional study of the thin foils with the extraordinary electrical properties,
- HVM Plasma, Prague, Czech Republic, ion beam analysis characterization of the superhard multi-layered coatings developed for the mechanical tools.

## **International research collaboration**

Both groups have collaboration in following international laboratories in the field of groups scientific scope.

The collaboration with ATOMKI, nuclear physics institute of the Hungarian Academy of Sciences is focused on the microbeam experiments with heavy energetic ions using micro machining for the preparation of advanced microstructures perspective in optics – common publications and experiments, instrumental know-how exchange.

Long-term fruitful collaboration with Helmholtz Zentrum Dresden-Rossendorf, Germany is established and based on common experiments realized at low energy implanters in HZDR, in IBA instrumentation development, common publications, instrumental know-how exchange, our team members serves as members of scientific user selection panel of Ion Beam Centre HZDR as well as members of Advisory board of RADIATE infrastructure (Horizon 2020 consortium) lead by HZDR and vice versa; the German colleagues serve as members of NPI (CANAM infrastructure) advisory and selection panel committees.

The nuclear analytical method characterization of materials modified by the multi-energetic ion implantation induced by plasma beam was realized in collaboration with University of Messina, Italy. The research was based on the trilateral agreements signed in 2015 by PALS (Prague Asterix Laser System, Prague, Czech Republic) and University of Messina, Italy and newly signed in 2018 as the bilateral agreement of common scientific collaboration between NPI and Uni Messina.

NPI is responsible for Uni Messina students training in nuclear analytical methods in the frame of Ph.D. study, our team members are taking parts as Ph.D. supervisors, Ph.D. committee members at Uni Messina.

Newly in 2019 was established cooperation with University of Oslo, Norway with group of Dr. Azarov, highly erudite and well known specialist in ion beam assisted defect engineering in semiconductors for micro and nanostructured optical and optoelectronic structure development. The common technological project was prepared and applied in Czech Technological Agency.

## Research activity and characterization of the main scientific results

Research activities in the period 2015-2019 can be divided in two areas:

1. Materials research
2. Instrumentation and methods for neutron diffraction

### 1. MATERIALS RESEARCH WITH HELP OF NEUTRON DIFFRACTION METHODS

Materials research carried out by the team is largely determined by its binding to the neutron scattering technique of investigation of matter, and to the operation of neutron diffraction facilities at the research reactor in Řež. Five team members are instrument scientists responsible for operation of five neutron diffractometers within the CANAM infrastructure of NPI. This fact determined largely the scope of materials research done by the team in the period 2015-2019, which can be categorized as:

- long term topics (brought by team members)
- ad-hoc topics (brought by external users of the neutron diffractometers)
- research topics of the project ESS-CZ-OP

#### 1.1 Long term topics

*High temperature alloys (Co-Re alloys, Ni-base superalloys)*

High-temperature alloys make a substantial category of technologically important materials which are indispensable for manufacturing of gas turbines. Mechanical properties and stability of these alloys are essential for a safe long-term operation of these expensive components. Further, the efficiency of turbines is determined by the temperature in the combustion chamber which is, in turn, dependent on the ability of turbine blade material to withstand increased temperatures and other severe conditions. This motivates development of novel high-temperature materials.

Excellent strength of Ni-based superalloys comes from their microstructure composed of  $\gamma'$ -precipitates embedded in solid-solution matrix. By in-situ Small Angle Neutron Scattering, volume fraction and morphology of  $\gamma'$  at high temperatures was determined in IN792-5A superalloy. It was found that additional precipitates are formed after reheating above 600°C when the superalloy was previously fast cooled from 900°C. These small precipitates explain the anomaly in the temperature dependence of the yield stress [1].

In order to enable a substantial increase of the turbine entry temperature, new types of materials are being tested. One of new high temperature materials are Co-Re base alloys. Our team contributed in the last years to testing of influence of various alloying elements to the stability of the Co-Re alloys at the foreseen operation temperatures (1200°C).

First, Ta and C additions were tested. TaC carbides, present in several morphological variants, were a candidate for strengthening precipitates in Co-Re turbine blades. Nevertheless, the fine TaC precipitate stability is crucial. The in-situ neutron diffraction and small-angle neutron scattering experiments determined the fine TaC morphology and volume fraction at operation temperatures and their evolution. The experiments proved the TaC suitability as a strengthening phase at the foreseen operation temperature [2], [3].

The second substantial alloying addition to Co-Re alloys which we tested was boron. Boron addition largely increases ductility. However, it could have an adverse effect on stability, particularly on temperature of hcp-fcc matrix transformation. In-situ neutron scattering experiment proved that - although there is a non-monotonic dependence of the transformation temperature on B content - the operation at 1200°C is still possible without cycling over the matrix transformation [4], [5].

In all these cases, our team contributed usually in the idea formulation (e.g. precipitate morphology study, carbides evolution, HT structure evolution with boron addition) as well as in

the planning and carrying out the neutron diffraction and SANS experiments. The team also carried out evaluation of the neutron-scattering data and participated largely in their interpretation, drawing conclusions and writing papers.

#### *Magnesium alloys and composites*

In the field of Mg alloys, it is of a large advantage to use in-situ neutron diffraction in combination with other techniques to investigate deformation mechanisms in these alloys. Twinning, which has a large contribution to plastic deformation, was the predominantly studied feature, but the other deformation mechanisms were studied as well.

In the case of Mg alloys, one of the complementary techniques to the neutron diffraction (which measures the twinned volume) is the acoustic emission (which detects the twin nucleation). By a combination of both methods, temperature dependence of twinning activity was studied. Particularly, the influence of temperature on the twin growth and twin nucleation was determined [6]. Additionally, the influence of the temperature and alloy composition on deformation mechanisms in Mg–Zn–Y magnesium alloys has been investigated at room temperature and 200°C. The results indicate that the share of twinning in the magnesium matrix and the kinking in the LPSO phase depends on the LPSO phase content and testing temperature [7].

A very important aspect in deformation mechanisms of Mg alloys is the loading mode. There exists an asymmetry of compression-tension deformation behaviour and it is one of the limiting factors for wider use of Mg alloys. This asymmetry is caused mainly by deformation twinning. One of the results within this topic is a description of the differences in the twinning activity in terms of nucleation and growth with respect to the loading direction and grain orientation [8]. Further, the unique experimental data obtained by in-situ neutron diffraction and acoustic emission brought information on dislocation slips and twinning in dependence on the loading mode. An elasto-plastic self-consistent model was used for quantitative comparison with measured data [9]. Both model calculations and experimental data explained the different deformation behaviour in tension and compression.

The last example regards the influence of the reinforcement short Saffil fibres on the deformation behaviour of Mg–Al–Ca alloy-based composite. Using in-situ neutron diffraction at room and elevated temperatures combined with FEM modelling and electron microscopy, the reinforcing mechanism was revealed. The experimental results provided an explanation for the fibre cracking and twinning dependence on fibre plane orientation and deformation temperature [10].

In all the cases, the method of in situ neutron diffraction combined with acoustic emission was developed in NPI by the team members. Neutron profile refinements and interpretation as well as other data evaluation (e.g. acoustic emission) were done by the team members. Neutron diffraction measurements were performed either in our laboratory in Řež or at neutron-physics laboratories abroad (in the latter case, the proposals of the experiments were prepared by NPI team members). Our team always participated in the preparation and execution of neutron diffraction experiments, as well as in the necessary modelling and electron microscopy. A large majority of the cited publications was written by the team members.

#### *Ti and Ti alloys*

Ti alloys play an important role in the aerospace, power generation and car industries thanks to their low density, high strength at elevated temperatures and corrosion resistance.

One of significant results was linking the mechanical properties of differently alloyed TiAl samples to their phase composition determined by neutron diffraction [11]. Changes in the microstructure (twin hardening) of  $\gamma$ -TiAl alloy during low-cycle fatigue was observed in-situ by the neutron diffraction technique [12].

Metastable  $\beta$ -Ti alloys are characterized by their ability to retain the high-temperature bcc phase above the  $\beta$ -transus temperature. Due to the metastable nature of the retained  $\beta$  phase, the mechanical properties can be tailored through careful control of the microstructure during heat treatments. The team members contributed to the understanding of the kinetics of nucleation and growth of the additional phases ( $\omega$ ,  $\alpha$ ) by in-situ neutron scattering experiments [13]. This understanding is essential for the control of the final microstructure and thus also the mechanical properties. One important aspect is size, shape and arrangement of  $\omega$  precipitates which significantly strengthen  $\beta$ -Ti alloys. We contributed significantly to determination of these parameters by Small-Angle Neutron Scattering (SANS) in single-crystal samples. This approach allowed to draw conclusions on the microstructure of the alloy after various annealing [14].

As a possible counterpart to (sometimes) expensive alloying elements, severe plastic deformation is a possible technique for improving mechanical properties of Ti pure metal. However, after such processing, residual stress field forms in the material which affects mechanical behaviour during further steps of processing or operation. Using neutron diffraction for measuring residual stresses, the ND team filled the gap still existing in determination of residual stresses after CONFORM ECAP processing of titanium [15]. Moreover, EBSD and X-ray studies were performed to clarify the microscopic background responsible for the stress field.

In all the cases the NPI team performed the neutron-diffraction structural and microstructural measurements (except SANS measurement of  $\beta$ -Ti alloys, which was done by our partners), including experiment proposal preparation, interpretation of results and, where relevant, phase transformation analysis. The ND team also helped with EBSD analysis and contributed significantly to drawing conclusions and writing manuscripts.

## **1.2 Ad-hoc topics**

*(problems solved by the external users of neutron diffractometers, at which the group members extensively participated)*

This category of results originates from the external user experiments at CANAM laboratory to which our team members contributed very significantly not only by carrying out the neutron diffraction experiments at our neutron diffractometers, but also by a full data evaluation and interpretation of the results, as well as by drawing conclusions from the experiment output for the given material.

The first significant result concerns magnetocaloric effect, in which field an extensive search for a suitable material exists. The study [16] was dedicated to the multi-technique investigation of a promising candidate (compound  $\text{AlFe}_2\text{B}_2$ ) for the magnetocaloric material usable in the magnetic refrigeration process. We determined the magnetic structure of the  $\text{AlFe}_2\text{B}_2$  a material for which the desired properties can be tuned to a certain extent.

Another topic broadly investigated by our users was perovskite structure, which, when properly doped, leads to a wide variety of materials with useful and exciting structural or magnetic properties. Some member of the triple-perovskite family showed the spin-liquid behaviour. Understanding of its formation was a driver for the research in which we participated. The nuclear and magnetic structures of doped Ru-Ir triple-perovskite compound was determined [17].

Similarly, complex metal oxides with perovskite-related structure have been of interest in the last decade due to the structural versatility of the perovskite lattice and remarkable properties originating from an interplay between spin, charge, and orbital degrees of freedom. One of studies was dedicated to the multiferroic candidate material - solid solutions  $\text{La}_{0.75}\text{Bi}_{0.25}\text{Fe}_{1-x}\text{Cr}_x\text{O}_3$ . The multi-technique approach to the investigation included also characterization by neutron diffraction and displayed a complete picture of this interesting system [18].

Properly designed advanced composites offer unique behaviour, different from the properties of the individual constituents. A novel composite of powders of semi-Heusler ferromagnetic shape memory alloy and pure Ti was successfully prepared by spark plasma sintering. It resulted in formation of small precipitates and intermetallic phases at the heterogeneous interfaces. Among other techniques, the structure was examined by SANS and by joint refinement of X-ray and neutron diffraction patterns [19].

Grain microstructure in the bulk of WC-Co composite material was studied using the Ultra-Small-Angle Neutron Scattering (USANS) facility MAUD of CANAM. Such cemented carbides are widely used as hard cutting tool materials. Conventional SANS instruments cannot be used due to high multiple scattering. Employing the USANS results, a method of linking the mean size of the grains to the inter-grain pockets was developed [20].

Residual stresses have a significant impact on engineering components during manufacturing and service and can reduce the component life. One of the performed studies evaluated residual stresses in heat treated 316L stainless steel specimens using finite element method (FEM), and compared them with stresses determined by the contour method. The FEM model was validated against neutron diffraction data. The results showed a good agreement in normal and tangential stress directions [21].

### **1.3 Research topics of the project ESS-CZ-OP**

The large research infrastructure *ESS Scandinavia-CZ* has been in part supported by the European Structural and Investment Funds project ESS-CZ-OP (*European Spallation Source - participation of the Czech Republic – OP*) focusing on delivery of technologies for the target station of ESS, but including also important research activities - *Research and development of in-situ experimental methods for characterization of processes in engineering materials*. While part of this research falls thematically within the long-term research topics and have been reported in the section 1.1 (e.g. the Mg alloys), there has also been research carried out solely by the team members working specifically on the project ESS-CZ-OP on part time contracts. We mention namely the methodical research in which thermo-mechanically loaded NiTi shape memory alloys were used as samples to develop in situ methods for engineering materials research. In this case, the authors from the ND team were at the same time members of the research teams working on this topic at collaborating institutions (FZU CAS, IT CAS, MFF UK). This fact is apparent from double affiliations on the publications.

The first result concerned the experiment and theory focusing on deformation mechanisms acting in thermomechanically loaded NiTi shape memory alloy at elevated temperatures and stresses. It summarized author's results from various thin NiTi wire experiments (thermomechanical tests, TEM, in-situ synchrotron x-ray diffraction), gave literature overview on the theory of transformation-plasticity coupling in NiTi and presented an original framework for it [22]. The team's share on the result creation: P. Šittner was invited by the journal editor to write this review based on his lectures on this topic. H. Seiner and P. Sedlák wrote the theoretical sections.

Cyclic martensitic transformation in thermomechanically loaded NiTi was a topic of the second important paper from this category. It deals with the plastic deformation accompanying the forward and reverse martensitic transformation in tensile tests on superelastic NiTi shape memory alloy wires. We achieved to evaluate these strains by designing and performing unique thermomechanical loading experiments on NiTi wires and interpreting the results via original theory explaining the activity of dislocation slip generated due to strain incompatibility at moving phase interfaces [23]. The team's share on the result creation: L. Kadeřávek participated in carrying out the thermo-mechanical experiment. P. Sedlák developed, in collaboration with H. Seiner, the theoretical framework explaining the origin of the plastic deformation accompanying the martensitic transformation under stress. P. Šittner wrote the manuscript.



In the finally listed very significant result in this section, the role of the deformation twinning in the martensite activated when martensitic transformation takes place at elevated temperatures and stresses was assessed. Original experimental and theoretical results were presented. Constitutive models capturing the coupled transformation-plasticity from the literature were overviewed and first version of an original constitutive model allowing for treating the thermomechanical functional behaviour of NiTi as a TRIP-like deformation was proposed [24]. The team's share on the result creation: The experiments were designed by L. Heller and carried out by 4 Ph.D. students - O. Tyc (thermomechanical tests), L. Kadeřávek (DIC), P. Sedmák (X-ray diffraction), M. Vronka (TEM). H. Seiner, P. Sedlák and P. Šittner developed the theoretical framework, P. Šittner coordinated writing of the manuscript.

## References:

*(Team members are underlined. Dashed underline denotes team members working on part time contracts at NPI with double affiliation)*

1. P. Strunz, M. Petrenec, J. Polák, U. Gasser, G. Farkas, Formation and Dissolution of gamma ' Precipitates in IN792 Superalloy at Elevated Temperatures. Metals. 2016, 6(2), 37. doi: 10.3390/met6020037 [ID 458662]
2. R. Gilles, D. Mukherji, L. Karge, P. Strunz, P. Beran, B. Barbier, A. Kriele, M. Hofmann, H. Eckerlebe, J. Rösler, J. Stability of TaC precipitates in a Co-Re-based alloy being developed for ultra-high-temperature applications. J. Appl. Cryst. 2016, 49(4), 1253-1265. doi: 10.1107/S1600576716009006 [ID 463723]
3. L. Karge, R. Gilles, D. Mukherji, P. Strunz, P. Beran, M. Hofmann, J. L. Gavilano, U. Keiderling, O. Dolotko, A., Kriele, A. Neubert, J. Rösler, W. Petry, The influence of C/Ta ratio on TaC precipitates in Co-Re base alloys investigated by small-angle neutron scattering. Acta Materialia. 2017, 132(JUN), 354-366. doi: 10.1016/j.actamat.2017.04.029 [ID 477404]
4. P. Strunz, D. Mukherji, P. Beran, R. Gilles, L. Karge, M. Hofmann, M. Hoelzel, J. Rösler, G. Farkas, Matrix Transformation in Boron Containing High-Temperature Co-Re-Cr Alloys. Metals and Materials International. 2018, 24(5), 934-944. doi: 10.1007/s12540-018-0121-8 [ID 492099]
5. P. Beran, D. Mukherji, P. Strunz, R. Gilles, L. Karge, M. Hofmann, M. Hoelzel, M. Rösler, G. Farkas, Additional Phases at High Boron Content in High-Temperature Co-Re-Cr Alloys. Metals. 2018, 8(8), 621. doi: 10.3390/met8080621 [ID 493524]
6. J. Čapek, G. Farkas, J. Pilch, K. Máthis, Temperature dependence of twinning activity in random textured cast magnesium. Mater. Sci. Eng. A 2015, 627(MAR), 333-335. doi: 10.1016/j.msea.2015.01.017 [ID 443223]
7. K. Máthis, D. Drozdenko, G. Németh, S. Harjo, W. Gong, K. Aizawa, M. Yamasaki, Y. Kawamura, In-situ Investigation of the Microstructure Evolution in Long-Period-Stacking-Ordered (LPSO) Magnesium Alloys as a Function of the Temperature. Frontiers in Materials. 2019, 6(11), 270. doi: 10.3389/fmats.2019.00270. [ID 517486]
8. K. Máthis, G. Csiszar, J. Čapek, J. Gubicza, B. Clausen, P. Lukáš, A. Vinogradov, S. R. Agnew, Effect of the loading mode on the evolution of the deformation mechanisms in randomly textured magnesium polycrystals - Comparison of experimental and modeling results. Int. J. of Plast. 2015, 72(SEP), 127-150. doi: 10.1016/j.ijplas.2015.05.009 [ID 448883]
9. J. Čapek, K. Máthis, B. Clausen, M. R. Barnett, Dependence of twinned volume fraction on loading mode and Schmid factor in randomly textured magnesium. Acta Materialia. 2017, 130(MAY), 319-328. doi: 10.1016/j.actamat.2017.03.017 [ID 475684]

10. G. Farkas, K. Máthis, J. Pilch, P. Minárik, P. Lukáš, A. Vinogradov, Deformation behavior of Mg-alloy-based composites at different temperatures studied by neutron diffraction. *Materials Science and Engineering A*. 2017, 685(FEB), 284-293. doi: 10.1016/j.msea.2017.01.010 [ID 474509]
11. A. Chlupová, M. Heczko, K. Obrtlík, J. Polák, P. Roupčová, P. Beran, T. Kruml, Mechanical properties of high niobium TiAl alloys doped with Mo and C. *Materials and Design*. 2016, 99(JUN), 284-294. doi: 10.1016/j.matdes.2016.03.079 [ID 458280]
12. P. Beran, M. Heczko, T. Kruml, T. Panzner, S. van Petegem, Complex investigation of deformation twinning in gamma-TiAl by TEM and neutron diffraction. *J. Mech. Phys. Solids*. 2016, 95(OCT), 647-662. doi: 10.1016/j.jmps.2016.05.004 [ID 464141]
13. P. Zháňal, P. Hrcuba, J. Stráský, J. Šmilauerová, P. Beran, T. C. Hansen, H. Seiner, M. Janeček, Transformation Pathway upon Heating of Metastable beta Titanium Alloy Ti-15Mo Investigated by Neutron Diffraction. *Materials*. 2019, 12(21), 3570. doi: 10.3390/ma12213570. [ID 518767]
14. P. Strunz, J. Šmilauerová, M. Janeček, J. Stráský, P. Hrcuba, J. Pospíšil, J., Veselý, P. Lindner, L. Karge, Evaluation of anisotropic small-angle neutron scattering data from metastable beta-Ti alloy. *Philosophical Magazine*. 2018, 98(34), 3086-3108. doi: 10.1080/14786435.2018.1520403 [ID 495738]
15. G. Németh, K. Fekete-Horváth, Ch. Hervoches, P. Cejpek, J. Palán, M. Duchek, K. Máthis, Characterization of the Microstructure, Local Macro-Texture and Residual Stress Field of Commercially Pure Titanium Grade Prepared by CONFORM ECAP. *Metals*. 2018, 8(12), 1000. doi: 10.3390/met8121000 ASEP [ID 500351]
16. J. Cedervall, M. S. Andersson, T. Sarkar, E. K. Delczeg-Czirjak, L. Bergqvist, T. C. Hansen, P. Beran, P. Nordblad, M. Sahlberg, M. Magnetic structure of the magnetocaloric compound AlFe<sub>2</sub>B<sub>2</sub>. *J. Alloys Comp.* 2016, 664(APR), 784-791. doi: 10.1016/j.jallcom.2015.12.111 [ID 458221]
17. P. Beran, S. A. Ivanov, P. Nordblad, S. Middey, A. Nag, D. D. Sama, S. Ray, R. Mathieu, Neutron powder diffraction study of Ba<sub>3</sub>ZnRu<sub>2</sub>-xR<sub>x</sub>O<sub>9</sub> (x=0, 1, 2) with 6H-type perovskite structure. *Sol. Stat. Sci.* 2015, 50(DEC), 58-64. doi: 10.1016/j.solidstatesciences.2015.10.011 [ID 454091]
18. S. A. Ivanov, P. Beran, G. V. Bazuev, R. Tellgren, T. Sarkar, P. Nordblad, R. Mathieu, Perovskite solid solutions La<sub>0.75</sub>Bi<sub>0.25</sub>Fe<sub>1-x</sub>Cr<sub>x</sub>O<sub>3</sub>: Preparation, structural, and magnetic properties. *J. Sol. Stat. Chem.* 2017, 254(OCT), 166-177. doi: 10.1016/j.jssc.2017.06.031 [ID 477646]
19. J. Kopeček, K. Bartha, R. Mušálek, Z. Pala, T. Chráska, P. Beran, V. Ryukhtin, P. Strunz, J. Nováková, J. Stráský, P. Novák, O. Heczko, M. Landa, H. Seiner, M. Janeček, M. Structural characterization of semi-heusler/light metal composites prepared by spark plasma sintering. *Scientific Reports*. 2018, 8(Jul), 1-13, 11133. [ID 501168]
20. A. B. Yildiz, J. Weidow, V. Ryukhtin, S. Norgren, G. Wahnstrom, P. Hedstrom, Very-small angle neutron scattering study on grain coarsening inhibition by V-doping of WC-Co composites. *Scripta Materialia*. 2019, 173(12), 106-109. doi: 10.1016/j.scriptamat.2019.08.005. [ID 509865]
21. J. Hodek, A. Prantl, J. Dzukan, P. Strunz, Determination of Directional Residual Stresses by the Contour Method. *Metals*. 2019, 9(10), 1104. doi: 10.3390/met9101104. [ID 517487]
22. P. Šittner, P. Sedlák, H. Seiner, P. Sedmák, R. Delville, L. Heller, L. Kadeřávek, On the coupling between martensitic transformation and plasticity in NiTi: Experiments and continuum based modelling. *Prog. Mater. Sci.* 2018, 98(10), 249-298. doi: 10.1016/j.pmatsci.2018.07.003 [ID 494430]

23. L. Heller, H. Seiner, P. Šittner, P. Sedlák, O. Tyc, L. Kadeřávek, On the plastic deformation accompanying cyclic martensitic transformation in thermomechanically loaded NiTi. *Int. J. Plast.* 2018, 111(12), 53-71. doi: 10.1016/j.ijplas.2018.07.007 [ID 499496]
24. L. Heller, P. Šittner, P. Sedlák, H. Seiner, O. Tyc, L. Kadeřávek, P. Sedmák, M. Vronka, Beyond the strain recoverability of martensitic transformation in NiTi. *Int. J. Plast.* 2019, 116(5), 232-264. doi: 10.1016/j.ijplas.2019.01.007. [ID 504077]

## 2. INSTRUMENTATION AND METHODS FOR NEUTRON DIFFRACTION

Generally, neutron scattering methods are much less supported by commercial sector in providing instruments and software tools when compared e.g. to analogical X-ray methods. Neutron laboratories thus have to rely more on self-developed instruments and methods. It is therefore not surprising that the ND team members engage significantly in activities and projects oriented on neutron instrumentation. These activities can be divided in two main areas: One is the participation in the construction of the European Spallation Source ERIC in Lund (Sweden) where NPI is responsible for realization of the contribution for the Czech Republic. The other area involves developments arising from the needs of the experiments carried out at the research reactor LVR-15 in Řež.

### 2.1 Instrumentation for European Spallation Source (ESS)

The involvement of the team in the construction of ESS is described in a broader scope in the section "*Participation in large collaborations*". Here we focus on the research and development activities which form a part of the project *ESS Scandinavia-CZ*. These activities have been aimed at supporting the development and delivery of the engineering diffractometer BEER as a part of the Czech in-kind contribution to the ESS construction. This instrument is dedicated to a non-destructive characterization of engineering materials and technological components, especially *in situ* and *in operando* during thermo-mechanical loading, i.e. under conditions that simulate real industrial processes, from manufacturing to operation. Related research in the areas of material science and development of experimental methods for the *in-situ* characterization of the structure and the structural changes of materials is described in the preceding sections. In the field of neutron instrumentation, the R&D activities focused mainly on two subjects:

- *Design and simulations of neutron optics* including development of the software for neutron ray-tracing simulations (SIMRES [1]). ESS employs long beam pulses in combination with a special low-dimensional moderator. Novel concepts in instrumentation optimized for this moderator were therefore required in order to fully benefit from the high source brightness. The ND team participated in the global optimization of 5 out of 23 neutron beam lines proposed for ESS, which served as a data base for decisions about the instruments actually scheduled for construction [2]. For the diffractometer BEER, the ND team developed the concept and detailed design of the neutron optics system [3, 4]. These results in a form of technical reports and software make part of the detailed design documentation of BEER.
- *Development of specialized deformation rigs for the diffractometer BEER*, which allows to employ neutron diffraction and imaging techniques during thermo-mechanical loading of materials in combination with other methods of characterization of physical processes in materials (acoustic emission, ultrasonic and imaging methods). A prototype of 100 kN uniaxial deformation rig with vacuum chamber allowing for various modes of deformation and heating together with wide acceptance angle for neutron beam has been designed and constructed by the ND team members by the end of 2019.

## 2.2 *Neutron diffraction instrumentation and methods at NPI*

### *Instrument upgrades*

The instrumental base for neutron diffraction at the reactor LVR-15 has been continuously upgraded with the aim to enhance experimental capacity and data quality. The major improvements include:

- Installation of large *bent crystal analyser* system allowing for wider Q-range of the SANS diffractometer.
- Installation and testing of a system for *induction heating*. It allows for fast (200 K/s) heating of samples under uniaxial load in a deformation rig on neutron beam.
- Installation of *oscillating radial collimator* in the secondary beam of stress diffractometer. This device allows for better definition of gauge volume, while leaving larger space for mapping residual stresses in large components.
- Commissioning of the *robotic arm* for accurate 3D positioning of samples at the strain diffractometer in its integration in the instrument control system.

### *Bragg diffraction optics*

The research focused on experimental studies of new types of high-resolution neutron monochromators / analysers employing dispersive configurations and multiple Bragg reflections. For example, a new dispersive monochromator based on the double reflection process in a two-slab sandwich pack of bent Si single crystals has been realized. It provides high resolution for powder diffractometry and freedom to combine different slabs for the double diffraction, which allows for a variety of selectable wavelengths. Our team carried out necessary calculations and the experimental tests, and participated in preparation of the publication [5].

### *Small-angle neutron scattering (SANS)*

Magnetic domains cause a strong multiple scattering of thermal neutrons which leads to significant broadening of diffraction peaks when scanning residual stresses in thick ferromagnetic materials like ferritic steels. Our experiments demonstrated that applying external magnetic field perpendicular to the neutron beam significantly reduces this effect and could thus be used to achieve larger sampling depths e.g. in large steel components. In this work, our team carried out all SANS measurements and data treatment and participated in preparation of the publication [6].

### *Analysis of residual stresses by neutron diffraction*

Neutron diffraction is an excellent tool for measuring crystal lattice strains which allows to analyse residual stresses that largely affect mechanical properties of metallic engineering components. This technique is - to a large extent - limited by resolution effects, which give rise to false observed strains if not treated properly. Modelling and treatment of these false strains made part of the collaboration project between the ND team and colleagues from TU München and KIT in Germany. A novel method and software combining neutron ray-tracing simulation with indirect deconvolution technique for treatment of the false strains has been developed at NPI [7]. The method permits to restore intrinsic strain distributions with resolution significantly better than the nominal instrumental gauge size, allowing to approach very small scan depths otherwise achieved only by X-ray diffraction or by using extremely high spatial resolution. Experimental validation [8] proved that gains in counting time of up to a factor of fifteen are possible when compared to high resolution measurements, without significant loss in the spatial resolution. The ND team also participated in optimization of special radial collimators for the diffractometer STRESS-SPEC at the FRM II reactor (TU München) which contributed to the significant improvement in suppression of the false strains problem at this instrument [9].

## References:

1. J. Šaroun, J., SIMRES - Neutron Ray-Tracing Program, <https://neutron.ujf.cas.cz/restrax/>
2. K. H. Andersen, M. Bertelsen, L. Zanini, E. B. Klinkby, T. Schonfeldt, P. M. Bentley, J. Šaroun, J. Optimization of moderators and beam extraction at the ESS. J. Appl. Cryst. 2018, 51(4), 264-281. doi: 10.1107/S1600576718002406 (ID 489155)
3. K. H. Andersen and 170 co-authors (ND team co-authors: P. Beran, J. Šaroun, P. Lukáš). The instrument suite of the European Spallation Source. Nucl. Instr. and Methods A 957 (2020) 163402, <https://doi.org/10.1016/j.nima.2020.163402>.
4. J. Šaroun, et al., *Neutron Optics Report for the BEER Instrument*, Technical report ESS-0238217, European Spallation Source, 2020.
5. P. Mikula, M. Vrána, J. Šaroun, B. S. Seong, W. Woo, V. Em, New type of dispersive sandwich monochromator for very high resolution neutron diffractometry. Physica. B. 2018, 551(12), 364-369. doi: 10.1016/j.physb.2017.12.039 (ID 500172)
6. W. Woo, V. Em, E. Shin, P. Mikula, V. Ryukhtin, Influence of multiple small-angle neutron scattering on diffraction peak broadening in ferritic steel. J. Appl. Cryst. 2015, 48(APR), 350-356. doi: 10.1107/S1600576715000813 (ID 443879)
7. J. Šaroun, J. Rebelo-Kornmeier, J., Gibmeier, M. Hofmann, Treatment of spatial resolution effects in neutron residual strain scanning. Physica. B. 2018, 551(12), 468-471. doi: 10.1016/j.physb.2018.01.013 (ID 500170)
8. J. R. Kornmeier, M. Hofmann, V. Luzin, J. Gibmeier, J. Šaroun, Fast neutron surface strain scanning with high spatial resolution. Materials Characterization. 2019, 154(8), 53-60. doi: 10.1016/j.matchar.2019.05.031. <https://doi.org/10.1016/j.matchar.2019.05.031> (ID 507629)
9. J. R. Kornmeier, M. Hofmann, W. M. Gan, J. Gibmeier, J. Šaroun, Non-destructive Neutron Surface Residual Stress Analysis. J. Nondest. Eval. 2019, 38(3), 79. doi: 10.1007/s10921-019-0617-2. <https://doi.org/10.1007/s10921-019-0617-2> (ID 510210)

## Research activity and characterisation of the main scientific results

The team is organizationally a part of the Department of Radiation Dosimetry, which focuses its research activities into three overlapping and complementary areas: dosimetry of complex radiation fields, radiation biophysics and biology, and environmental dosimetry. The part of the researcher capacity in the department dealing with environmental dosimetry and radiocarbon dating is for purposes of the present evaluation administered separately.

The main research activities in dosimetry of complex radiation fields focus on studies of cosmic radiation, related radiation protection issues on board aircraft and spacecraft, dosimetric and microdosimetric description of therapeutic charged particle beams.

I. Ambrožová coordinates the participation of the research team in international experiments focused mainly on passive dosimetry on board the International Space Station (ISS). Our team is involved in several international projects focused on the determination of dosimetric characteristics onboard ISS and various satellites. One of them is ESA (European Space Agency) project DOSIS 3D (3D dose distribution onboard ISS), which aims to determine temporal and spatial variations of the radiation environment within the European Module Columbus using various passive and active detector systems. NPI researchers were responsible for providing and analyzing passive detectors (three types of thermoluminescent detectors and two types of plastic nuclear track detectors), which have been, together with detectors from other participants, placed at 11 positions inside the Columbus module [ID 468234, 474529]. Our passive detectors were placed also at other parts of ISS and onboard a biological satellite BION-M1 [ID 485809, 486343, 499093, 506944]. Data obtained in these studies bring valuable information about the radiation situation in space and help to estimate the radiation risk of crewmembers.

In our experimental studies, we often apply track-etched detectors as LET spectrometers. The methodology of passive dosimetry using these detectors has been continuously upgraded [ID 485807, 492464, 523893].

Since December 2016, most of the activities in this domain have been covered by project CRREAT (Research Center of Cosmic Rays and Radiation Events in the Atmosphere, [www.creat.eu](http://www.creat.eu)) funded from the European Structural and Investment Funds by means of the Ministry of Education, Youth and Sports, Operational Programme Research, Development and Education in combination with the institutional support of the Nuclear Physics Institute of the CAS, the Institute of Atmospheric Physics of the CAS, and the Czech Technical University in Prague. The aims of the project are to deepen the knowledge about the relation between atmospheric phenomena and ionizing radiation in thunderstorms, and second, to clarify phenomena causing variations of the secondary cosmic particles (SCP) in the atmosphere. For this purpose, the activities focus on measurements and theoretical studies of cosmic radiation and high-energy radiation generated in thunderstorms at several altitude levels: in space (at low-Earth orbit mentioned above but also flights to Moon [ID 506042] and Mars [ID 494426]), in stratospheric balloons, at flight altitudes of passenger aircraft, at high-mountain observatories, and at ground level.

Thunderstorm activity on the ground was studied using the existing radiation monitoring network (RMN) in the Czech Republic [ID 523905]. It was found that the Early Warning Network of the RMN was able to detect radiation enhancements with short- and long-lasting responses during thunderstorms. Observations during the thunderstorms indicated that strong

thundercloud electric fields can significantly increase exposure levels through both lightning discharges and the TGE, whereas the radon progeny alone cannot explain the observed enhancements. Another on-ground study of the thunderstorm radiation activity via correlations between secondary cosmic ray rates measured with SEVAN and strong electric fields at Lomnický štít was published in [ID 480081].

Studies on variations of SCP measured on the ground were published in [ID 490151, 503152, 504076, 504409, 497094]. The first two papers [ID 490151, 503152] describe characteristics of the GLE on 10 September 2017 based on the available data both from satellite GOES-13 and from selected neutron monitors, including Lomnický štít. In the paper [ID 497094], quasi-periodicities in cosmic rays and time lag of the solar activity at neutron monitors, including Lomnický štít, were described. Power spectral analysis indicated the presence of several mid-term quasi-periodicities, including Rieger type and Quasi-biennial oscillations. The paper [ID 477481] has successfully demonstrated the implementation of a hierarchical Bayesian spatio-temporal model and a Kriging interpolation technique to forecast the trapped particle flux distribution at medium LEO altitudes.

Our team members perform dosimetry studies in complex radiation fields on board aircraft, compliant with the 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 requested to monitor them (see Atomic law n. 263/2016 and Decree on radiation protection n. 422/2016). Annual effective doses received by aircrew are routinely calculated using the computer code CARI-7. Our team provides evaluation of effective doses of personnel of all airlines registered in the Czech Republic and the Slovak Republic. Our results obtained since 1997 are summarized in [ID 523911]. The fact that radiation dosimetry methods onboard aircraft and spacecraft are to some extent similar is discussed in [ID 445843].

The calculations are regularly validated by experimental measurements. Verification measurements on board aircraft were performed in December 2015, June 2016, and December 2019 using various active and passive detectors. The flights were also used for comparing the response and sensitivity of different radiation detectors, see [ID 445842]. Calibrations of these detectors in terms of ambient dose equivalent were performed in CERN'S High-Energy Reference Field (CERF) facility in 10/2015, 11/2016, 8/2017 and 6/2018. An improved calibration method for PIN-diode detectors was proposed in [ID 445838]. Calibration methods of pixel detectors based on Timepix technology used in mixed radiation fields including cosmic radiation and radon progenies are described in [ID 484292, 495729, 497560, 458113].

We allow free access to our long-term measurements with the silicon spectrometer Liulin onboard aircraft also by means of a database available online at <http://cr10.odz.ufj.cas.cz/> [ID 523910]. This online tool enables to compare time dependencies of quantities measured on board aircraft using Liulin with neutron monitor data at high-mountain observatory at Lomnický štít, Slovakia. The database covers measurements since 2001, which is longer than the usual duration of the solar cycle period. The database comprises over 130 thousand individual records of energy deposition spectra, absorbed dose rates, and ambient dose equivalent rates including also information on about flight parameters. Since 2017, the database was extended by measurements onboard aircraft using several dosimeters Airdos developed at our department [ID 503705]. A different approach to evaluate the radiation risk of aircraft crews

based on continuous measurements with a neutron monitor at Lomnický štít was published in [ID 471141].

Since 2015 novel active dosimeters for mixed radiation fields have been developed by team members. These dosimeters are intended for long term measurements on board aircraft and spacecraft. Two versions of AIRDOS dosimeters were developed, calibrated, tested [ID 503705] and routinely deployed on board aircraft. Two versions of SPACEDOS dosimeters were launched in 2019 to Earth orbit. One SPACEDOS dosimeter was sent to the Socrat-R cubesat mission (2019-038-AE) in July 2019 in cooperation with the Moscow State University. Another SPACEDOS dosimeter was placed at the International Space Station from September 2019 to February 2020. SPACEDOS 01 is intended for measurement on board vacuum/open space satellites and SPACEDOS 02 is intended for crewed flights, for measurement inside a pressurized cabin of spacecraft. In addition, novel methods of measurement were invented during the development, and one of them was patented [ID 499195].

HIMAC in Japan is not only an excellent cancer-treatment facility using the carbon beam but also a facility to perform experiments related to radiation therapy, space radiation protection and basic nuclear physics. HIMAC BIO is an irradiation room used for experiments related to both radiobiology and physics. When performing such experiments, it is essential to know the experimental setup, as well as the beam characteristics, in detail. O. Ploc et al. [ID 479652] described the beam-line and characterized the fragmentation from heavy ion beams calculated with PHITS and measured with Liulin. Depth-dose distributions and LET spectra in carbon ion beam acquired using CR-39 were compared to Geant4 calculations [ID 450487].

Pixel detector Timepix is a promising technology in characterization of the mixed radiation field due to its small dimension, fast response, information on both energy deposition and track of the traversing particle. A method to calculate the LET spectra using Timepix was successfully proposed and tested via intercomparison with standard detector – the tissue-equivalent proportional counter (TEPC) Hawk in [ID 495581].

Large share of our research is performed in the frame of the European Radiation Dosimetry Group (EURADOS). The team members actively contribute mainly to working groups WG9 – Radiation dosimetry in radiotherapy and WG11 – High energy radiation fields. Individual activities of team members are described more in detail further in section Participation in large collaborations.

Our team organized on 29<sup>th</sup> November 2017 an international experiment “Aircraft campaign REFLECT” focused on the influence of cosmic radiation on board aircraft. The response of more than 20 different detectors was investigated during a flight on board a small aircraft under stable flight conditions. Sixteen institutes from the whole Europe participated, several of them representing the leading research groups in aviation dosimetry in their respective countries. As a result, REFLECT is the largest campaign of this type ever performed. The flight campaign enabled measurement in uniform, well-defined conditions on board an aircraft and comparison of new instruments with those routinely used. The results of the experiment will contribute to the further development of the most accurate standardized dosimeter to be flown on board commercial aircraft and will provide valuable insight into further development of air transport safety. This campaign was a part of the research activities of EURADOS Working Group 11 and the CRREAT project [ID 533918].

Another big experiment of WG11 has been carried out at the Lausanne University Hospital (CHUV) in September 2017, where the response of various active and passive dosimeters to



electron LINAC have been compared. Team members participated with thermoluminescent detectors, ionization chamber, Candy detector and Timepix [ID 525560].

Responses of conventional dosimeters (films, polyallyldiglycol carbonate, electronic personal dosimeter) to proton bunches of up to 30 MeV energy produced by South Korean PW laser system at the Advanced Photonics Research Institute, Gwangju Institute of Science and Technology were studied, both by Monte Carlo simulations and experimentally. The capacity of working in pulsed fields of pulse length below 1 ps, in a single-shot regime up to the repetition rate of 1 kHz, has been evaluated [ID 467004].

Within WG9 collaboration, the response of different passive dosimetry systems in mixed radiation field induced by proton pencil beam inside anthropomorphic phantoms representing 5 and 10 years old children was studied. Doses were measured in different organs with thermoluminescent (MTS-7, MTS-6 and MCP-N), radiophotoluminescent (GD-352 M and GD-302M), bubble and poly-allyl-diglycol carbonate (PADC) track detectors. Results showed that RPL detectors are less sensitive to neutrons than LiF TLDs and can be applied for in-phantom dosimetry of gamma component. Neutron doses determined using track-etched detectors, bubble detectors and pairs of MTS-7/MTS-6 are consistent within the uncertainty range. This was the first study dealing with measurements on child anthropomorphic phantoms irradiated by a pencil scanning beam technique [ID 492463].

Systematic 3D mapping of out-of-field doses induced by a therapeutic proton pencil scanning beam in a  $300 \times 300 \times 600 \text{ mm}^3$  water phantom was performed using a set of thermoluminescence detectors (TLDs): MTS-7 ( $^7\text{LiF:Mg,Ti}$ ), MTS-6 ( $^6\text{LiF:Mg,Ti}$ ), MTS-N ( $^{\text{nat}}\text{LiF:Mg,Ti}$ ) and TLD-700 ( $^7\text{LiF:Mg,Ti}$ ), radiophotoluminescent (RPL) detectors GD-352M and GD-302M, and polyallyldiglycol carbonate (PADC)-based ( $\text{C}_{12}\text{H}_{18}\text{O}_7$ ) track-etched detectors. Neutron and gamma-ray doses, as well as linear energy transfer distributions, were experimentally determined at 200 points within the phantom. In parallel, the Geant4 Monte Carlo code was applied to calculate neutron and gamma radiation spectra at the position of each detector. For the cubic proton target volume of  $100 \times 100 \times 100 \text{ mm}^3$  (spread out Bragg peak with a modulation of 100 mm) the scattered photon doses along the main axis of the phantom perpendicular to the primary beam were approximately 0.5 mGy/Gy at a distance of 100 mm and 0.02 mGy/Gy at 300 mm from the center of the target. For the neutrons, the corresponding values of dose equivalent were found to be  $\sim 0.7$  and  $\sim 0.06 \text{ mSv/Gy}$ , respectively. The measured neutron doses were comparable with the out-of-field neutron doses from a similar experiment with 20 MV X-rays, whereas photon doses for the scanning proton beam were up to three orders of magnitude lower [ID 489292].

EURADOS WG9 carried out a large measurement campaign at the Trento Centro di Protonterapia (Trento, Italy) in order to determine the neutron spectra near the patient using two extended-range Bonner sphere spectrometry (BSS) systems. In addition, the work focused on acknowledging the performance of different commercial active dosimetry systems when measuring neutron ambient dose equivalents,  $H^*(10)$ , at several positions inside (8 positions) and outside (3 positions) the treatment room. Detectors included three TEPCs - tissue equivalent proportional counters (Hawk type from Far West Technology) and six rem-counters (WENDI-II, LB 6411, RadEye NL, a regular and an extended-range NM2B). Meanwhile, the photon component of stray radiation was deduced from the low-lineal energy transfer part of TEPC spectra or measured using a Thermo Scientific FH-40G survey meter. Experiments involved a water tank phantom ( $60 \times 30 \times 30 \text{ cm}^3$ ) representing the patient that was uniformly

irradiated using a 3 mm spot diameter proton pencil beam with 10 cm modulation width, 19.95 cm distal beam range, and 10×10 cm<sup>2</sup> field size [ID 444984, 473762].

The environmental doses from stray neutrons in the vicinity of a solid slab phantom as a function of beam energy, field size and modulation width, using the proton pencil beam scanning (PBS) technique have been determined. Measurements were carried out using two extended range WENDI-II rem-counters and three tissue equivalent proportional counters. Detectors were suitably placed at different distances around the RW3 slab phantom. Beam irradiation parameters were varied to cover the clinical ranges of proton beam energies (100 – 220 MeV), field sizes ((2×2) – (20×20) cm<sup>2</sup>) and modulation widths (0–15 cm) [ID 488861].

Long-term collaboration is maintained with the Joint Institute for Nuclear Research (JINR), Dubna, Russia. M. Davidková co-supervised Ph.D. studies of C. Oancea performed in collaboration between our laboratory, Dzhelepov Laboratory of Nuclear Problems JINR, and the Faculty of Physics, University of Bucharest, Bucharest, Romania. C. Oancea successfully defended her thesis in October 2018. Perturbations of radiation field caused by metallic implants in pencil proton beam therapy have been studied using track-etched detectors applied as LET spectrometers. Detectors were placed behind simple phantoms containing stainless steel and titanium materials used as hip and dental implants [ID 488757, 477475]. Specific nuclear interactions in photographic emulsions were investigated in cooperation with Veksler and Baldin Laboratory of High Energy Physics JINR. At first, calibration of ion ranges in emulsions has been performed and manual measurements were compared with automated image processing measurements [ID 486347]. Research continued with computer measurements of ranges and angles of collinear cluster tri-partition of heavy nuclei implanted in emulsions along with fragmentation of boron atoms caused by thermal neutrons [ID 458942]. Next work was focused mainly on the ternary fission in emulsions irradiated with <sup>252</sup>Cf source [ID 484258]. The latest topic of interest was estimation of neutron fluxes using standard photoemulsions and emulsions enriched with boron [ID 523896]. International cooperation on nuclear track emulsions is performed within the Becquerel project [becquerel.jinr.ru].

The team works in close contact with other departments and research groups within NPI. Together with colleagues from the Department of Accelerators, we contributed to the development of two novel methods of mass production of fluorescent nanodiamonds. First, a proton beam irradiation of a circulating aqueous colloidal solution was employed [ID 458079]. Second, an easily scalable method for rapid isotropic irradiation of nanomaterials by light ions using in-situ nuclear reaction was developed [ID 498523].

In the framework of informal cooperation with the Institute of Physics of CAS, the Institute of Plasma Physics of CAS and the Faculty of Electrical Engineering, Czech Technical University in Prague, team members H. Orčíková, K. Turek, and R. Wagner participated in fusion technology experiments with Z-pinch plasma devices. The experimental studies of intense laser interactions with plastic targets were performed at the PALS facility (Prague Asterix Laser System). Team members contributed by measurements of energies of produced ions using solid-state nuclear track detectors, calibration of track detectors in the neutron field of the Am-Be source and calibration of radiochromic films by <sup>60</sup>Co gamma rays [ID 443444, 471462, 501864, 520833, 501858].

Biological effects of ionizing radiation depend crucially on microscopic radiation quality, namely the spatial structure of energy depositions along the particle tracks. As part of our basic

research, we seek to define links between radiation track structure and multi-scale biological consequences of irradiation.

Our long-term interest are biological consequences of radiation action on the subcellular level, where we use DNA plasmids as a model repair-free experimental system. In cooperation with Prof. L. Sihver from the Chalmers University of Technology, Sweden, European Space Agency, and Dr. E. Ukraintsev from the Institute of Physics of the CAS, we have continued in studies of clustered DNA damage by different radiation sources (heavy ions and gamma) under different scavenging conditions. We have particularly focused on proton-induced effects. We have complemented previously published results on the yields of strand breaks and base damage with fragmentation yields detected using atomic force microscopy. The yields of DNA damage were measured in solution of coumarin-3-carboxylic acid, a scavenger of hydroxyl radicals, to control the extent of the indirect radiation effects. The scavenger was also used to precisely measure hydroxyl radical yields, which were compared with Monte Carlo simulations. The results revealed that under the given conditions, the indirect effects caused by radical attack are responsible for most of the DNA damage [ID 450488, 448614]. Further, we have developed an algorithm for image analysis of plasmid molecules or similar objects imaged with AFM [ID 499497]. The results have revealed that the yields of radiation-induced DNA fragments estimated by standard measurement techniques underestimate the yields observed with atomic force microscopy (AFM) or calculated by track-structure studies [ID 509919].

In a follow-up project, partially funded by the Czech Science Foundation (project n. 17-03403Y), we focused on the effect of concentration and length of the DNA plasmid molecule. While the results demonstrated the impact of the plasmid length, no significant difference was experimentally observed between two used concentrations of the plasmid in the solution [ID 523903]. The experimental work was complemented by the development of a Geant4 application targeted at improving the dosimetry part of radiobiological experiments [ID 494791, 489134] and a framework for computation of radiation induced damage on dynamic models of plasmid DNA described at atomic level [ID 491161].

In collaboration with the group of Ing. L. Juha, Ph.D. from the Institute of Physics of the CAS, we participated in the studies of primary processes of radiation damage caused by extreme UV and soft X radiation. We contributed to a testing of a new compact laser plasma source of soft X-rays for radiobiology studies. The source developed in the Institute of Optoelectronics, Military University of Technology (Warsaw, Poland) is based on a laser produced plasma as a result of irradiation of a double-stream gas puff target with nanosecond laser pulses from a commercially available Nd:YAG laser. The source allows irradiation of samples with soft X-ray pulses in the “water window” spectral range (wavelength: 2.3–4.4 nm; photon energy: 280–560 eV) in vacuum or a helium atmosphere at very high-dose rates and doses exceeding the kGy level. Single-strand breaks (SSB) and double-strand breaks (DSB) induced in DNA plasmids pBR322 and pUC19 have been measured [ID 454692, 464879]. Dose-rate effects in breaking DNA strands by short pulses of extreme ultraviolet laser pulses were also studied [ID 448547, 490027]. The yields of single- and double-strand breaks (SSB and DSB) were determined as a function of the incident photon fluence. DNA cross-linking revealed by gel electrophoresis was confirmed also by AFM. Both SSB and DSB yields decreased with dose rate increase. Quantum yields of SSBs at the highest photon fluence were comparable to yields of DSBs found after synchrotron irradiation. The average SSB/DSB ratio decreased only slightly at elevated dose rates.

Experimental radiobiology studies at the cellular level have been successfully carried out especially to study the effects of protons and heavy charged particles. In order to describe effects of low energy ions to cell population, a particular setup for irradiation of cell monolayers at microbeam of Tandetron accelerator 4130 MC at the Laboratory of Nuclear analytical methods NPI have been designed and tested. The first results on effects of low energy protons and alpha particles have been obtained [ID 502236].

Detailed analysis of cell response to heavy ion irradiation has been carried out in collaboration with biologists from the Institute in Biophysics of the CAS in Brno, namely with the team of RNDr. M. Falk, Ph.D. Using advanced immunofluorescence techniques, the complexity of DNA damage induced by boron and neon ions accelerated at similar LET values ( $\sim 135 \text{ keV}/\mu\text{m}$ ) and low energies (8 and 47 MeV/n, respectively) have been studied [ID 492530].

An important and worthy direction of research is radiobiology of stem cells. Radiotherapy plays a significant role in brain cancer treatment. However, the use of this therapy is often accompanied by neurocognitive decline that is, at least partially, a consequence of radiation-induced damage to neural stem cell populations. Our findings describe features that define the response of neural stem cells to ionizing radiation [ID 509936]. Our findings describe the increased transcriptional activity of p53 targets and proliferative arrest after irradiation. Moreover, we showed that most cells do not undergo apoptosis after irradiation but rather cease proliferation and start a differentiation program. The current knowledge about neural stem cells and the molecular mechanisms underlying changes in neural stem cell niches after brain radiotherapy have been summarized in [ID 509893].

We performed also a comparison of breast cancer cell line MCF7 and human adipose-derived stem cells (ADSC) response to irradiation by the same doses of megavoltage X-rays cells. The cell growth, the induction of apoptosis and the expression of selected genes were analyzed. Irradiated MCF7 related to their control sample grow slower than ADSC and they undergo apoptosis in much higher levels than ADSC. This was confirmed by real-time PCR as well, where the expression of apoptotic genes was found to be considerably higher for MCF7 than for ADSC [ID 525572].

Many of our experiments have been focused on the biological efficiency of spread-out Bragg peaks of clinical proton beams. The experiments in active scanning pencil beams at the Proton Therapy Center in Prague (PTC) have been carried out. We have performed precise dosimetry measurements to position cell monolayers at the beginning, at the middle and at the distal edge of the spread out Bragg peak (SOBP) and we have followed different biological endpoints in irradiated normal human skin fibroblasts [ID 477333]. 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 investigated clinical implications of a variable relative biological effectiveness (RBE) on proton dose fractionation [ID 459898]. Human fibroblasts (AG01522) at four positions along a clinical SOBP were subjected to various fractionation regimens with an interfraction period of 24 hours. Cell killing RBE variations were measured using standard clonogenic assays and parameterized using a linear quadratic formalism. Significant variations in the cell killing RBE for fractionated exposures along the proton dose profile have been observed. RBE increased sharply toward the distal position, corresponding to a reduction in cell sparing effectiveness of fractionated proton exposures at higher LET. The effect was more pronounced at smaller doses per fraction. Experimental survival fractions were adequately predicted using a linear quadratic formalism assuming full repair between fractions. Our studies [ID 444984,

473762, 459898, 477333, 488757, 477475, 489292] provide valuable datasets that can be used by the modeling community for the optimization of proton therapy planning.

Our long-term fruitful cooperation with MedAustron, particle therapy center in Wiener Neustadt, Austria, mainly with Dr. M. Puchalska, resulted in mobility project supported by Ministry of Education, Youth and Sports in 2019 (project n. 8J19AT019, 2019-2020). The project aims on radiobiological and dosimetric comparison of proton beams operated in MedAustron, Wiener Neustadt, Austria and Proton Therapy Center Czech, Prague, Czech Republic. Using in vitro cellular plasmid DNA models and passive track etched dosimeters we address variations of relative biological effectiveness and linear energy transfer outside and inside the clinical proton beams.

Biological dosimetry is a method of retrospective, individual dose assessment. Cytogenetic methods are well established and accepted as biodosimetry techniques of humans therapeutically, occupationally or accidentally exposed to ionizing radiation. The number of radiation-induced micronuclei, small extranuclear bodies resulting from chromosome fragments or the whole chromosomes secluded from daughter nuclei during mitosis, reflects the level of chromosomal damage and relates to an absorbed dose and quality of incident ionizing radiation. We determined the micronucleus formation in normal human fibroblasts exposed to 30 MeV protons and  $^{60}\text{Co}$  gamma radiation. We found a linear increase in binuclear cells containing micronuclei for absorbed doses from 1 to 5 Gy for both radiation modalities. However, the total number of micronuclei in binuclear cells follows a linear-quadratic dose dependence. In case of human exposure to mixed radiation fields or high LET radiation, the proportion of binuclear cells containing micronuclei from all binuclear cells can serve as a good biomarker of radiation induced DNA damage [ID 448253]. We participated also in large experimental comparison of the induction and persistence of different radiation exposure biomarkers in human peripheral blood in vivo [ID 488736].

Simulation tool RADAMOL developed by our team has been maintained and extended by a module on charge transfer simulation [ID 465449]. In order to share our experiences in the domain of DNA radiation damage modelling with a wide scientific community, we collaborate with Dr. Sebastien Incerti, developer of Geant4 toolkit and spokesperson of Geant4-DNA collaboration (<http://geant4-dna.org/>) [ID 454108]. As a member of the Geant4-DNA collaboration, V. Štěpán contributed to the development of biological target models (Czech Science Foundation project n. 17-03403Y). We also participated in the Standard DNA Damage (SDD) data format development [ID 504301], that aims to provide data interchange structure in between different radiation DNA damage evaluation codes.

In 2018, the team was joined by P. Kunderát, who has been involved in the development of PARTRAC biophysical simulation tool at the Helmholtz Zentrum Munich since 2008. PARTRAC belongs to the most advanced track-structure based codes for the simulations of radiation-induced biological effects. It ranges from modelling particle tracks over assessing direct and indirect damage to DNA to following the repair of DNA double-strand breaks and the formation of chromosome aberrations. Continuing his fruitful international collaboration, Dr. Kunderát's research activities are mainly directed at further developing this tool towards the critical endpoint of radiation-induced cell killing and towards enabling its wider applications in radiation biology and medicine [ID 523897]. In addition, he has contributed to the assessment of personalized long-term health risks from radiotherapy [ID 523892].

## Research activity and characterisation of the main scientific results

### Cyclotron U-120M

U-120M is a multipurpose multiparticle accelerator which can be tuned according to the type of particles (p, D,  $^3\text{He}^{2+}$ ,  $^4\text{He}^{2+}$ ) and the use (internal/external beam) in a wide range of energies (1–55 MeV). This cyclotron is a unique facility because it is operated both in positive (extraction p, D,  $^3\text{He}^{2+}$ ,  $^4\text{He}^{2+}$ ) and in negative mode (acceleration  $\text{H}^-$  resp.  $\text{D}^-$  and subsequent extraction of p, D). Accelerated beams with currents from a few nA up to tens of  $\mu\text{A}$  were extensively used within the frame of the CANAM „Open Access“ for a wide range of experiments in basic and applied research. A list of basic and applied research experiments follows:

- production of fluorescent nanodiamonds (FND) [1–8],
- irradiation of biological samples [9],
- astrophysical experiments,
- production of homologues of super heavy elements (rarely accessible beams of  $^3\text{He}^{2+}$ ) [10],
- measurement of excitation functions and nuclear data [15–22],
- testing of cosmic rays detectors (mainly TimePix and MediPix type) [12,13],
- determination of radiation hardness of electronic components [11],
- calibration sources [23–27],
- determination of damage to proton-irradiated samples (DPA),
- fusion relevant neutronics experiment,
- experimental simulation of neutron fields of future fusion material tester IFMIF [14],
- production of conventional and unconventional radionuclides for production and research of radiopharmaceuticals [28–29].

In connection with neutron targets, the U-120M cyclotron is a unique intensive source of fast neutrons. An average beam time is approx. 3 000 hours/year.

### Target technology

For experimental groups following targets and related systems were designed, tested and implemented:

- solid and liquid targets for production of fluorescent nanodiamonds [1–8],
- a prototype of a target for production of fluorescent nanodiamonds cooled by liquid nitrogen,
- a target for proton irradiation of W and Fe samples for DPA studies,
- various holders for irradiation of biological materials and samples [9],
- a new Be target with neutron flux up to  $1 \times 10^{11}$  resp.  $1 \times 10^9 \text{ n cm}^{-2} \text{ s}^{-1}$  at the sample site. For this target a new neutron collimator (thickness approx. 2.6 m) was designed and installed. This system enables collimation and extraction of fast neutron fluxes into a hall with low electromagnetic interference and free space approx. 20 m. This layout enables to perform neutron Time Of Flight (nTOF) spectrometric measurements even with the existing time structure of the U-120M beam.
- a new PET target with a water beam energy degrader,
- a new extended PET target.

### Cyclotron TR-24

The TR-24 cyclotron provides proton beams with energies from 18 MeV to 24 MeV. It is equipped with an axial injection system with an external ion source of the CUSP type, which significantly increases available current of the accelerated beams (up to 300  $\mu\text{A}$ ).

Within the Open Access regime of the project CANAM the TR-24 beams were mainly used for testing new target stations intended for production of new medical longer-lived radionuclides. The beam time was also intensively used for testing of the Be-based High Power Neutron Converter being developed for production of high fluxes of fast neutrons.

A commercial production of PET radionuclide  $^{18}\text{F}$  and generator  $^{81}\text{Rb}/^{81\text{m}}\text{Kr}$  for lung ventilation studies was implemented on the cyclotron as well.

### Target technology

Following the successful commissioning of the TR-24 cyclotron, considerable efforts were made to a design of technological subsystems necessary for the implementation and operation of new target stations. The systems include autonomous high-pressure (10 bar) and low-pressure (3.5 bar) water cooling circuits and a He cooling circuit for cooling the separating target foils with He gas.

A design and implementation of the new targets including high-power ones for production of novel medical radionuclides and special calibration sources have been carried out and tested:

- a new target for production of  $^{81}\text{Rb}/^{81\text{m}}\text{Kr}$  generator
- a target for production of  $^{83}\text{Rb}$  (86.2 d, reaction  $^{\text{nat}}\text{Kr}(p,xn)^{83}\text{Rb}$ ). The radionuclide serves for manufacturing of  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  sources, where the daughter  $^{83\text{m}}\text{Kr}$  (1.83 h) provides unique set of monoenergetic electrons suitable for calibrations crucial for the large experiments KATRIN and XENON.

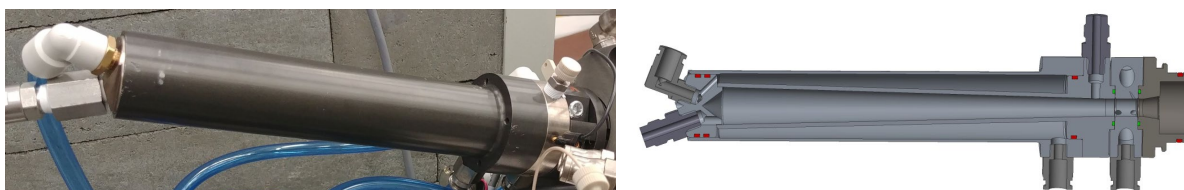


Fig. 1 A new gaseous target developed for large-scale production of  $^{83}\text{Rb}$ .

A system of control, management and remote handling of the irradiated liquid product was designed for a high-power liquid target for the production of  $^{18}\text{F}$  as well as for the target for production of  $^{81}\text{Rb}$  for manufacturing  $^{81}\text{Rb}/^{81\text{m}}\text{Kr}$  generator.

### New projects

During this period in question, very intensive development and implementation of a research program: **Modernization of cyclotron-based neutron generators** solved within the CANAM OP project was solved. The project includes the development of the U-120M cyclotron proton beam bunching system for neutron spectrometry using the TOF method and the development of a High power proton-neutron converter for production of fast neutrons on the TR-24 cyclotron.

### Project of a new bunching system with multi-orbital proton beam extraction from the U-120M cyclotron

The system is based on a unique pulsed vertical deflection of the selected final orbits of the internal accelerated beam of the  $\text{H}^-$  ions to an extractor-stripper (a thin carbon foil positioned below the cyclotron median plane). A set of home-made programs have been developed for simulations and parameters determination (i.e. dimensions of the deflection system, parameters of the pulsed high voltage power supply, position of the stripper, beam trajectories, beam parameters, beam losses, Be target position etc.). The system was successfully implemented and tested. It provides beam bunch interval up to 1000 ns range of a defined beam time structure (up to beam bunch period to beam bunch width ratio min 100). The parameters of the bunching system will be supplemented with the parameters of European nTOF devices (GELINA Geel, NFS Ganil).



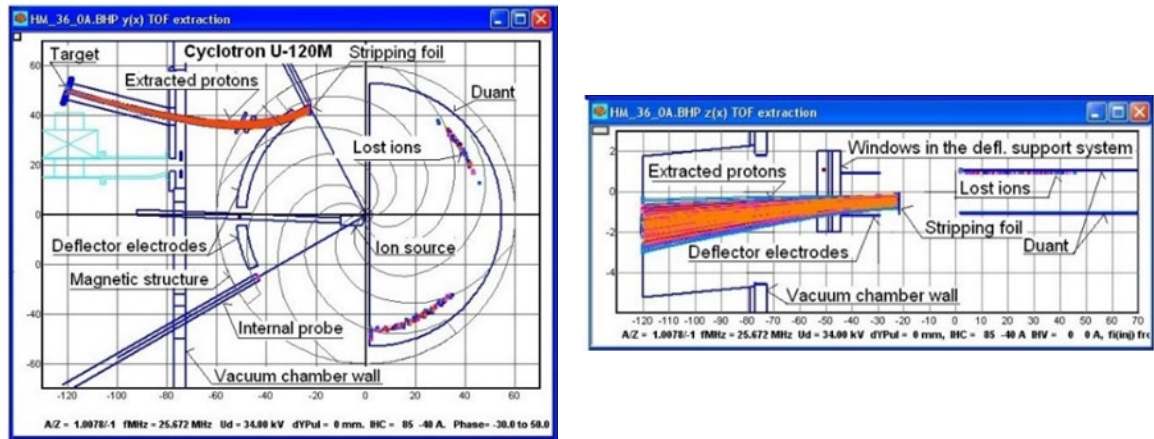


Fig. 2 TOF extraction system layout.

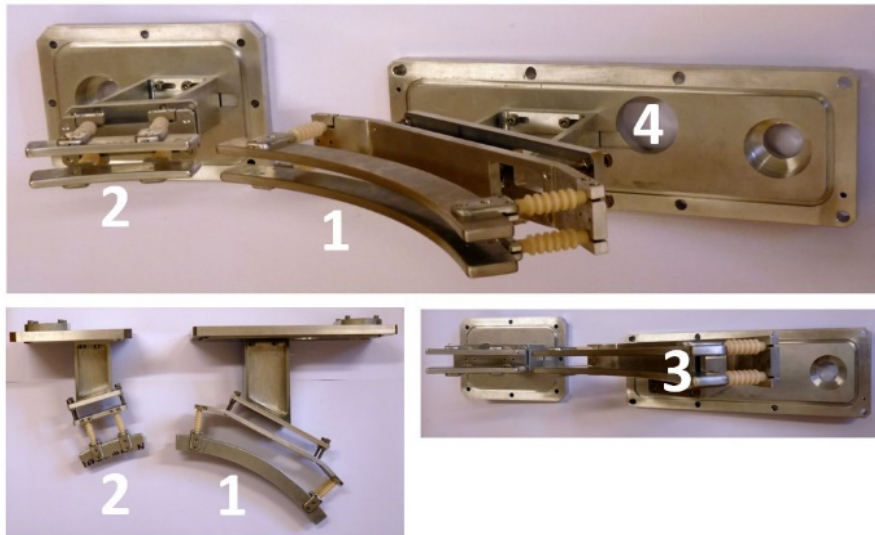


Fig. 3 Two section of the deflection bunching system: 1 – 1<sup>st</sup> deflector section, 2 – 2<sup>nd</sup> deflector section, 3 – beam entry, 4 – beam exit window

Bunching system includes design and implementation of deflection electrodes of internal accelerated  $H^-$  ion beam supplied by the high voltage 12kV pulse with duration of 40 ns. A unique high-power high voltage pulsed power supply (HV switch), working to the capacitor load, based on the SiC power MOSFET transistors was also developed.



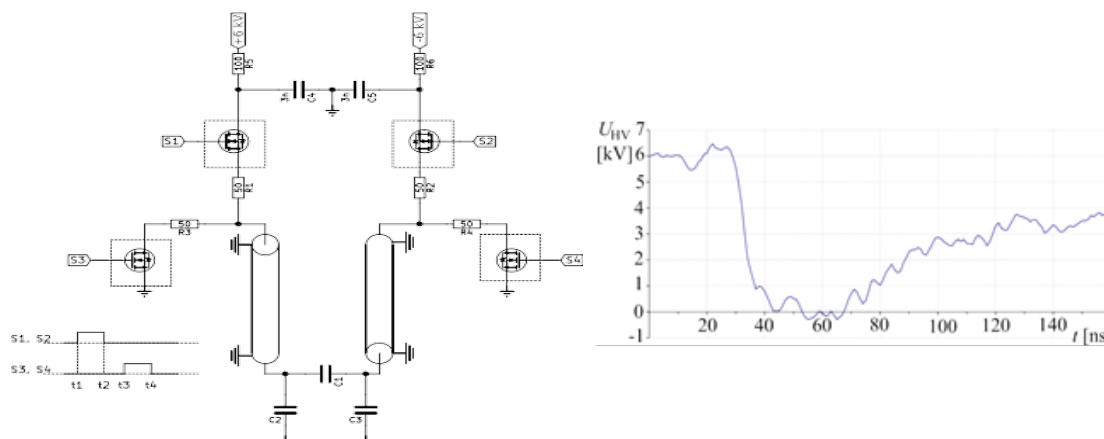


Fig. 4 Wiring diagram of HV switcher with deflector and measured rising edge of the  $\frac{1}{2}$  HV switch pulse.

### The high-power proton-neutron converter (HPNC) based on the TR-24 cyclotron for testing ITER diagnostic components

The HPNC uses high intense proton beam of the TR-24 cyclotron (reaction  $p(24\text{MeV}) + \text{Be}$ ) for production high fluxes of fast neutrons. The solution and subject of the stage was the original development and construction of a target cooler enabling the installation of irradiated samples at a minimum distance from the target and capable of dissipating extremely high heat load of the target by a proton beam ( $\leq 4 \text{ kW/cm}^2$ ). This value several times exceeds the value of  $\leq 0.5 \text{ kW/cm}^2$  characterizing converters cooled by convection flow of medium.

The generator will provide a neutron flux density up to  $10^{12} \text{ n cm}^{-2} \cdot \text{s}^{-1}$ . It will be the highest value compared to current or completed top generators in the energy range of thermonuclear neutrons (NFS Spiral-2 Ganil France, LENS University Indiana USA and University Jyväskylä Finland). With its spectral composition of the field ("ITER-like"), it will offer development of a new approach to radiation tests of ITER diagnostics so far performed at fission research reactors with unsuitable spectral composition of neutron field.

For the design of the converter cooling system, a research analysis of heat transfer by convection for a nested nozzle was performed and critical values of the heat transfer coefficient were defined. Data for computational simulation of the function of the cooling nozzle of the neutron converter were prepared. In cooperation with HVM Plasma s.r.o., a simulation of the kinematic characteristics of the cooling nozzles (ANSYS code) was performed and evaluated, a physical project was processed and subsequently the neutron converter chamber in the test variant was designed and manufactured.

The efficiency of the proposed unique cooling system for high heat dissipation from Be target (protons of 24 MeV energy and 230  $\mu\text{A}$  beam current) was verified for safety reasons using diagnostics performed on an Al dummy target. The dummy target was equipped with three sensors positioned axially in drilled holes that monitor target temperature during the tests. A four-collimator was also designed and implemented for on-line monitoring of the high current beam position during irradiations.

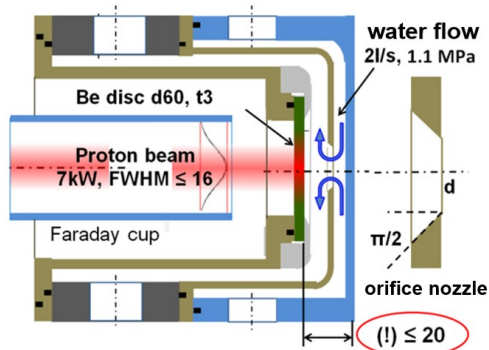


Fig. 5 Arrangement of target chamber with Be disc, Faraday cup and orifice nozzle.

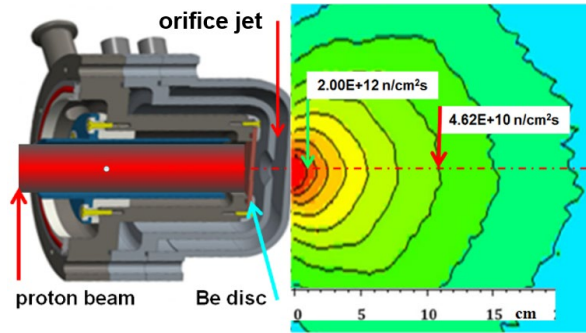


Fig. 6 Simulated neutron field.

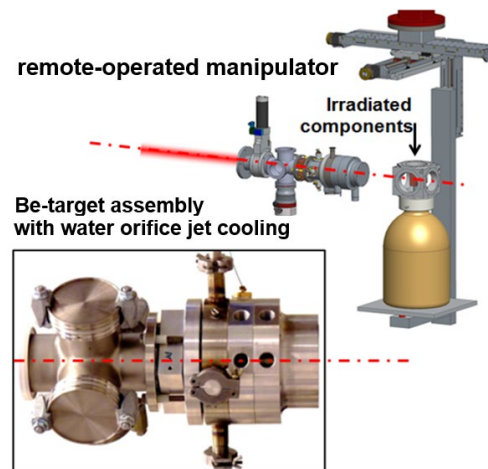


Fig. 7 Model of arrangement and picture of High-Power Neutron Converter.

A manipulator of irradiated samples and local shielding of target irradiation positions on the TR-24 cyclotron beam lines were completed as well.

Production of neutrons with a Be target was successfully verified at the beam current 100  $\mu\text{A}$ , the corresponding neutron flux was  $6 \times 10^{11} \text{ n cm}^{-2} \text{ s}^{-1}$ . Even at one-third of the cyclotron power, the TR-24 HPNC is currently the most efficient fast neutron radiation generator and potential tester of ITER diagnostic technology components (with a maximum flux of  $2 \times 10^{12} \text{ n cm}^{-2} \text{ s}^{-1}$  at 300  $\mu\text{A}$ ).

### Microtron MT-25

In 2015-2019, the microtron served as a source of electron and photon beams for a wide range of experiments. Various materials were irradiated for the radiation polymerization. For example, it was successfully irradiated a conceptually new, microfibrinous, biodegradable functional material prepared from a modified polysaccharide showing strong potential as material for wound healing. Several dozens of irradiations were performed for photon activation analysis (PAA), which allows determining selected elements in different materials. This post ensures fast sample transport between the irradiation position and the HPGe detector. For this method a pneumatic post in microtron laboratory was installed. This system will greatly extend IPAA capabilities, as it will allow determination of the short-lived isotopes. A methodology for routine irradiation of  $\text{PbWO}_4$  crystals was developed and then several thousands of these crystals were analyzed. Different types of detectors in electron and photon beams were tested, especially Timepix and Medipix and also the Liulin silicon detector, specially designed to measure cosmic rays on aircraft decks. Luminescent nanodiamonds were also regularly produced on the microtron.

### Radiochemical laboratories

A complex of the radiochemical laboratories was built over the cyclotron TR-24 – it wasn't only routine supply of commercially available items, but an attempt to combine established technologies with new solutions (two remotely controlled target systems connected by pneumatic post with the hot cells and fume hoods, and automated transport of the samples from the radiochemical to analytical laboratory). The result is a compromise between the budget and our vision. The new complex will serve for the production and research of novel positron emitters and theranostic radionuclides.



Fig. 8 Radiochemical laboratory over the cyclotron TR-24 – a view on the four hot cells and two radiochemical fume hoods intended for target processing, separations and labellings.

### Nuclear reaction data

Within the IAEA Co-Ordinated Research Project no.17461 we re-measured with great care the excitation functions of deuteron-induced reactions on naturally monoisotopic  $^{89}\text{Y}$  and proton-induced reactions on natural molybdenum. Besides major focus on medically relevant  $^{89}\text{Zr}$ ,  $^{99\text{m}}\text{Tc}$  and  $^{99}\text{Mo}$  and beam monitor  $^{96\text{m}+g}\text{Tc}$ , we obtained altogether 36 excitation functions, some of them measured for the first time (e.g. formation of the long-lived  $^{97\text{m}}\text{Tc}$ ) [15,16]. The experimental material was compared with previously published data and prediction of the nuclear reaction model code TALYS. Critical evaluation of the available cross-sections resulted in our recommended excitation function and thick target yields for cyclotron production of  $^{99\text{m}}\text{Tc}$  and for the monitoring reaction  $^{\text{nat}}\text{Mo}(p,x)^{96\text{m}+g}\text{Tc}$  and in recommendations regarding optimized production of the medical radionuclides. Experiments revealed also discrepancies between the recommended cross-sections deuteron beam monitoring reactions.

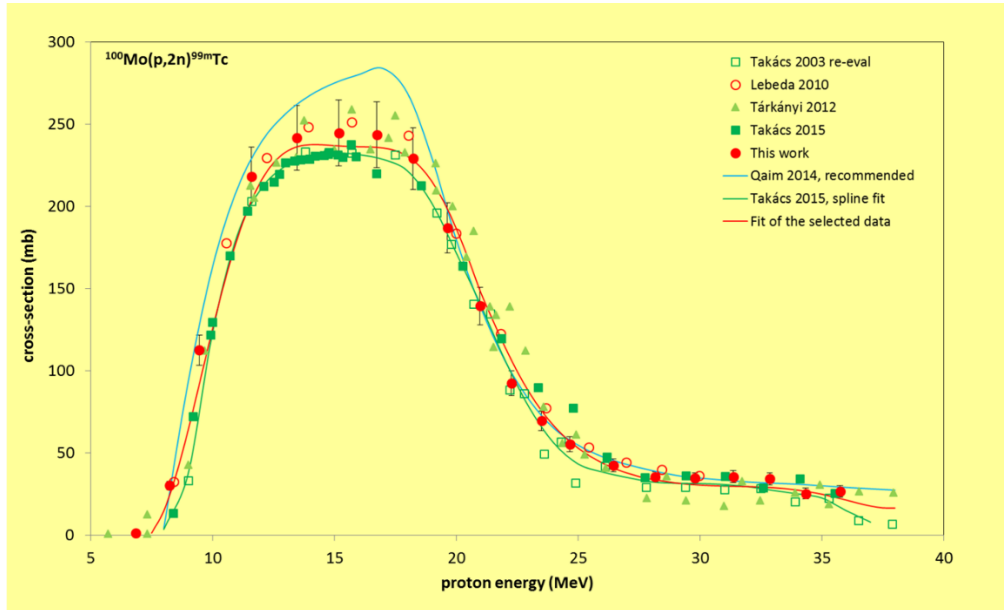


Fig. 9 Selected experimental cross-sections for the  $^{100}\text{Mo}(p,2n)^{99\text{m}}\text{Tc}$  reaction and their fit in comparison with previously published recommended cross-sections [16].

The ambitious IAEA project encompassed critical evaluation of wide spectrum of monitoring reactions and reactions for production of diagnostic and therapeutic radionuclides providing more reliable data for many of them. It was summarized in four extensive publications [17–20].

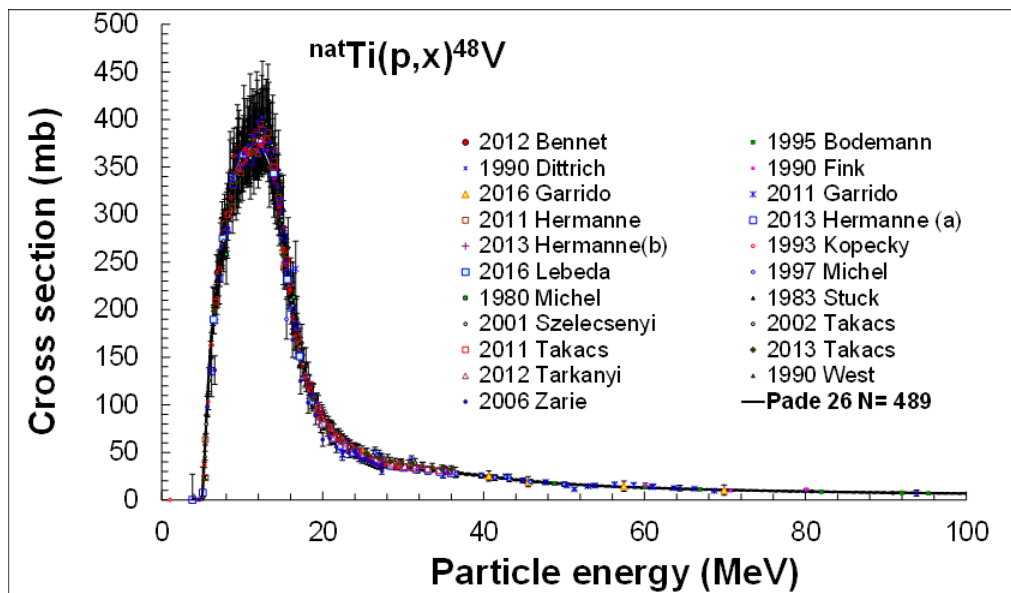


Fig. 10 Selected experimental data for the monitoring reaction  $^{\text{nat}}\text{Ti}(p,x)^{48}\text{V}$  and their Pade fit defining recommended cross-sections [17]

In the framework of the CANAM OP project (CZ.02.1.01/0.0/0.0/16\_013/0001812), we measured proton- and deuteron-induced reactions on naturally monoisotopic gold (altogether 14 excitation functions) with special regard to formation of novel theranostic radionuclide  $^{197\text{m,g}}\text{Hg}$  [21,22]. The data were critically evaluated and compared with TALYS prediction and previously published values. The measurement revealed significant discrepancy in the  $^{197\text{m}}\text{Hg}$  decay scheme that initiated its revision. Moreover, measurement provided a new data for the  $^{\text{nat}}\text{Cu}(d,x)^{63}\text{Zn}$ .

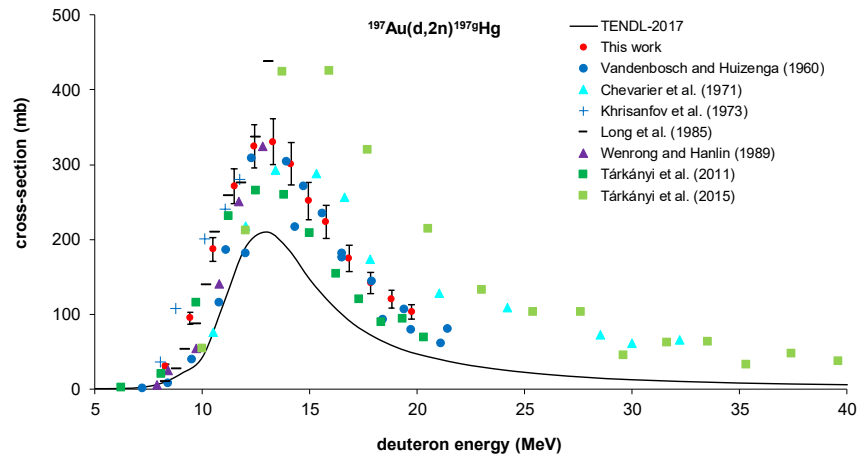


Fig. 11 Cross-sections for the  $^{197}\text{Hg}$  formation in gold activation by protons. Obvious scattering of the available experimental material and limits of the TALYS nuclear reaction model code [21].

All the measured data were included in the data base EXFOR.

### Radionuclides production for physics and medicine

A lot of attention was paid to production of  $^{83}\text{Rb}$  and manufacturing of calibration sources  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  for the KATRIN experiment. We prepared several generators  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  based on zeolite spherules with activities exceeding 1 GBq and delivered them to KIT, Karlsruhe. KATRIN spectrometer was put in operation in July 2017 with one of the sources [23,24] and since that time calibration of the system with  $^{83\text{m}}\text{Kr}$  conversion electrons plays a key role in the data acquisition reliability [25]. The results allowed for the first improvement of the neutrino mass upper limit [26]. Besides the gaseous source of  $^{83\text{m}}\text{Kr}$ , we provided  $^{83}\text{Rb}$  in tungsten furnaces for production of the implanted solid calibration sources at the university of Bonn.

The solid/gas  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  generators has found its use also in XENON experiments and related fields, so we provided several academic sites with the custom-made zeolite-based sources that seem to be rather versatile research tool [27].



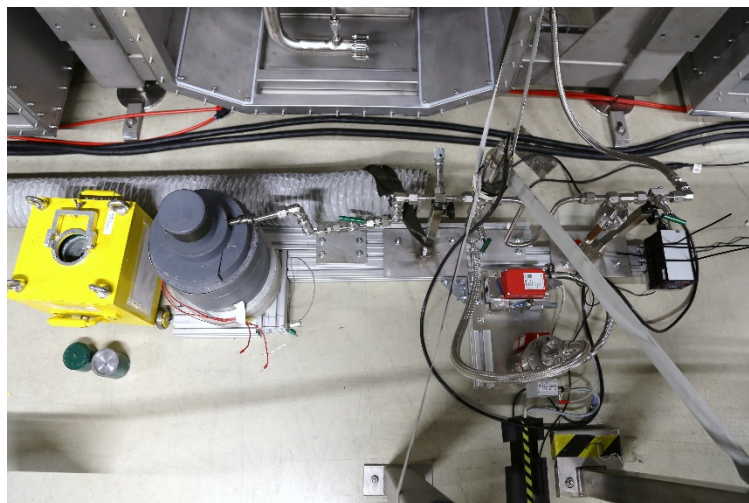


Fig. 12 Generator  $^{83}\text{Rb}/^{83\text{m}}\text{Kr}$  – setup at the first measurement of the conversion electrons from decay of gaseous  $^{83\text{m}}\text{Kr}$  in the KATRIN main spectrometer in July 2017

Regarding medically relevant radionuclides, production of  $^{64}\text{Cu}$ ,  $^{89}\text{Zr}$ ,  $^{197\text{m,g}}\text{Hg}$  and  $^{203}\text{Pb}$  has been studied and implemented. In the latter two cases, the superiority of deuteron over proton activation (in terms of the yield, isomeric ratio and radionuclidic purity) resulted in choice of this beam for their production. The radionuclides  $^{64}\text{Cu}$ ,  $^{89}\text{Zr}$  were provided to IMTM Olomouc in the framework of the EATRIS project,  $^{197\text{m,g}}\text{Hg}$  to HZDR Rossendorf (open access, CANAM) and  $^{203}\text{Pb}$  to Semmelweis University Budapest.

In 2019, a commercial collaboration on a novel separation method for high specific activity  $^{177}\text{Lu}$  production with IOCHB has been established and continues.

### Labelled compounds

The monoclonal antibody IgG M75 specific towards human carbonate dehydratase IX (CA IX) present in many hypoxic tumours was successfully conjugated with novel copper-specific chelator “phosphinate”. This immunoconjugate was easy to label with positron emitters  $^{61}\text{Cu}$  and  $^{64}\text{Cu}$  in high radiochemical yield providing the product stable in vitro in human serum at 37 °C. In vitro uptake in the HT-29 and NIH 3T3 cell lines demonstrated specific binding to the carbonate dehydratase IX. Finally, the biodistribution of the radioimmunoconjugate  $^{64}\text{Cu}$ -SCN-PS-IgG M75 in the mouse model inoculated with HT-29 cells imaged with  $\mu\text{PET}/\text{CT}$  exhibited increasing tumour to background ratio in time. The obtained results suggest high potential of this radioimmunoconjugate for diagnostics of the CA IX expressing tumours [28,29].

Within the EATRIS project, we have implemented production of  $^{18}\text{F}$ FDDNP, an Alzheimer plaques tracer that is provided to a private Israel company for evaluation of a new method of their removal on regular basis.

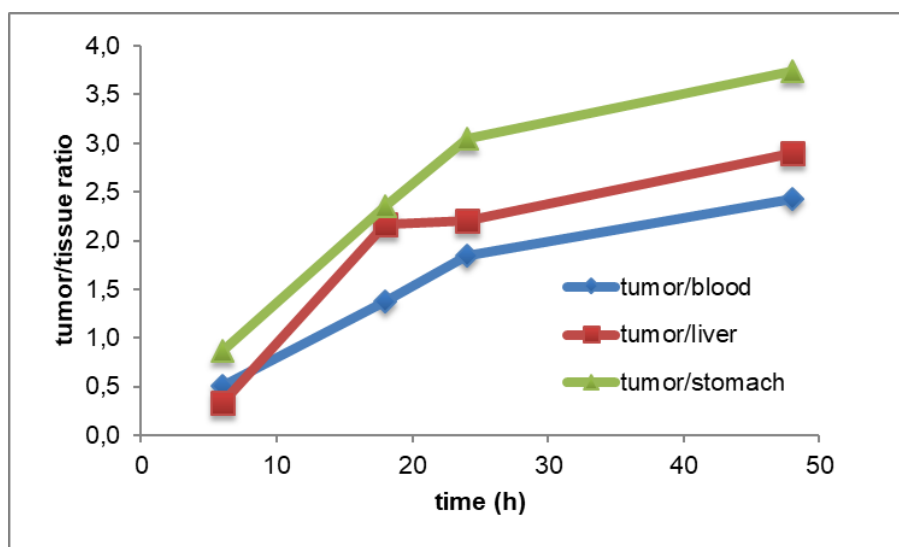


Fig. 13 Accumulation of the monoclonal antibody IgG M75 labelled with  $^{64}\text{Cu}$  using the chelator “phosphinate” in tumour tissue (subcutaneously implanted human colorectal carcinoma, HT-29) increases in time compared to other tissues. As an example, we display ratio of the accumulation in tumour tissue and in blood, liver and stomach as a function of time [29].