



BOOK OF ABSTRACTS

PLASMA CHEMICAL TECHNOLOGIES
NANOMATERIALS & HYDROGEN PRODUCTION

H_2

EPR

*“It is through science that we prove, but through intuition that we
discover”*

Jules Henri Poincaré

3rd international workshop: “Plasma Chemical
Technologies as the Important Approach to the
(Nano)Materials and Hydrogen Production
(PLASCHEMAT)”

Editor: Dr. hab. Maksym Buryi, Ph.D.

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Foreword

It is with great pleasure that we welcome you to this workshop dedicated to **Nanomaterials and Hydrogen Production**, a field that lies at the intersection of advanced materials science and the urgent global pursuit of sustainable energy solutions. This event gathers researchers, engineers, and thought leaders from around the world to share insights, foster collaboration, and advance the frontiers of innovation.

Nanomaterials, with their unique physical and chemical properties, are proving to be key enablers in this space enhancing catalytic activity, improving energy efficiency, and enabling novel technologies across the hydrogen value chain. Hydrogen, as a clean and versatile energy carrier, is increasingly seen as a cornerstone of the future low-carbon economy. Its production, storage, and utilization present both opportunities and challenges that demand interdisciplinary solutions.

This abstract book reflects the breadth and depth of research being undertaken across these critical domains. From novel synthesis techniques and functional nanostructures to emerging thermal plasma hydrogen production pathways including photocatalysis, and biomass reforming, the contributions collected here showcase a vibrant scientific community committed to transformative change.

We hope that the discussions sparked during this workshop will not only deepen our collective understanding but also inspire new collaborations that drive practical applications and scalable solutions. As the world seeks to transition to cleaner energy systems, the role of fundamental and applied research has never been more vital.

We thank all contributors, speakers, and participants for their engagement and look forward to a productive and inspiring exchange of ideas.

In Prague, 08.06.2026



Sincerely,

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Effects of Thermal Plasma Treatment on Structural and Surface Properties of Oxide Materials

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Thermal plasma treatment offers a powerful approach for tailoring structural, morphological and defect-related properties of materials under extreme thermochemical conditions, enabling transformation of both inorganic and organic systems into potentially value-added products [1,2]. In inorganic systems, selected oxide materials including ZnO, WO₃, Y₂O₃ and Al₂O₃ are treated as powders or surface layers deposited on substrates. Plasma exposure leads to surface restructuring, modification of defect populations and changes in crystallinity; in some cases, partial volatilisation followed by condensation results in the formation of new phases or nanostructured features [1,3]. Plasma processing of organic feedstocks, for instance tomato waste, enables the formation of carbon-rich nanostructured materials, such as carbon nanoparticles, with broad application potential [2,4], and under suitable conditions these materials can serve as precursors for advanced carbon-based systems, including carbon quantum dots relevant for photoluminescence, sensing and optoelectronics [4]. The influence of plasma treatment is analysed using a combination of structural and spectroscopic techniques, providing insight into defect states, morphology and phase composition. Previous work has shown strong sensitivity of defect-related properties of oxide materials to plasma exposure, and this study extends the approach to additional oxide systems with different chemical and structural characteristics [1,5]. The results demonstrate the versatility of thermal plasma for controlled modification of inorganic and organic materials, enabling the design of functional materials for applications in electronics, optics and energy technologies.

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Characterization of NMC Black Mass as a Potential Catalyst for Plasma Pyrolysis

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NMC black mass is a complex powder derived from the mechanical processing of spent nickel–manganese–cobalt (NMC) lithium-ion batteries. It consists mainly of active electrode materials after the removal of outer casings, current collectors such as aluminium and copper foils, and plastic insulation. Although this material is traditionally targeted for metal recovery and battery recycling, its high content of transition metals also makes it an interesting candidate for alternative upcycling routes. This project explores the potential use of NMC black mass as a cost-effective catalyst for plasma pyrolysis, with the aim of providing a more sustainable alternative to expensive primary transition metal compounds. To evaluate its suitability for this application, the material was subjected to comprehensive physicochemical characterization before and after thermal treatment. All analytical characterizations were performed on campus, utilizing the institution's available machinery and equipment. A major challenge identified during the study was the significant concentration of fluorine in the black mass. Fluorine-containing species may originate from electrolyte residues, such as LiPF_6 , as well as from LiF or other fluorinated compounds. Their presence is problematic due to potential environmental concerns and, particularly, the risk of corrosion and damage to the plasma reactor and related equipment. Thermal treatment successfully reduced the overall carbon and fluorine content, however, residual fluorine was still detected. Therefore, future work will focus on chemical purification procedures aimed at isolating cleaner metal oxide fractions from the black mass and further assessing their suitability for catalytic plasma pyrolysis.

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Mass Production Process Development of Thin Film Si Solar Panels

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Solar cells or modules, are one of the key technologies for generating electricity in an environmentally friendly way. Their development in the past two decades has moved them from a supplementary energy source to the mainstream technology. At a certain stage of development, an interesting alternative (with potentially lower production costs) was the technology of thin Si layers based on the tandem (two-layer) concept of a-Si:H / uc-Si:H layers [1]. This technology was taken over by the Swiss industrial corporate Oerlikon by hiring the complete R&D team from the Neuchatel University in 2004 [2]. In the following years, this technology was further improved for industrial deployment using the unique concept of the PECVD chamber originally designed for flat panels. By 2012, Oerlikon Solar had sold complete turnkey equipment for 10 factories for thin-film Si modules (1.4 m²) and these activities had some continuation under the Japanese company TEL within 2013-2015.

The lecture describes the basic technological steps in the production of thin-film panels based on photovoltaic layers of amorphous and microcrystalline silicon. ZnO was used as a contact conductive and transparent layer, the structuring of which into cells was carried out by the laser scribing technology. These active layers were enclosed between two supporting glass panels by a lamination foil. The process of preparing thin silicon layers using the PECVD method, i.e. vapor phase deposition, where the source gas is SiH₄ and consisting of 5-12 layers created using 20-50 process steps, will be presented in detail. The basic characterization methods and required criteria for individual layers used in this type of solar cell will also be mentioned. The phenomenon of degradation of silicon layers and their influence on the final stabilized performance of the panels will also be briefly described. Examples of optimization changes in individual layers and their influence on the overall efficiency of the solar cell will be shown [3]. These intensive development activities led to the production of a large commercial module with a record efficiency of 12.34% [4] for a two-layer configuration and also to 13.46% [5] in the case of a small solar cell with a three-layer configuration.



Fig.1. Layout of module production fab (a), a-Si and tandem solar panels (b), Efficiency improvements (c).

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Formic Acid Production via Molecular Robson-Type Dual-Metal Catalysts: Integrated Design, Green Synthesis, and Electrolyzer Validation

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Electrochemical CO₂ reduction using renewable electricity produces useful chemicals such as formic acid (HCOOH), methanol (CH₃OH), ethanol (C₂H₅OH), and carbon monoxide (CO). Formic acid (HCOOH) is attractive because it is efficient, scalable, and can serve as both a chemical feedstock and a hydrogen carrier [1,2].

A new class of molecular bimetallic Robson-type catalysts was developed for selective conversion of CO₂ to formate (HCOO⁻). Their electronic structure is tunable, and computational screening guides the catalyst design. The catalysts are synthesized below 80 °C using a pyrolysis-free, environmentally friendly method with earth-abundant elements. Standard characterization techniques confirm their structure.

Electrochemical tests in H-cells and flow cells show strong performance. Current densities reach ~200 mA cm⁻², Faradaic efficiencies exceed 96%, and stable operation is maintained for more than 100 hours. After electrolysis, the Co–Cu catalyst largely retains its structure and supports continuous production of concentrated formate and formic acid.

Studies on cobalt phthalocyanine (CoPc) on carbon show that catalyst–carbon interactions strongly affect stability and CO₂ reduction activity. Solvent-free ball milling improves catalyst dispersion, while higher precursor loading forms protective regions that stabilize active sites during heating. These insights support the development of stable electrocatalysts for scalable CO₂ conversion.

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From Diagnostics to Industrial Application: Plasma Arc Cutting Research in Collaboration with Fronius GmbH

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Research on plasma arc cutting in collaboration with Fronius GmbH was carried out in the Thermal Plasma Department (since 2018 Plasma Chemical Technologies Department) between 2008 and 2011. This work produced a substantial body of experimental and theoretical results, documented both in confidential internal reports and in peer-reviewed publications [1, 2, 3]. The present contribution provides a concise overview of these activities. Comparison of different metal cutting technologies is given and an attempt to introduce plasma arc system based on steam plasma is presented. The collaborative research included experimental studies of arc cutting of mild steel, an investigation of the role of the exothermic oxidation of iron during oxygen cutting, and optical emission spectroscopy of the plasma jet generated by a steam arc cutting torch. Additional spectroscopic measurements were performed by observing the plasma inside the kerf during stainless-steel cutting. Together, these studies significantly advanced the fundamental understanding of several key aspects of the plasma arc cutting process and enabled the direct transfer of this knowledge into technologies developed by Fronius GmbH.

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Application of Carbon Quantum Dots in Next-Generation Scintillation Material

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Carbon quantum dots (CQDs) have recently attracted significant attention as emerging nanomaterials for scintillation and radiation detection applications owing to their exceptional optical, electronic, and structural properties. Their strong photoluminescence, tunable emission wavelengths, low toxicity, excellent water solubility, and facile synthesis make them promising alternatives to conventional inorganic scintillators. Recent studies have demonstrated that CQDs exhibit efficient fluorescence, phosphorescence, and delayed luminescence behaviors that are highly beneficial for converting ionizing radiation into detectable optical signals. In addition, surface functionalization and heteroatom doping have been shown to improve quantum yield, emission stability, and radiation response characteristics. CQD-based nanocomposites and hybrid materials further enhance scintillation efficiency through improved energy transfer mechanisms and reduced self-absorption losses. These materials have shown potential applications in X-ray and gamma-ray detection, medical imaging, particle physics experiments, environmental radiation monitoring, and optoelectronic devices. Furthermore, the lightweight nature, flexibility, and low-cost fabrication of CQD-based systems offer significant advantages for next-generation portable and flexible radiation detectors. Despite notable progress, challenges including optimization of light yield, radiation hardness, and long-term stability remain active areas of investigation. This review highlights recent advancements in the synthesis, luminescence mechanisms, and scintillation performance of carbon quantum dots while discussing their future prospects as sustainable and high-performance scintillating materials for advanced radiation detection technologies.

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Low-Carbon Hydrogen Production

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Low-carbon hydrogen is defined as hydrogen produced from non-renewable energy sources that achieves at least a 70% reduction in greenhouse-gas (GHG) emissions relative to the fossil comparator of 94 g CO₂/MJ, corresponding to a maximum lifecycle carbon intensity of 3.38 kg CO₂ per 1 kg H₂. This category includes blue hydrogen from natural gas with carbon capture and storage (CCS), hydrogen produced via electrolysis using grid electricity, and hydrogen from methane pyrolysis. A specific open issue concerns low-carbon hydrogen produced by electrolysis using nuclear electricity (often referred to as “nuclear/pink” hydrogen): at present, there is no dedicated methodology for demonstrating the supply of low-carbon electricity via power purchase agreements (PPAs) for this pathway. The European Commission is expected to launch a public consultation on a proposed methodology by June 2026, assessing impacts on the energy system, emissions savings, and a level playing field with RFNBO rules.

The key motivation for using nuclear electricity is to improve predictability and economics of hydrogen production. When relying solely on renewables, electrolyser utilization can be low (approximately ~15% in a pessimistic case to ~45% in an optimistic case), amplifying uncertainty on both the producer and off-taker side and worsening the “green premium” challenge. Contracts therefore often require volume flexibility and take-or-pay structures to balance bankability with buyer risk. In the short term, combining baseload and load-following nuclear generation can enable more stable electrolyser operation in an optimal load range (~60–80%), reducing levelized cost of hydrogen (LCOH) and commercial risk. In the medium term, further LCOH reductions may be enabled by high-temperature electrolysis, benefiting from higher overall efficiency (lower electricity consumption per unit of H₂).

Overall, nuclear electricity can strengthen cost competitiveness, operational reliability, and supply security of low-carbon hydrogen - supporting both near-term deployment and longer-term cost decline.

First-principles and machine learning methods for description of optical materials

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The transition metal and rare earth ions with the unfilled 3d and 4f electron shells, respectively, are extremely important for applications in optical materials. In this work an overview of basic electronic and spectroscopic properties of these ions in a free state and in crystal fields of various symmetries will be given [1]. Special attention is paid to the energies of electronic transitions used for getting visible emission for lighting and location of those energy levels in the host's band gap. Several examples of the Density Functional Theory (DFT) based calculations are described in detail to unveil the changes in the electronic properties of hosts after doping and to locate the impurity's ground state and its excited states with respect to the host's band structure (Fig. 1) [2-5]. Additionally, examples of recently emerged machine learning methods for prediction of the emission properties of impurity ions in crystals are also shown [6].

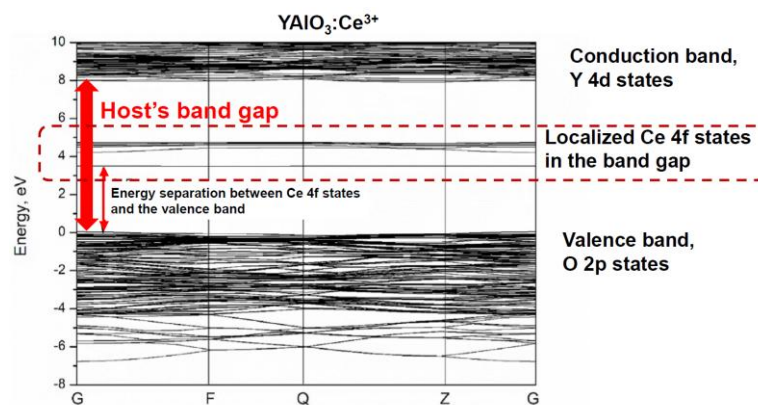


Fig. 1. Calculated band structure of Ce³⁺-doped YAlO₃ [2].

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Processing of Fine Plastic Fractions from WEEE Using Plasma Technology

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The contribution addresses the issue of processing fine plastic fractions generated during the recycling of waste electrical and electronic equipment (WEEE), as well as other difficult-to-recycle plastic streams. These fine fractions, often contaminated with impurities and characterized by heterogeneous composition, represent a significant challenge for conventional recycling technologies and are typically directed to energy recovery or landfilling. The presentation will introduce the typical properties and composition of fine plastic fractions from WEEE, including their sources and current management practices. Particular attention will be paid to the possibilities of their material or chemical recovery using advanced technologies, especially plasma processing. This method enables the efficient decomposition of organic components at high temperatures and the conversion of waste into synthesis gas and an inert solid residue. The aim of the contribution is to evaluate the potential of plasma technology for the utilization of fine plastic fractions, identify its advantages and limitations, and discuss its role in the context of the circular economy and landfill reduction. Keywords: WEEE, fine plastic fractions, plasma processing, recycling, circular economy.



Application of Multiscale Multiphase CFD Modeling Including Phase Transfer for Plasma-Driven Thermal and Reactive Systems

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Plasma-assisted processes are emerging as key technologies for sustainable chemical transformations, advanced materials processing, and energy conversion. Many of these applications such as plasma assisted boiling, plasma–liquid interaction, and plasma-enhanced heat and mass transfer are governed by complex multiphase phenomena involving strong coupling between phase change, transport processes, and interfacial dynamics. In particular, the formation, growth, and interaction of vapor structures play a decisive role in process efficiency, selectivity, and thermal management. This work presents the application of the GENTOP (GENeralized TwO-Phase) modeling framework to multiscale multiphase flows with phase transfer, with a focus on conditions relevant to plasma-driven thermal and reactive systems. The approach combines dispersed and interface-resolving multiphase modeling within a unified multifield formulation. Small vapor structures are described using an inhomogeneous Multiple Size Group (iMUSIG) model, enabling the representation of polydisperse bubble populations and interfacial transport processes. Larger coherent gas structures are treated as continuous phases with resolved interfaces, allowing the simulation of complex flow regimes encountered in plasma–liquid and high-heat-flux environments. The model incorporates advanced descriptions of interfacial momentum exchange as well as heat and mass transfer, including wall boiling formulations for phase change processes. This enables the consistent prediction of evaporation dynamics, bubble-induced mixing, and heat transfer enhancement; key mechanisms influencing plasma–liquid reactivity and process performance. The applicability of the approach is demonstrated for representative configurations, including heated flow channels, pool boiling systems, and closed-loop evaporation–condensation cycles. These configurations serve as proxies for plasma-relevant environments, where rapid energy deposition and localized heating lead to strong phase change and multiphase interactions. The simulations capture flow regime transitions, vapor structure formation, and coupled evaporation–condensation processes, providing detailed insight into the multiscale dynamics governing such systems. Results highlight the importance of accurately resolving both dispersed and continuous gas phases for predicting transport processes and thermal behavior under conditions relevant to plasma-assisted technologies. The framework provides a basis for improving the design and optimization of plasma reactors, particularly with respect to heat management, phase distribution, and process efficiency. Ongoing developments focus on extending the model toward plasma-specific applications by incorporating additional physics, such as localized energy input and enhanced interfacial transport mechanisms. This paves the way for predictive, CFD-based design of plasma-driven systems supporting sustainable chemical processing, energy efficiency, and advanced materials production.



Recent Advances in Plasma-Assisted Materials Synthesis at the Institute of Plasma Physics

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This contribution presents recent progress in the plasma-assisted synthesis of metal-halide perovskites (AMX₃) achieved over the past year at the Institute of Plasma Physics. The work focuses on both technological aspects of the synthesis process and the resulting material properties. Particular attention is given to the design of the plasma setup, including reactor geometry, precursor delivery, and substrate configuration, which critically influence the formation pathways and final morphology of the deposited layers.

A range of compositions based on AMX₃ perovskites were investigated, where A represents alkali or small cations (e.g., Cs, Li), M corresponds to metal centers (Pb, Cu, Mg, Zn), and X denotes halides (Br, Cl). The plasma-assisted approach enables rapid synthesis under non-equilibrium conditions, offering unique opportunities to tailor composition, crystallinity, and defect structure compared to conventional solution-based or melt-processing techniques.

The study demonstrates the successful preparation of perovskite-based layers on various substrates, with emphasis on controlling phase purity, crystallite size, and surface coverage. The influence of plasma parameters on halide retention, cation incorporation, and structural stability is discussed. In addition, selected results highlight the potential of plasma processing to stabilize non-conventional compositions and to introduce dopants in a controlled manner.

Overall, the presented results underline the versatility of plasma-assisted synthesis as a promising route toward advanced functional materials, particularly for optoelectronic and photonic applications, where precise control over structure–property relationships is essential.

Activated Lignin-Derived Carbon Nanofibres for Electrochemical and Sensing Applications

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Recent advances in sustainable nanomaterials have highlighted lignin as a promising bio-derived platform for advanced carbon and hybrid nanostructures [1]. Due to its aromatic structure and rich surface chemistry, lignin can interact with nanoparticles, quantum dots, dyes, and biomolecules through π - π interactions, hydrogen bonding, electrostatic interactions, and covalent modification [2]. Electrospun lignin-derived carbon nanofibres are particularly attractive because carbonization forms porous conductive structures with high specific surface area and abundant active surface sites [3].

This contribution discusses lignin-derived carbon nanofibres and hybrid nanostructures for electrochemical applications, especially in energy storage, electrolyzers, and biosensing. Surface activation increases porosity and introduces reactive functional groups, enabling immobilization of catalytically and biologically active species.

Particular attention is devoted to integrating semiconductor quantum dots and other functional nanomaterials with activated lignin-derived carbon nanofibres. Their tunable electronic and optical properties can enhance charge transfer and electrochemical responses, while the porous structure enables efficient anchoring of nanoparticles and biomolecules.

Such lignin-derived conductive nanostructures show strong potential for supercapacitors, electrocatalytic systems, electrolyzers, electrochemical biosensors, and advanced sensing interfaces [4].

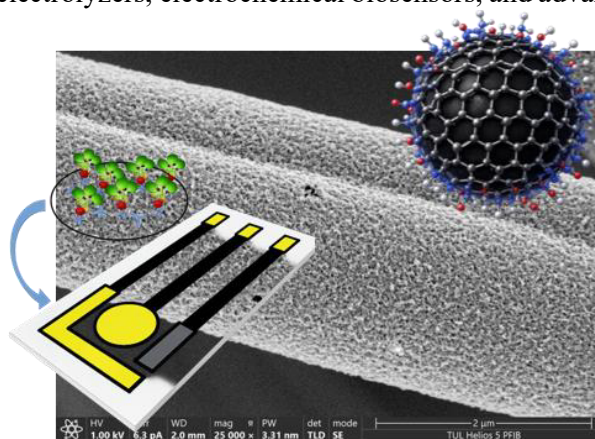


Fig. 1. SEM of carbon fiber microporosity.

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Optically Induced Phenomena in Graphene

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Graphene exposed to intense near-infrared laser radiation exhibits a variety of strongly non-linear optical and photoelectronic phenomena, including broadband white-light emission, hot-electron generation, photocurrent formation, and laser-assisted catalytic reactions. Recent studies demonstrated that graphene foams and graphene aerogels irradiated by continuous-wave lasers at 808 and 980 nm undergo multiphoton ionization leading to coherent broadband emission extending from the visible to near-infrared spectral range [1]. The observed laser-induced white emission (LIWE) is characterized by an excitation threshold, exponential growth of intensity with laser power, and simultaneous generation of photocurrent associated with the emission of hot electrons [2]. The proposed mechanism involves multiphoton absorption in graphene followed by the formation of ionized graphene states, electron–photon coupled pairs, and thermal emission.

These effects reveal the exceptional capability of graphene to convert optical excitation into collective electronic and photonic processes, opening perspectives for compact broadband light sources, photonic devices, and optoelectronic emitters based on carbon nanostructures.

An important extension of these studies concerns laser-induced hydrogen generation from methanol vapor and liquid alcohols using graphene aerogel as both the optical target and catalytic electrode [3]. Experiments showed that laser irradiation combined with an external electric field significantly enhances methanol dissociation and hydrogen production efficiency.

In the hybrid laser-induced ionization/electric-field ionization (LII+EFI) process, hydrogen generation increased more than twofold compared with individual excitation mechanisms, while maintaining relatively low CO₂ and CH₄ emissions. The process is driven by hot electrons generated during laser excitation of graphene, which initiate efficient dissociation of methanol molecules and plasma-assisted conversion reactions. The combination of ultrafast optical excitation, broadband coherent emission, and photocatalytic hydrogen generation demonstrates that graphene constitutes a unique multifunctional platform for future energy-conversion and photonic technologies. The interplay between laser-driven charge dynamics, coherent emission, and catalytic activity may open new routes toward efficient hydrogen production systems and graphene-based broadband optoelectronic devices.

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Evaporation of Zinc During Aerodynamic Levitation Melting of Aluminosilicate Glasses

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Aerodynamic levitation (ADL) is a method for preparation of new materials by melting. A small bead of material is levitated in jet of carrying gas and heated by contactless means such as microwaves or lasers. When laser is used as a heating source, temperatures obtained can be as high as 3000 K, maintaining cooling rates in order of $10^2 \text{ K}\cdot\text{s}^{-1}$. ADL is therefore a useful method in research of metastable phases and glasses that are difficult or impossible to obtain by conventional melt-quenching. Apart from higher cooling rate, the absence of melt-container interface also lowers tendency to crystallization due to limitation of nucleation sites [1].

However, if prepared material or starting chemicals contain volatile compounds, the composition of the batch changes during melting. The problem of volatilization has already been solved for binary alkali-silicate systems [2]. In this contribution we focus on ternary $\text{ZnO}-\text{Al}_2\text{O}_3-\text{SiO}_2$ system. We observe effect of two different carrying gases on composition and discuss mass losses as a function of melting time. Homogeneity issues arising from insufficient temperature or melting time are also briefly addressed.

The composition is checked by EDS, homogeneity is assessed by SEM and optical microscopy.

Acknowledgements. This work was supported by the Barrande Fellowship Program coordinated by the French Institute in Prague (IFP) and the Czech Ministry of Education, Youth and Sports (MEYS).

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Decomposition of Methane in a Multichamber Plasma Reactor

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The work presents a numerical simulation of the decomposition of methane (CH₄) in a mixture of methane, nitrogen, and argon generated in a microwave torch with an output power of approximately 3 kW. One of the principal goals of the research is the production of carbon black and carbon nanoparticles.

Numerical model was created in the ANSYS FLUENT 2024 R2 software package [1]. The model is fully three-dimensional and solved by stationary iterations. The flow is subsonic, generally compressible, turbulent, with the gas transport and thermodynamic properties dependent on temperature at atmospheric pressure. The overall chemical scenario of methane decomposition and the production of its byproducts is introduced in ANSYS Fluent by a non-equilibrium chemistry.

Results of calculation provide distribution of temperature, velocity field, pressure, density, turbulence quantities and species concentrations. The first calculation was performed for a CH₄-Ar-N₂ gas mixture with the respective flow rates of 3, 10, and 45 slm, an output microwave power of 2.325 kW, and an average inlet gas mixture temperature of 1773 K. The temperature of the gas mixture drops significantly only in the last third of the chamber's length, whereas the turbulent viscosity ratio reaches its maximum in the third of the chamber's length from the inlet.

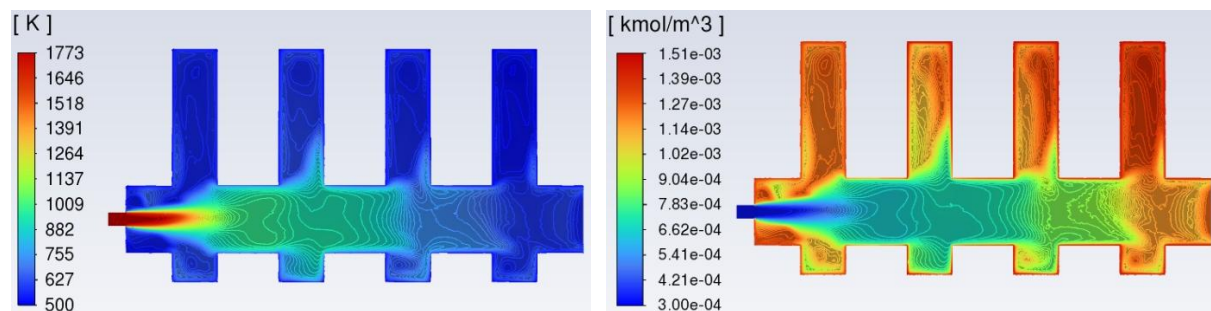


Fig. 1. Static temperature contours (left) and CH₄ molar concentration (right) and in a chamber cross-section for a 2.3 kW microwave power and CH₄-Ar-N₂ gas flow rates of 3, 10, and 45 slm respectively.

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Frequency Resolved UV Photoluminescence of NV Rich Single Crystal Diamond

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Results (Fig. 1) show the residual UV excitation band around 365 nm and the diamond Raman band at 384 nm (1332 cm^{-1} shift).

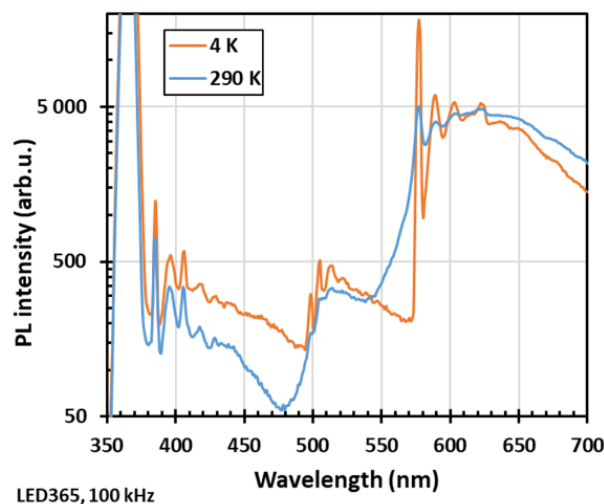


Fig. 1. Frequency resolved photoluminescence of NV rich single crystal diamond measured with LED365 excitation (10mW focused on 0.1 mm diameter spot) at 100 kHz.

PL features in the 490–520 nm range are most commonly nitrogen-aggregate/deformation-related color centres. In particular, the 491 nm PL is related to plastic deformation-related PL (“decorated slip traces”), the 496 nm PL to H4 centre (N–V–N–V–N) with zero-phonon line (ZPL) and 503 nm PL to the H3 centre (neutral N–V–N) ZPL. H3 and H4 centres are typical for type Ia (nitrogen-rich) diamonds. The NV^0 centers in diamond produce in red spectral region broad phonon sidebands related to sharp ZPL at 577 nm. In contrast, there is no obvious NV^- feature at 637 nm; the signal is decreasing through 630–645 nm without a distinct local maximum at 637 nm.

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A Self-Consistent Non-Equilibrium Numerical Framework for Microwave Plasma Dynamics and Electron Kinetics

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This work presents a comprehensive, self-consistent numerical framework designed to simulate the strongly non-equilibrium (non-LTE) dynamics of microwave (MW) plasma flows. Even at atmospheric and sub-atmospheric pressures, the classic assumption of Local Thermodynamic Equilibrium (LTE) fails to capture the true physical nature of MW discharges. This limitation stems from the profound thermodynamic decoupling between the electron temperature (T_e) and the heavy-particle gas temperature (T_g), alongside the highly non-Maxwellian nature of the electron energy distribution function (EEDF). Consequently, an accurate description of the reactor physics requires a tight, simultaneous coupling of state-to-state chemical kinetics and electron-impact processes.

Using molecular nitrogen as a rigorous physical benchmark, the model accounts for the dominant electron-molecule and heavy-particle collisional channels. A primary focus is placed on electron-impact vibrational excitation driven by the low-energy shape resonance ($e + N_2 \rightarrow N_2^- \rightarrow N_2(v) + e$). This resonant mechanism efficiently pumps energy into the lower vibrational levels of the ground electronic state. The energy is subsequently redistributed via rapid Vibration-Vibration (V-V) exchanges, leading to the formation of a strongly non-equilibrium Treanor-like population distribution and a highly populated vibrational plateau. These vibrationally excited states significantly accelerate gas heating via Vibration-Translation (V-T) relaxation and lower the effective thresholds for ionization and dissociation, deeply governing the macroscopic plasma behavior.

Crucially, this macro-thermodynamic fluid loop is coupled self-consistently with the advanced kinetic Boltzmann solver LoKI-B [1,2]. The local EEDF is dynamically updated based on a thoroughly revised and validated database of electron collision cross-sections, ensuring that all electron transport coefficients and rate constants precisely reflect the non-equilibrium state of the discharge. The underlying macroscopic fluid equations account for gas expansion, vortex-driven flow boundary conditions, and regenerative gas preheating effects, with thermal conduction to the reactor walls acting as the primary energy sink in the current phase. This framework builds upon and expands foundational methodologies established in non-equilibrium plasma modeling [3,4].

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Effect of Hydrogen Substitution in a Hybrid Plasma Torch

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Thermal plasma represents a promising technology for the pyrolysis and gasification of waste materials, enabling the production of syngas with high concentrations of H₂ and CO [1,2]. Plasma torches based on electric arcs are widely used for these applications, while their efficiency and lifetime are strongly affected by the method of plasma stabilization. Besides gas-flow stabilization, water-vortex stabilization can be employed to reduce the thermal load on torch components. Hybrid-stabilized plasma torches combine the advantages of both approaches [3]. Hybrid water/gas-stabilized torches are commonly operated with Ar/H₂O mixtures [4]. However, replacing argon with hydrogen, resulting in H₂/H₂O plasma, may improve the overall process efficiency and increase the purity of the produced syngas.

The effect of plasma composition on the arc column can be assessed using a simplified integral model, expressed by following equation:

$$\frac{G\bar{h}}{L} + 2\pi\bar{S} + 4\pi^2 R^2 \bar{\epsilon}_n = \pi R^2 \bar{\sigma} E^2 = \frac{I^2}{\pi R^2 \bar{\sigma}},$$

The individual terms represent the contributions of axial heat convection, radial heat conduction, and radiation losses to the overall arc energy balance [5].

Replacing argon with hydrogen increases the relative importance of axial heat convection compared with radial heat conduction, which can significantly enhance plasma generation efficiency. At the same time, the higher thermal conductivity of hydrogen-containing plasma may lead to increased heating and erosion of torch materials.

These findings indicate that hydrogen is a promising alternative to argon as a stabilizing gas in hybrid water/gas-stabilized plasma torches. The expected improvement in plasma generation efficiency and the favorable impact on syngas composition may outweigh the increased demands on torch materials.

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Gas-Phase FTIR Spectroscopy

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Infrared (IR) spectroscopy serves as a versatile and non-destructive analytical technique employed for the qualitative identification and quantitative determination of chemical species across gaseous, liquid, and solid phases. The method relies on the interaction between infrared radiation and the vibrational modes of molecules, where the fundamental physical requirement for absorption is that a vibration must induce a net change in the molecule's permanent dipole moment. When the frequency of IR radiation matches a bond's natural vibrational frequency and a dipole change occurs, energy is transferred, elevating the molecule to a higher vibrational state. Consequently, homonuclear diatomic molecules like N_2 and O_2 , or noble gases such as Ar and He, are "IR inactive" because they cannot undergo a change in dipole moment, making them invisible to this method. Modern instruments utilize Fourier Transform Infrared (FTIR) technology, which captures all frequencies simultaneously via an interferometer to produce a raw signal called an interferogram. This is mathematically converted into a spectrum where absorbance is plotted against wavenumbers (cm^{-1}), providing an intuitive format for human interpretation. Analyzing gases presents specific challenges due to lower molecular density compared to condensed phases, which directly correlates to weaker absorption. This is typically mitigated by increasing the optical path length using specialized cells with internal mirrors, which can achieve path lengths of tens of meters. However, these systems are highly sensitive to dirt and require precise optical alignment. Sensitivity is also limited for molecules with small dipole moments, resulting in lower detection limits. Furthermore, the ubiquitous presence of water vapor creates significant interference, as its complex spectrum of overlapping peaks can mask target analytes.

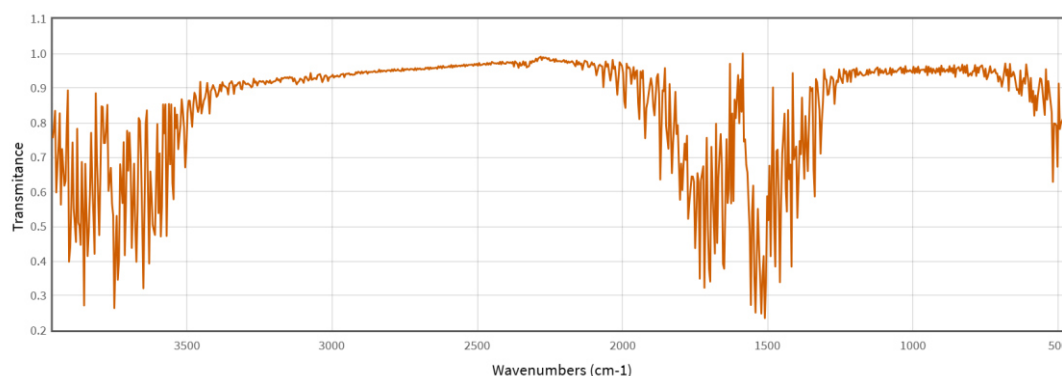


Fig. 1. Water infrared spectrum [1].

Physical conditions also play a role; while temperature does not shift peak positions, it alters the population levels leading to changes in peak intensity that necessitate strict temperature control. While FTIR is an exceptional tool for monitoring specific functional groups and known mixtures, its limitations in overall unknown analysis mean it is often complemented by other methods like Mass Spectrometry to provide a comprehensive chemical fingerprint.

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Chalcogenide Materials for Next-Generation Electronics, Storage and Energy Conversion

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The intensively investigated two dimensional and bulk (2D and 3D) chalcogenides have been discovered exhibit a wide range of properties and applications. Chalcogenides offer a promising route to next-generation computing and sensing, thanks to their topological, magnetoelectric, excitonic, and spintronic properties. Integration of 2D materials with other functionalities, such as ferromagnetic, ferroelectric, topological insulators and superconductors, has attracted significant attention as the promising part of multi-stable devices and elements of the functional electronics. From the other side, the infrared transparency and high non-linear optical responses enable innovative applications in photonics and energy-efficient systems. Due to low-cost fabrication methods supports the development of environmentally conscious and scalable solutions i.e. energy conversion and storage (thermoelectricity, solar cells, batteries and supercapacitors). An interesting and useful feature of these materials is the possibility of using them for high-performance electrochemical and photoelectrochemical water splitting.

As global demand grows for sustainable materials, chalcogenides offer a versatile platform to drive progress in next-generation electronic and energy technologies.

In my talk, I will focus on the influence of composition (non-stoichiometry, high configurational entropy, structure defects), size (2D, nano), temperature or stress on the various useful properties. Finally, examples of the promising materials interesting for energy conversion, superconductivity, electronics applications, remotely temperature or pressure sensing will be presented.



From CAD to Experiment: Prototyping Tools at IPP PCHT

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Modern research in plasma technology, materials synthesis, and experimental device development increasingly requires rapid and flexible prototyping capabilities bridging conceptual design and functional laboratory implementation. In response to these demands, our department has expanded its in-house manufacturing infrastructure, enabling accelerated development of experimental hardware, reactor components, cooling systems, holders, electronic enclosures, and custom laboratory equipment without dependence on external suppliers.

This presentation summarizes recent improvements and practical experiences related to additive manufacturing, resin printing, and compact CNC machining technologies implemented at our department. The presented approaches include fabrication of functional polymer components from standard and engineering-grade materials, including thermally resistant and ESD-safe variants, together with post-processing methods such as conductive and protective metal coatings for electromagnetic shielding, microwave applications, and improved thermal or electrical conductivity.

The presentation further demonstrates machining and prototyping capabilities for plastics, acrylic glass, brass, aluminum alloys, plastic composites, and soft metals, together with applications of standard, high-strength, high-temperature, and ceramic-filled resins. Practical limitations associated with thermal resistance, dimensional stability, chemical compatibility, and post-processing are also discussed. Overall, the presentation demonstrates how modern prototyping technologies can shorten development cycles, reduce manufacturing costs, and improve flexibility in the design and fabrication of laboratory infrastructure for scientific and engineering applications.

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Thermal Plasma Approach as a Branch of Nanotechnology

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Thermal plasma technologies represent one of the most dynamic and promising branches of modern nanotechnology due to their capability to create extreme physicochemical environments enabling rapid synthesis, modification, and functionalization of advanced nanomaterials. Thermal plasmas are characterized by very high temperatures, elevated energy densities, strong nonequilibrium chemical activity, and extremely fast heating and cooling rates, which together provide unique conditions for controlling nucleation, crystal growth, phase composition, and defect engineering at the nanoscale. Compared with conventional wet-chemical or solid-state synthesis routes, plasma-based approaches often offer solvent-free processing, reduced contamination, shorter synthesis times, continuous operation, and improved scalability for industrial applications.

This contribution presents an overview of thermal plasma approaches as an important technological platform for nanomaterial production and plasma-enabled nanomanufacturing. The fundamental principles of plasma generation are discussed, including microwave plasma, radiofrequency plasma, inductively coupled plasma, and arc plasma systems. Special attention is devoted to microwave thermal plasma due to its electrode-free configuration, high plasma density, relatively low contamination risk, rapid response, and suitability for continuous-flow synthesis. The interaction between plasma species and precursors is analyzed with emphasis on evaporation–condensation mechanisms, plasma pyrolysis, plasma-assisted gas-phase reactions, and defect formation processes.

The presentation highlights the synthesis of various classes of nanomaterials using thermal plasma technologies, including carbon nanostructures, graphene-related materials, carbon quantum dots, semiconductor nanoparticles, metal oxides, perovskites, nanocomposites, photocatalytic materials, and luminescent nanostructures. Plasma-assisted doping and hydrogen-related defect engineering are discussed as powerful tools for tailoring electronic, optical, magnetic, and catalytic properties of nanomaterials. Particular emphasis is placed on the role of plasma-induced defects and paramagnetic centers, which can significantly influence charge transport, recombination pathways, luminescence efficiency, photocatalytic activity, and radiation response.

Thermal plasma technologies also provide significant opportunities for sustainable nanotechnology and circular economy applications. The abstract discusses plasma-assisted conversion of waste materials, including plastics, biomass, sewage sludge, textile waste, and industrial residues, into valuable products such as hydrogen, synthesis gas, carbon nanoparticles, and functional nanostructures. Plasma-driven methane pyrolysis, dry reforming of methane with CO₂, and plasma gasification are presented as emerging pathways combining nanomaterial production with clean energy generation and carbon valorization. The possibility of integrating plasma technologies with renewable energy systems and hydrogen economy concepts is also addressed.

In addition to experimental developments, the importance of advanced plasma diagnostics, multiscale computational fluid dynamics (CFD) modeling, plasma chemistry simulations, optical emission spectroscopy, hyperspectral imaging, and artificial intelligence-assisted process optimization is emphasized.

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Electrochemically Active Electrospun Amorphous SiO₂ Fibers for All-solid-state Batteries

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All-solid-state batteries are expected to be the future of energy storing as they can offer significantly higher power densities, and enhanced safety and lifetime compared to liquid electrolyte Li-ion batteries. However, slow interface kinetics is hindering industrial adoption of this technology, along with production and durability issues, and content of hazardous elements like sulfur. Fibrous or connected-pore structures are reported to be an efficient approach, since they serve as a net of conductive pathways, but they currently mostly utilize organic materials, which are naturally flammable and inferior to inorganic materials in terms of chemical and thermal stability. Further, they often rely on hazardous components such as fluorine, chlorine, or sulfur, which complicates production and subsequent disposal of end-of-life materials. Our research focuses on electrochemically active submicron- or nano- scale amorphous SiO₂ fibers which, while still durable, aren't flammable, and offer remarkable thermal and chemical stability. Moreover, they are suitable for activation through various methods. Additional advantage lies in production method – electrospinning – which has a highly versatile setup options allowing large number of approaches and tuning of properties options. Furthermore, it should allow continuous production of whole segment-interface-free cells with gradient distribution of active materials, simply by changing the feed's sol composition accordingly. Si, lithium phosphate glass, and NMC particles were used as active materials for anode, electrolyte, and cathode respectively, while TEOS sol was used as electrospinning solution. There's, however, still need for significant improvement as interfacial resistance between bulk metal current collectors and electrode materials is high, and the particles doping process currently complicates production of mechanically durable fibers with simultaneously sufficient content of active material. At the moment we are focusing on lowering the resistance between current collectors and electrodes by metal coating the fibers, and lowering battery inner resistance by optimizing the doping process and combing more activation methods. Carbon nanostructures from plasma pyrolysis are also a promising doping material to be tried since formation of triaxial structure (PVP-GPNs-PVP) at 16.7 m.% doping level with commercial GNPs (graphene nanoplatelets) was reported in literature.



Destructing Chemical Additives in WEEE Plastics

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Plastics are versatile, lightweight materials that enable extensive use in various applications. Their broad applicability allows producers to use different additives based on the qualities they offer in their products. More than 13.000 chemicals are used as additives in plastics [1], some of which are being banned. The products are promoted on their removable labels as “without” polybrominated diphenyl ethers (PBDEs), Pb, Cd, per- and polyfluoroalkyl substances (PFAS), and bisphenol A (BPA), among others. Still, these claims are not printed on the plastic material. Therefore, when they are recycled without knowledge of which chemicals may be present, they can pass as legacy contamination in the recyclates [2], and they reenter the market in products that include recycled polymers. Treating plastics with plasma chemical technologies has shown that the chemical additives are destroyed and accumulated as salts or oxides in the output materials. We analyzed 33 elements present in chemicals of high concern due to their toxicity to human health and their persistence and environmental pollution. They were analyzed in the input material, WEEE mixed plastics, and the output materials sampled in the cyclone, bag filter, and reactor. 21 elements were identified, 11 of which are included in the European Parliament's critical raw materials (CRM) list [3]. Si and Al were the higher elements concentrated in the output materials. They were present as oxides, as well as Ti. 5 are considered elements of concern; 3 are included in the Restriction of Hazardous Substances (RoHS) Directive [4], and Br is included as PBDEs. Br and Cl are included in the Stockholm Convention as PBDEs and chlorinated paraffins. These results showed that plasma chemical technologies could be a destructive technology for chemicals of concern used as additives in plastics, with the advantage that some of the elements are valuable as they are included in the CRM list.

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NAA and PAA Research Applications at NPI Řež

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Neutron activation analysis (NAA) is a robust and sensitive method for simultaneous multi-element determination in both organic and inorganic materials. In combination with the photon activation analysis (PAA), more than 40 elements could be determined in total. NAA and PAA allow the identification and quantification of both major and trace elements in a sample by their activation, following by the measurement of characteristic gamma rays whose energy and intensity reveal the element's presence and concentration (mass fraction).

NAA includes a wide variety of modifications, e.g., instrumental and radiochemical, with thermal, epithermal, and fast neutrons, with short- and long-time irradiation. The most employed thermal NAA mode has advantages in high activation cross-sections, the absence of interfering reactions (employing only (n, γ) reactions), and the spectral transparency of a common sample matrix. The need for a powerful irradiation facility and disturbance of the neutron flux by highly absorbing samples are the biggest issues. At NPI, NAA employs the LVR-15 research nuclear reactor operated by the Research Centre Řež.

NAA has been considered as a primary method of measurement. The quality control procedure for NAA has been described in detail in the IAEA (2022) protocol. Nowadays, conventional spectrometric methods such as ICP-OES and ICP-MS have become more widespread, particularly for biological samples and shorter series of soluble geological samples. However, NAA is the best choice for hardly dissolvable samples, low trace element content determination, e.g., in high-purity materials, and a large series of similar samples (e.g., tens or hundreds of meters deep land, ocean bottom, or polar ice drill cores).

PAA is a complementary method to NAA applied in assay of elements hard to determine by NAA. At NPI, bremsstrahlung - high energy photon radiation produced from electrons accelerated at the MT25 microtron accelerator - is used for the irradiation.

This presentation will cover a theoretical background of the activation analysis method, its in-house implementation in the NPI Řež, and a representative set of topics, researched by the Radioanalytical Methods group using NAA and PAA.