Description of the main research directions investigated by the Institute

In the period from 2015 to 2019, the research areas of IT CAS covered fluid dynamics, thermodynamics, dynamics of mechanical systems, mechanics of deformable solids, material diagnostics, interdisciplinary problems (e.g., fluid-structure interaction, environmental aerodynamics, biomechanics, and mechatronics), and power electromechanical systems (with emphasis on electric machines, fuel cells, energy storage, electrical instruments and other equipment). The Institute consists of six scientific departments supplemented by seven joint laboratories with universities and other CAS institutes, Aerodynamic Laboratory in Nový Knín, and the *CeNDYNMAT Center of Excellence*. The evaluated research teams are defined as follows:

- *D1 – Fluid Dynamics* (involving the detached Aerodynamic Laboratory in Nový Knín),
- *D2 – Thermodynamic*s,
- *D3 – Dynamics and Vibration*,
- *D4 – Impact and Waves in Solids* together with the *CeNDYNMAT Center of Excellence*,
- *D5 – Ultrasonic Methods*,
- *D6 – Electrical Engineering and Electrophysics*.

Most of the main results of the Institute's research teams were published in relevant impacted journal articles. The fundamental research is supported by the grants provided predominantly by the Czech Science Foundation (GACR) and Operational Programs and international programs of the Ministry of Education, Youth and Sports (MEYS). Due to the focus on applied physics, a considerable part of the Institute's outputs found a direct relevance in the applied research and development. The applied results were achieved either within the joint projects of applied research and experimental development supported mostly by the Technology Agency of the Czech Republic (TACR) and the Ministry of Industry and Trade (MIT) or from the direct commercial contracts. The Institute collaborates with private companies ranging from large enterprises such as the Czech primer energy producer ČEZ, steam turbine manufacturer Škoda Doosan Power, or car producer Škoda Auto to medium-sized and small companies. The outputs of the applied research were described in research and technical reports, sometimes of a confidential character, and in scientific and conference articles. Some of the results are also patented.

The following summary provides description of the main research results of IT CAS during the reported period. More details are provided in the description of six research teams of the Institute in section *3.4 – Reports on the research activities of the teams*.

2015

Power control of grid-connected converters under unbalanced voltage conditions

A grid current control technique for power converters has been developed. The analysis deals with the control of positive and negative current sequences in a grid-connected converter during voltage sags. The method assures proper exchange of active and reactive power without ripple, the mitigation of harmonic distortion of currents, and also enables control of grid current peaks. Simulation and experimental results are reported to validate theoretically predicted performance of the control strategy.

- Valouch V., Bejvl M., Šimek P., Škramlík J.: Power control of grid-connected converters under unbalanced voltage conditions. **IEEE Transactions on Industrial Electronics** 62 (2015) 4241-4248.

Dynamics of the flow-field in the vicinity of vibrating airfoil NACA 0012

By the PIV and the Oscillation Pattern Decomposition (OPD) methods a strong interaction between the airfoil and the flow-field including the wake was found. The flow field spatial dynamics is characterized by the OPD modes of oscillating and non-oscillating characters, capturing traveling and pulsating patterns. Each mode is characterized by its own complex topology, eigenfrequency and damping. The unsteady velocity field is determined by both wing vibrations and inherent flow dynamics.

- Uruba V.: Near wake dynamics around a vibrating airfoil by means of PIV and Oscillation Pattern Decomposition at Reynolds number of 65000. **Journal of Fluids and Structures** 55 (2015) 372-383.

Determination of elastic moduli of thin micro- and nanostructured layers

The mechanical properties of few micrometers thick sputtered Al and NiTi layers were studied, both promising candidates for applications in micromechanics. The spectra of vibrations of substrates with these layers were measured by resonant ultrasound spectroscopy (RUS) and inversely analyzed that enabled determination of the elastic moduli. For the NiTi alloy, the evolution of Young's modulus with temperature was studied. For Al layers, the correlation between the modulus and porosity was analyzed. Similarly, nanoporous semiconductors were studied.

- Ben-David E., Landa M., Janovská M., Seiner H., Gutman O., Tepper-Faran T., Shilo D.: The effect of grain and pore sizes on the mechanical behavior of thin Al films deposited under different conditions. **Acta Materialia** 87 (2015) 321-331.
- Thomasová M., Sedlák P., Seiner H., Janovská M., Kabla M., Shilo D., Landa M.: Young's moduli of sputter-deposited NiTi films determined by resonant ultrasound spectroscopy: Austenite, R-phase, and martensite. **Scripta Materialia** 101 (2015) 24-27.
- Janovská M., Sedlák P., Kruisová A., Seiner H., Landa M., Grym J.: Elastic constants of nanoporous III-V semiconductors. **Journal of Physics D-Applied Physics** 48 (2015) 24.

2016

Numerical models of inelastic processes in shape memory alloys

Within a long-term collaboration with the Institute of Physics CAS, RWTH Aachen (Germany), and ESRF Grenoble (France) numerical models of inelastic straining processes in polycrystalline shape memory alloys and their localization were developed. These models were applied to various geometries and loading modes using finite element methods. The comparison of the model predictions with the results of 3D X-ray diffraction tomography were published in the prestigious journal Science.

- Sedmák P., Pilch J., Heller L., Kopeček J., Wright J., Sedlák P., Frost M., Šittner P.: Grain-resolved analysis of localized deformation in nickel-titanium wire under tensile load. **Science** 353 (2016) 559-562.
- Frost M., Sedlák P., Kadeřávek L., Heller L., Šittner P.: Modeling of mechanical response of NiTi shape memory alloy subjected to combined thermal and non-proportional mechanical loading: A case study on helical spring actuator. **Journal of Intelligent Material Systems and Structures** 27 (2016) 1927-1938.
- Frost M., Benešová B., Sedlák P.: A microscopically motivated constitutive model for shape memory alloys: Formulation, analysis and computations. **Mathematics and Mechanics of Solids** 21 (2016) 358-382.

Model for gas hydrates relevant to CCS technologies

A thermodynamic model for the properties and phase equilibria of gas hydrates was developed in collaboration of the Institute of Thermomechanics of the CAS with the Ruhr-Universität Bochum and the Technische Universität Dresden. The new model for eight gas hydrates is compatible with accurate multiparameter equations of state for fluid phases and ices. The model was implemented in the software package TREND 2.0 and can be used for practical design of CCS (Carbon Capture and Storage) technologies.

- Vinš V., Jäger A., Span R., Hrubý J.: Model for gas hydrates applied to CCS systems part I. Parameter study of the van der Waals and Platteeuw model. **Fluid Phase Equilibria** 427 (2016) 268-281.

- Jäger A., Vinš V., Span R., Hrubý J.: Model for gas hydrates applied to CCS systems part III. Results and implementation in TREND 2.0. **Fluid Phase Equilibria** 429 (2016) 55-66.
- Vinš V., Jäger A., Hrubý J., Span R.: Model for gas hydrates applied to CCS systems part II. Fitting of parameters for models of hydrates of pure gases. **Fluid Phase Equilibria** 435 (2017) 104-117.

Wave motion in a thick cylindrical rod undergoing longitudinal impact

A new formulation and the comprehensive analytical solution to longitudinal impact of thick elastic rods is presented. The solution is derived based on the exact 3D theory without using the Skalak's decomposition. The resulting formulas for all the quantities are derived using the residue theorem. Their numerical evaluation is made in such a way that the accuracy of obtained results is very high. Based on these results, the transient wave phenomena occurring in the rods are discussed in detail.

- Červ J., Adámek V., Valeš F., Gabriel D., Plešek J.: Wave motion in a thick cylindrical rod undergoing longitudinal impact. **Wave Motion** 66 (2016) 88-105.

2017

Impact of roof height non-uniformity on pollutant transport between a street canyon and intersections.

Special experimental methods applied on models in the aerodynamic tunnel investigated the impact of the uneven roof-height of courtyard buildings (typical for the centers of Central European cities) on pollutant transport from traffic between the street canyons and intersections. The results confirmed that uneven buildings have a significant impact on pollutant transport and determined the details of the transport, including new discoveries for the horizontal pollutant transport by turbulence.

- Nosek Š., Kukačka L., Jurčáková K., Kellnerová R., Jaňour Z.: Impact of roof height non-uniformity on pollutant transport between a street canyon and intersectionsle. **Environmental Pollution** 227 (2017) 125-138.

Optimization of the fluid jet actuators

Cooling of miniature electronic components can be realized by periodic fluid jets generated by a resonant cavity driven by an oscillating diaphragm. An optimization obtained a significant enhancement of the energetic efficiency up to 2.5 times higher values comparing to available devices. The theoretical results were confirmed experimentally. The investigation was based on experimental and numerical methods performed in Prague and Sydney, respectively. The device has been designed and patented.

- Kordík J., Trávníček Z.: Optimal diameter of nozzles of synthetic jet actuators based on electrodynamic transducers. **Experimental Thermal and Fluid Science** 86 (2017) 281-294.
- Trávníček Z., Broučková Z.: Způsob a zařízení pro chlazení těles válcového tvaru proudem chladicí tekutiny. [The method and the device for cooling of cylindrical objects by means of the cooling fluid jet.], Patent č. 306506, 2017.
- Broučková Z., Trávníček Z., Vít T.: Synthetic and continuous jets impinging on a circular cylinder. **Heat Transfer Engineering** 40 (2019) 13-14.
- Kordík J., Trávníček Z., Timchenko V., Ismail N.A.: The predominant effect of stroke length on velocity profiles at the exit of axisymmetric synthetic jet actuators. **International Journal of Heat and Fluid Flow** 66 (2017) 197-208.

Elastic properties of magnetic shape memory alloys

Properties of ferromagnetic shape memory alloys were investigated by ultrasonic methods with the aim to analyze the soft phonon structure in the low-temperature phases (martensites). The results are in good agreement with theoretical ab-initio predictions and confirm that the non-modulated martensite of the NiMnGa alloy exhibits strong elastic anisotropy with shear instability related to the soft acoustic phonons mediating the reverse transition.

- Sedlák P., Seiner H., Bodnárová L., Heczko O., Landa M.: Elastic constants of non-modulated Ni-Mn-Ga martensite. **Scripta Materialia** 136 (2017) 20-23.

2018

Implosive magneto-cumulative generator

A unique laboratory-scale implosive thermal plasma source for a magnetohydrodynamic or magneto-cumulative generator of electricity has been developed and tested. The thermal plasma is currently created from a combustible stoichiometric mixture of hydrogen and oxygen by the spherical implosion of convergent detonation wave. In addition, other mixtures and advanced configurations of the device for effective conversion of plasma jet into electricity were investigated.

- Tesař V., Šonský J.: No-moving-part commutation of gas flows in generating plasma by cumulative detonations (survey). **Energy** 157 (2018) 493-502.

Methods and facilities for calibration of non-contact vibration diagnostics systems of machine blades

New methods and equipment for calibration and laboratory testing of the non-contact vibro-diagnostics systems for the diagnosis of rotating blades of large blade machines were developed. The appliances were verified as prototypes for measuring the static and dynamic deformations of rotating blades. An electromagnetic simulator of rotating machine blades was developed. Developed impulse electromagnetic exciter is characterized by an increased excitation force.

- Procházka P.: Electromagnetic Simulator of Rotating Machine Blades for Noncontact Sensor Dynamic Testing. **IEEE Transactions on Instrumentation and Measurement** 67 (2018) 1506-1508.
- Procházka P.: Methods and Facilities for Calibration of Noncontact Blade Vibration Diagnostic Systems, **IEEE Transactions on Instrumentation and Measurement** 67 (2018) 2345-2352.
- Procházka P.: Impulse exciter of Rotating Blades with an Increased Excitation Force. **IEEE Transactions on Instrumentation and Measurement** 67 (2018) 1-3.

Calibration of a simple directional distortional hardening model for metal plasticity

Directional distortional hardening (DDH) is the change of shape of the yield surface such that a region of high curvature develops roughly in the loading direction while a region of lower curvature develops in the opposite direction. A simple model of DDH involving six material parameters was calibrated by analytical means. Analytical integration resulted in equations for the stress–strain curve, the hysteresis loop and the cyclic stress–strain curve inherent to the model.

- Parma S., Plešek J., Marek R., Hrubý Z., Feigenbaum H.P., Dafalias Y.F.: Calibration of a simple directional distortional hardening model for metal plasticity. **International Journal of Solids and Structures** 143 (2018) 113-124.

2019

Model of short-term gas release by industrial accidents for an idealized urban canopy

Emergency services need to know an evolution of the incident in case of toxic gas leakages during industrial accidents or terrorist attacks. Emergency models utilized up to now can predict only the situation for long-term leakages, e.g., gas from a stack. Hence, a new unique emergency model enabling to predict the situation for short-term gas leakages, i.e. providing probability density functions of individual puff characteristics at exposed places, was developed for the Czech rescue services.

- Chaloupecká H., Jakubcová M., Jaňour Z., Jurčáková K., Kellnerová R.: Equations of a new puff model for idealized urban canopy. **Process Safety and Environmental Protection** 126 (2019) 382-392.

Ultrasound characterization of growth of omega-phase nanoparticles in single crystals of titanium alloys

Structural changes in titanium-molybdenum alloys at elevated temperatures were studied. The aim was to monitor in-situ the growth of nanoscopic particles of the omega-phase. It was shown that the contact-less laser-ultrasonic methods can reliably detect the nucleation and growth of these particles. This enabled to monitor the evolution of the phase composition of single crystals of the given alloy in thermal cycles and, based on this measurements, to study kinetics of the omega-transition.

- Nejezchlebová J., Janovská M., Sedlák P., Šmilauerová J., Stráský J., Janeček M., Seiner H.: Elastic constants of beta-Ti15Mo. **Journal of Alloys and Compounds** 792 (2019), 960-967.

Crack growth in Fe-Si single crystals on macroscopic and atomistic level

The effect of T-stress on fracture behavior of an edge crack loaded in tension mode I, both on the macroscopic (experimental) and atomistic scale was assessed. Both the experimental results and 3D atomistic simulations showed that the emission of blunting dislocations is more difficult in the specimens with $T > 0$ compared to samples with $T < 0$. Consequently, fracture toughness is larger in the specimens with $T > 0$, which complies with the continuum predictions.

- Ševčík M., Zídek J., Nejezchlebová J., Štefan J., Machová A., Seiner H., Uhnáková A., Čapek J., Lejček P.: Crack growth in Fe-Si (2 wt%) single crystals on macroscopic and atomistic level. **Results in Physics** 14 (2019) 102450.

The overview of solved **research projects** is given in part *3.2 – A List of grant and program projects*.

The results of the applied research are summarized in part *3.3 – Research for practice* including list of applied research projects supported from the commercial contracts, collaborative projects, and patents and inventions. Important outputs of applied research are also described in the reports of the Institute’s six research teams, i.e. section *3.4*.

Research activity and characterisation of the main scientific results

Main research activities are of both theoretical and experimental character accompanied with numerical modelling, often with direct impact on industrial applications. Main activities and results can be shortly divided into several groups, reflecting the division of the team into laboratories.

Laboratory of Internal Flows *(head: Assoc. Prof. Martin LUXA)*

The main research activities in considered period was focused mainly on turbine profile cascades for supersonic flow fields, highly loaded turbine blade cascades, problems of transonic flow fields both in turbine blade cascades and valves, axial compressor transonic blade cascades (international contract - Doosan Heavy Industry Seoul Ltd., South Korea), flow in complicated geometries of valves intended for large turbomachines (contracts - Doosan Skoda Power. Ltd.) and also blade flutter in turbomachines. Furthermore, research in relatively very narrow channels was realized. Also further development of advanced experimental methods (e.g., constant temperature anemometry - hot-film measurement in transonic flow fields) was realized.

1. The influence of the stabilization device tie-boss on transonic flow field in the interblade channel consisting of ultra long turbine rotor blades.

   The investigation was focused on aerodynamic properties of tie-boss stabilization devices for ultra-long rotor blades. It covered measurements on multiple blade cascades and CFD simulation of the flow past these cascades. Conclusions were drawn from results of the measurements and CFD and from the knowledge of prior investigation of the used blade cascade. Main focus was to describe influence of a tie-boss stabilization device on flow field in interblade channel. Tie-boss with more massive shape proved to cause lesser losses, while tie-boss with a tailored trailing edge showed lesser influence on flow turning.

   - Radnic, T., Hála, J., Luxa, M., Šimurda, D., Fürst, J., Hasnedl, D., Kellner, J. Aerodynamic effects of tie-boss in extremely long turbine blades (2018), Journal of Engineering for Gas Turbines and Power-Transactions of the ASME, 140/11 art. No. 112604.
   - Radnic, T., Hála, J., Luxa, M., Šimurda, D., Hasnedl, D., Kellner, J. Preliminary experiments on transonic cascade with damping device tie-boss (2016), The Application of Experimental and Numerical Methods in Fluid Mechanics and Energy 2016. Proceedings of the International Scientific Conference, University of Žilina, pp. 197-200.

2. Mapping of flow unsteadiness during operation of steam control valves at wide range of regimes

   Result of contract with Doosan Skoda Power, Ltd. in Pilsen. Assessment of influence of protective screen in control steam valve on dampening of unsteady structures in the flow field.

   - Šimurda, D., Hála, J., Luxa, M. Unsteady measurement on valve I (2017), Czech Acad Sci, Inst Thermomech, research report No. Z-1583/17.

3. Optimized hub section for ultra-long turbine rotor blade

   The optimized geometry of the hub section was intended for the ultra-long turbine rotor blade for last stage of steam turbine with large output. The important limiting condition was the requirement of a straight fire-tree dovetail, whose application significantly improves the resistance to low cycle fatigue. The optimisation led not only to the smaller sensitivity to the flow separation under off–design condition but also to increasing of aerodynamic loading of the profile. Simultaneously, the kinetic energy loss decreases.

- Hála, J., Luxa, M., Šimurda, D., Bobčík, M., Novák, O., Rudas, B., Synáč, J. Optimization of root section for ultra-long steam turbine rotor blade (2018), Journal of Thermal Science, 27/ 2, pp. 95-102.

Laboratory of Turbulent Shear Flows *(head: Prof. Václav URUBA)*

The complex flows of various types have been studied using advanced experimental techniques. The attention has been paid to control of flow in order to achieve an optimised structure from the perspective of turbulence or boundary layer detachment. Special experimental methods based on the use of hot-wire sensors and optical principles (PIV) were applied both in fundamental research and applied research in real turbo-machines measurements in situ (turbines and compressors).

1. Dynamics of the flow-field in the vicinity of a moving body
   Flow around steady and vibrating airfoil NACA 0012 with a 10 degrees angle of attack has been studied experimentally, using a time-resolved PIV technique at Reynolds number of 65 000. In this situation, a strong interaction between the airfoil and the flow-field is typically observed. Dynamics of flow in the airfoil wake has been investigated in details. Besides statistical analysis of the flow field point-by-point in space, we have explored complex spatial dynamics of the flow using the Oscillation Pattern Decomposition (OPD) method applied on the entire velocity vector field. The flow field spatial dynamics is characterized by the OPD modes of oscillating and non-oscillating characters, capturing traveling and pulsating patterns. Topology and frequencies of dynamical modes were investigated. The unsteady velocity field is affected by both wing vibrations and inherent flow dynamics. Role of the airfoil vibrations in the flow dynamics is demonstrated.
   - Uruba, V., Near wake dynamics around a vibrating airfoil by means of PIV and Oscillation Pattern Decomposition at Reynolds number of 65 000 (2015), Journal of Fluids and Structures. 55(May), pp. 372-383.
2. 3D Instability of Flow in the Vicinity of an Airfoil Suction Side
   The nonstationary flow close to the suction side of an airfoil has been analyzed in details. Various types of nonstationary structures have been detected in the form of more or less regular waves of vortices oriented either in span-wise or stream-wise directions. Those dynamical structures have important effect on static pressure distribution in the airfoil vicinity. To fulfil the above task the new special analytical methods have been developed, allowing analysis of nonstationary velocity fields by their decomposition.
   - Uruba, V., Procházka, P., P., Skála, V. On the boundary layer structure on suction side of an airfoil (2019), EPJ Web of Conferences. Paris: EDP Sciences, art. No. UNSP 02088.
3. New principle of lift generation on an airfoil
   A new hypothesis [*Hoffman et al., New theory of flight (2015), Journal of Mathematical Fluid Mechanics, 18(2)*] of physical mechanism of flight relies on existence of streamwise vortical structures above the wing and inside the wake. The vortices origin as a consequence of flow instability inside the boundary layer developed under adverse pressure gradient. These structures are highly dynamical in nature, they change position and size very rapidly. A simple airfoil in the form of a flat plate with moderate angle of attack is considered in our research. Stereo PIV time resolved measurement technique was used to capture high-dynamic data in several planes which are located in the wake and are perpendicular to freestream or parallel to the airfoil. Distinct flow patterns with associated kinetic energy were described as well as their role in the studied case. The results of our experiments and mathematical modelling support the new theory, however the real flow-field is even more complex, it contains structures not presented in the model.

- Uruba, V., On aerodynamic forces physical mechanism (2016), AIP Conference Proceedings, New York: American Institute of Physics Inc., art. No. 020011.1768.
- Procházka, P., Uruba, V., Streamwise and spanwise vortical structure merging inside the wake of an inclined flat plate (2019), Mechanics & Industry. Vol. 20/7, art. No. 705.

Laboratory of Environmental Aerodynamics *(head: Stěpán NOSEK, Ph.D.)*

The team of the Laboratory of Environmental Aerodynamics has addressed four national projects and has been participating on two international networks (COST actions) during the evaluation period (2015-2019). Two projects have finished within the period, while the second two projects and the two international networks are currently under progress.

1. Experimental study of organized structures in turbulent boundary layer with free-steam turbulence
   The goal was to provide a better understanding of the physical phenomena associated with grid-generated external turbulence and roughness-generated internal turbulence. Particularly, the turbulent kinetic energy (TKE) and momentum flux by means of coherent structure detection methods and their combinations were analysed. A new methodology was developed: how to find a statistical representation of boundary layer, to assess its parameters and their uncertainties. The main goal of the project was to develop a strategy for identification of both the external and internal turbulence and to localize the interface in-between. By means of modified wavelet analysis together with correlation and integral length scale, it is possible to differentiate the coherent structures within the external turbulence from those in the internal turbulence; to manifest the unified character of the structures within each of the turbulent layer and demonstrate their growth with the increasing distance from the fences; localise the interface as a place where destructive mixing of both types of structures takes place; to evaluate the number of structures, their onset and cessation and the longitudinal dimension directly from the analyses. The estimation their vertical extent is possible indirectly from a correlation. The Quadrant analysis in combination with the wavelet analysis verified the existence of large scale motions (LSM) and very large scale motions (VLSM). The Proper Orthogonal Decomposition (POD) confirmed that the energy content inside studied structures reaches up to 80% within the investigated boundary-layer volume. An advanced validation technique comprising the coherent detection methods for large eddy simulation (LES), evolved in Charles University in Prague (Department of Atmospheric Physics, Faculty of Mathematics and Physics) was further developed. The necessity of in-depth validation procedure was demonstrated, which considers also the statistics of transient phenomena, and not only of the mean values. The project proved the ability of the model to reliably simulate the large dominant events despite its sparse spatial resolution.
   - Kellnerová, R., Fuka, V., Uruba, V., Jurčáková, K., Nosek, Š., Chaloupecká, H., Jaňour, Z., On street-canyon flow dynamics: advanced validation of LES by time-resolved PIV (2018), Atmosphere, 9(5), art. No 161.
   - Nosek, Š., Kukačka, L., Kellnerová, R., Jurčáková, K, Jaňour, Z., Impact of roof height non-uniformity on pollutant transport between a street canyon and intersections (2017), Environmental Pollution, Vol. 227, pp. 125-138.

2. Short-term toxic gas leakages into atmosphere
   The main aim was to develop a new fast emergency dispersion model for short-term gas leakages. The model was based on the relations between short-term and long-term gas releases being found utilizing wind-tunnel experiments. The model is written into a standalone .exe execute MATLAB-code. The standalone code will be utilized by the Ministry of Interior of the Czech Republic in the daily use of the emergency services – the Emergency Call Centre 112.

In the year 2018, the relations between characteristics of short-term and long-term gas leakages for an urban area were searched, the data from the international database COST ES1006 were utilized. Then, releases of short-term and long-term gases for a rural area were performed using wind-tunnel modelling. A dimensionless Database I was created from the data.
In the year 2019, the dispersion of short-term and long-term gas releases in an industrial area was studied in the wind-tunnel. The measured data were analysed and the second dimensionless Database II was created. Both the Database I and Database II were utilized for the validation of the model. The software written as a standalone MATLAB code was written as the main goal of the project.

- Chaloupecká, H., Jakubcová, M., Jaňour, Z., Jurčáková, K., Kellnerová, R., Equations of a new puff model for idealized urban canopy (2019), Process Safety and Environmental Protection, 126(June), pp. 382-392.

3. Impact of Atmospheric Boundary Layer Parameters on Ammonia Emissions from Livestock Buildings
Naturally ventilated livestock buildings (NVLB), such as cattle barns, represent one of the most significant sources of ammonia emissions. While higher concentrations of ammonia pose severe health and environmental issue, the dispersion processes even of passive pollutant within NVLBs are still not well understood. Therefore, the main objective of this ongoing project is to investigate the passive pollutant dispersion in a model of a cattle barn using a wind tunnel experiment method. This objective was designed according to the objectives and needs of the ongoing COST project CA16106 „Ammonia and Greenhouse Gases Emissions from Animal Production Buildings". The results show that the type of atmospheric boundary layer and sidewall opening height have a significant impact on the pollutant dispersion in the barn, while the presence of animals and doors openings are insignificant under conditions of winds perpendicular to the sidewall openings. The observed relations will be implemented in a new software for the prediction of ammonia emissions from cattle barns.
   - Nosek, Š., Kluková, Z., Jakubcová, M., Yi, Q., Janke, D., Demeyer, P., Jaňour, Z., The impact of atmospheric boundary layer, opening configuration and presence of animals on the ventilation of a cattle barn (2020), J. Wind Eng. Ind. Aerodyn. Vol. 201.

Laboratory of Computational Fluid Dynamics *(head: Dr. Jan PECH)*

The research activities in the laboratory were focused mainly on development of mathematical models for transonic flow, high order simulations of flow with variable properties, development of mathematical models for incompressible flow, high-order Galerkin method, and implementation of turbulent model into a high order numerical solver.

1. Development of mathematical models for transonic flow in turbomachinery applications
Numerical simulations were focused on modelling of transonic flows in turbine blade cascades corresponding to mid and tip blade sections of low-pressure part of the steam turbine of a large output. Various transition models based on the intermittency coefficient were tested for the modelling of transition in attached and separated flows with respect to the interaction of the shock wave with boundary layers. A special attention was given to the separation induced transition. Further the effect of the computational domain on the modelling of flow through the turbine blade cascade with a supersonic inlet was studied. Computational domains were formed partly by the blade cascade only and partly by the substantial part of the test section with the blade cascade and with the permeable wall for the suppression of shock waves reflections. Simulations were carried out for 2D and 3D flows through blade cascades by means of SST and EARSM turbulence models. The k-kL-omega turbulence model was modified for the pressure-gradient effect and tested for compressible flow with heat transfer. The

algebraic transition model proposed in the last period was modified for the effect of wall roughness including a short rough strip. Proposed correlations were verified by experiments in various boundary conditions including heat transfer.

- Louda, P., Příhoda, J., On the modelling turbulent transition in turbine cascades with flow separation (2019). Computers & Fluids, 181(March), pp.160-172.

2. <u>High-order simulations of flow with variable properties</u>
Original numerical scheme based on spectral/hp element method was developed for high-order simulations of flow with variable properties. High-order approximations to CFD solutions bring accuracy, efficiency and direct insight to error estimate in spatial coordinates through decays in coefficient spectra. Material properties (viscosity, density and thermal conductivity) in the Navier-Stokes-Fourier system were considered as temperature-dependent. Dependence of density on pressure was neglected, but divergence of velocity was non-homogeneous as a consequence of thermal expansion. Convergence properties of the scheme were thoroughly tested on manufactured solutions and it was already applied in simulations of flow around heated/cooled bodies in unsteady regimes of laminar-turbulent transition. Temporal evolution of various parameters, e.g. Strouhal, Nusselt number, flow separation points, was studied and results contributed to understanding of laminar-turbulent transition of fluid flow exposed to temperature change. Structure of the Navier-Stokes-Fourier system has multiple common features with some models of turbulence, therefore modification of the solver for models of turbulence has begun.

- Pech, J., On computations of temperature dependent incompressible flows by high order methods (2016), EPJ Web of Conferences, 114 02089.
- Pech, J., Louda, P., Comparison of finite volume and spectral/HP methods on Navier - Stokes equations for unsteady incompressible flow (2018), Proceedings Topical Problems of Fluid Mechanics 2018, pp. 223-230.

3. <u>Development of mathematical models for incompressible flow in environmental applications</u>
Development of mathematical models for incompressible flow in environmental applications was carried out during the whole period in cooperation with Laboratory of Environmental Aerodynamics. Model for turbulent transport of pollutant originating in a building has been developed. Its implementation on OpenFOAM platform is tested and improved progressively. Applied finite volume method used in this research provides numerically stable results and coincidence between numerical and experimental data is traced.

4. <u>High-order Discontinuous Galerkin (DG) study of compressible flow around an aerodynamic profile</u>
DG method is a modern approach which gets a lot of attention in computational community during last years. It is capable to approximate discontinuous flow fields and provides stable simulations of unsteady flows at high speed regimes without additional turbulent models. Combination of DG approach and locally high-order spatial approximation (spectral/hp elements) then brings combination of numerical stability and high-order spatial accuracy.

The research in above listed areas was supported by the following **grant projects**:

1. National Centre for Energy, Technology Agency of the Czech Republic, project No. TN01000007, 2019-2020
2. Turbine Profile Cascades for Supersonic Flow Fields, Technology Agency of the Czech Republic, project No. TH02020057, 2017-2020
3. Aerodynamics of Highly Loaded Blade Cascades, Technology Agency of the Czech Republic, project No. TA03020277, 2013-2016

4. Impact of Atmospheric Boundary Layer Parameters on Ammonia Emissions from Livestock Buildings, Ministry of Education, Youth and Sports of the Czech Republic, project No. LTC118070, 2018-2021
5. Ammonia and Greenhouse Gases Emissions from Animal Production Buildings European Cooperation in Science and Technology, project No. COST CA 16106, 2017-2021
6. Profiling the atmospheric Boundary layer at European scale, European Cooperation in Science and Technology, project No. COST CA 18235, 2019-2023
7. Large structures in the boundary layers over complex surfaces in high Reynolds numbers, Czech Science Foundation, project No. GA18-09539S, 2018-2020
8. Experimental study of organized structures in turbulent boundary layer with free-stream turbulence, Czech Science Foundation, project No. GA15-18964S, 2015-2019
9. Short-duration leakage of hazardous gases into atmosphere, Technology Agency of the Czech Republic), project No. TJ01000383, 2018-2019
10. Advanced experimental research on synchronous and non-synchronous blade vibration, Ministry of Education Youth and Sports of the Czech Republic, project No. LTAUSA19036, 2019-2022
11. Intake and outlet structures of pump and turbine facilities, Ministry of Industry and Trade of the Czech Republic, project No. FV30104, 2018- 2021
12. Flow control of boundary layer using DBD plasma actuators, Czech Science Foundation, project No. GA14-25354P, 2014-2016
13. High order numerical simulations of heated flow and fluid-structure interaction, Czech Academy of Sciences, project No. MSM100761901, 2019-2020
14. Direct eddy simulation in turbochargers via MILES-WBF method, Technology Agency of the Czech Republic, project No. TA04011437, 2014-2017
15. Investigation of flows in a multi-stage axial turbine stages arrangement, Technology Agency of the Czech Republic, project No. TA04020129, 2014-2017
16. 3D Instability of a shear layer in adverse pressure gradient, GA17-01088S, 2017-2019
17. Effect of complex boundary conditions on the laminar/turbulent transition, Czech Science Foundation, project No. GAP101/12/1271, 2012-2016

Research activity and characterisation of the main scientific results

The research in the Department of Thermodynamics concerns various aspects of heat and mass transfer, fluid flow, material properties, phase transitions, and complex processes requiring specialized, mostly self-designed, experimental apparatuses, thorough theoretical understanding and expertise in mathematical modelling. The research activities are primarily concentrated in four laboratories: The Laboratory of Thermophysical Properties (LTP) led by Dr. V. Vinš, the Laboratory of Heat and Mass Transfer (LHMT) led by Assoc. Prof. Z. Trávníček, the Laboratory of Phase Transitions (LPT) led by Dr. J. Hrubý, and the Laboratory of Energy Storage (LES) led by Dr. J. Kordík. The laboratories share personnel depending on the needs, individual skills and availability of projects. Besides the laboratory heads, the team had several outstanding personalities – Prof. F. Maršík (former department head, part time), Prof. V. Tesař (part time), Prof. T. Roubíček (part time), and Assoc. Prof. A. Fedorchenko, who were loosely connected with the laboratories and performed their research individually or with small ad hoc groups.

This report represents only a narrow selection from the output of the team. In the evaluated period, the Department of Thermodynamics generated 103 articles in renowned journals and 7 patents covering a broad range of equilibrium and non-equilibrium thermodynamics, heat and mass transfer, fluid flow, and other engineering science disciplines.

Laboratory of Thermophysicial Properties (LTP) was led by Dr. J. Pátek and later by Dr. V. Vinš. In the evaluated period, the research in LTP focused primarily on thermophysical properties of ionic liquids. Ionic liquids are currently subject of intense research efforts because of their remarkable potential for various applications. Two experimental facilities were used: (i) a constant volume apparatus to measure pressure-volume-temperature relations of liquids, (ii) a tensiometer to measure the volume-temperature relation at atmospheric pressure by the buoyancy method and the surface tension-temperature relation by Wilhelmy plate and du Noüy ring method. The constant volume apparatus, designed in LTP has several unique features: it makes possible measurements at temperatures down to –90 °C, the temperature of the sample can be defined and measured with the accuracy of 0.005 K, the relative expanded combined uncertainty at 95% confidence level of the resultant density is 0.1 %. The measurements are typically conducted in the temperature interval from 200 to 353 K and from 0.1 to 60 MPa in pressures. Further equipment of the laboratory consists of commercial instruments for measurement of pressure-volume-temperature-composition relationship, surface tension, and viscosity. The LTP team develops own calibration procedures in order to obtain accurate reliable data. Tensiometer Krüss K 100 allows for measurement of surface tension with the Wilhelmy plate method and the du Noüy ring technique in the temperature range from app. –15 to 150 °C. A buoyancy density measurement at atmospheric pressure with a single-crystal silicon can be carried out in addition.

Surface tension and density was studied for several ionic liquids [6][8] in frame of project [K]. A group contribution and parachor analysis of experimental data on densities and surface tension has been performed for several homologous series of ionic liquids [5], providing a tool for estimating these properties for a broader class of ionic liquids. Besides, recommended values for the surface tension of ordinary water were generated based on all available experimental data including own new measurements using nonparametric regression [6]. Starting from this data set, a new equation has been developed representing the surface tension of ordinary water in the complete temperature range. This work is highly relevant for the International Association for the Properties of Water and Steam (IAPWS) and also it has links to the activity of LPT laboratory as discussed later.

Laboratory of Heat and Mass Transfer (LHMT) was led by Assoc. Prof. Z. Trávníček. An important field of study of LHMT were synthetic jets (SJs). SJ is a fluid flow generated by pushing and pulling fluid from a cavity through an orifice or a nozzle. The cavity is typically bounded at one end by a rigid wall with an emitting orifice and at the other end by an actuating surface (a diaphragm or piston). The flow in the orifice reverses its direction after each stroke while the time-mean mass flux in the orifice is zero. SJ offers potential advantages for various applications of active control of flow/thermal fields such as heat/mass transfer applications (drying technologies or cooling of highly loaded electronic devices or gas turbine blades). Besides the zero-mean-flux SJ, also so called hybrid SJ with non-zero net mass flux were studied. These devices use fluidic diodes or other means of passive flow control to enhance the directional flow.

In frame of consecutive projects [M] and [L], control of flow by means of fluid oscillation was studied and the pulsatile jet actuation has been optimized. The experiments used flow visualization, single-sensor hot-wire measurements, and mass transfer measurements on the wall using the naphthalene sublimation technique. The local heat transfer expressed in terms of a Nusselt number was evaluated using the heat and mass transfer analogy [7]. Additional experiments were performed using the laser Doppler vibrometry [15]. For theoretical analyses, lumped element models were used [10]. In a study of energetic efficiencies of synthetic and hybrid synthetic jet actuators driven by electrodynamic transducers [10], the hybrid synthetic jet actuator achieved a 15-23% increase in the velocities and a 41 to 48% increase in the energetic efficiency, both in comparison with an ordinary synthetic jet actuator working at the same input real power. The flow field of SJ was investigated by visualization experiments [15] parameterized in terms of the Reynolds (Re) and Stokes (S) numbers. Four regimes of oscillatory suction and extrusion were distinguished and presented by means of a Re-S parameter map: (a) creeping flow without SJ formation, (b) SJ formation and propagation without vortex rollup, (c) SJ with vortex rollup, and (d) vortex structure breakdown, instability and transition to turbulence. Quantitative study of velocity profiles at the exit of axisymmetric synthetic jet actuators [19] performed in a collaboration with group of Prof. V. Timchenko (UNSW Sydney) showed that the average-to-centerline velocity ratio depends mainly on the dimensionless stroke length, with a minor dependence on the Reynolds number. Results of both experimental and numerical approaches are in reasonable agreement showing variation this ratio in the range of 0.7-1.3. Further contribution to quantitative studies of SJ was development of a relatively simple experimental method for evaluating synthetic jet (SJ) characteristic velocity and fluxes of time-mean momentum and kinetic energy [25] using a direct measurement of the SJ thrust by means of precision scales. Performed quantitative studies of SJs allowed to proceed to their optimization [18] based on maximizing an objective function which was alternatively selected from the four integral quantities: volumetric flux, momentum flux, kinetic energy flux, and energetic efficiency. With respect to potential applications for active flow control and heat transfer enhancement, the most appropriate objective function was suggested to be the momentum flux. Because of the intrinsic non-linearity of SJ actuators, it appears feasible to improve their performance by non-harmonic excitation [22]. An axisymmetric synthetic jet actuator based on a loudspeaker was driven by a waveform whose shape was derived from a pulse-width modulated signal. Based on a newly introduced dimensionless nozzle diameter, a criterion was found that states conditions under which it is advantageous to use the suggested non-harmonic excitation.

A new systematically developed direction of research was improving technology by adopting arrangements found biological systems. A novel variant of a synthetic jet actuator was designed [21] employing a bio-inspired nozzle whose oscillating lip is formed by a flexible diaphragm rim. The proposed actuator showed an increase in the momentum flux by 18 % compared with that of a conventional synthetic jet actuator.

Besides the research targeted at synthetic jets, several general topics has been addressed in LHMT. Recently introduced idea of secondary invariants was used to bypass this limitation the Buckingham pi-theorem for flow similarity. This new approach was demonstrated on a family of nozzles which are mutually not fully geometrically similar [26]. A new arrangement of high-frequency no-moving-part fluidic oscillators has been proposed [9]. It employs a stationary rotating vortex inside the chamber bounded by two attachment walls. Three distinct regimes were identified with oscillation frequencies ranging from1.7 kHz to 8.2 kHz.

Several patents were awarded for inventions with potential applications. These include cooling of cylindrical objects with help of synthetic jets [30], new fluidic oscillator [31], new arrangement of a small-scale blade-less steam turbine [33], fluidic sensors of particles and substances [34], flow control using high frequency electrical current [32], and a new method of additive manufacturing using small droplets of molten metals [35]. The last two inventions have been achieved in collaboration with Dr. J. Šonský from Dept. 6-Electrical Engineering and Electrophysics.

Laboratory of Phase Transitions (LPT) was led by Dr. V. Vinš and later by Dr. J. Hrubý. Main research activities of LPT are connected with theoretical and experimental investigation of the thermophysical properties of metastable fluids, phase transitions, particularly nucleation of droplets and bubbles. Several LPT researchers are active members of the International Association for Properties of Water and Steam (IAPWS, http://www.iapws.org/) and much of the research at LPT is motivated by the needs of IAPWS. The participation in IAPWS was supported by travel grants [I] and [E].

A large part of the experimental work at LPT focused on investigation of thermophysical properties of pure water and aqueous mixtures under the metastable supercooled liquid conditions as a part of activities of consecutive projects [K] and [N]. Two in-house designed apparatuses have been developed for measurement of surface tension and density of supercooled water and aqueous mixtures. These apparatuses were further improved over the present evaluation period. Experiments on the surface tension of supercooled water were continued by two alternative methods: a counterpressure capillary rise method [1] and the horizontal capillary tube method [2]. Application of these methods required considerable development efforts. The importance of using the alternative methods was in confirming previous results of this laboratory, in particular regarding the question of the existence of the second inflection point (SIP) in the temperature dependence of the surface tension. The counterpressure capillary rise method used helium to balance a change of capillary elevation due to a change of surface tension. It circumvented an uncertainty connected with possibly varying cross section of the capillary tube along its length. The horizontal method imitated experiments by P. T. Hacker, which were a main dataset supporting the hypothesis of SIP existence. The SIP as observed by Hacker was not confirmed, but certain straightening of the surface tension curve indicated a possible inflection at lower temperatures. A major achievement was finalization of highly accurate measurements of density of heavy water [3] including the metastable supercooled region from 254 to 298 K and up to 100 MPa. The expanded (k=2) uncertainty of these measurements was 50 ppm. Measured data was used together with selected literature values of the speed of sound to develop an equation of state for the region of liquid water.

Besides experiments, modelling work was an important part of LPT activities. In a series of papers on gas hydrates modeling [4], several aspects of the thermodynamics of these clathrate structures were investigated in collaboration with Prof R. Span and coworkers from Ruhr-Universität Bochum (RUB) and Technische Universität Dresden (TUD). Phase equilibria with fluid phases and crystalline phases were computed and compared to literature data. The model has been implemented in the software package TREND (Thermodynamic Reference and Engineering Data) maintained at RUB.

In frame of projects [H] and [C], nucleation (first stage of phase transition) was studied in systems relevant to carbon capture and storage or utilization (CCS/U). Experimental work involved development of expansion chambers, in which supersaturation needed for nucleation of droplets is developed by adiabatic expansion. Theoretical studies of nucleation were based on modifications of the classical nucleation theory, in which some of its crude approximations were replaced by more realistic ones. In particular, curvature-dependent surface tension needed for computing the formation work of clusters was modelled for multicomponent systems relevant to CCS using density gradient theory [13][20]. Long-term collaboration with Eindhoven University of Technology (TU/e) continued by a study of the effect of pressure and carrier gas on homogeneous water nucleation rates [14].

Laboratory of Energy Storage (LES) was led by Dr. J. Kordík. LES was established during the present evaluation period (2015-2019) as an action of the Strategy AV21 aiming at strengthening of collaboration of the Czech Academy of Sciences with state and public institutions as well as with commercial subjects, and at strengthening the collaborations among various institutes of the Czech Academy of Sciences. The topic of thermal energy storage was selected because it is of great importance for the energy policy: almost half of primary energy is consumed for heating purposes. Daily or even seasonal energy storage can provide a major contribution to energy savings. In addition, thermal energy storage can participate in “peak-shaving” of the power production and consumption curves. High temperature thermal storage is an important part of concentrated solar power plants, compressed air energy storage, and batch-wise industrial processes. LES has been established as an application oriented laboratory which is in the intersection of the research fields of the three existing labs – LTP, LHMT, and LPT.

LES succeeded in receiving support through a fundamental research project [A] focussing on low-temperature thermal storage materials [29] and in an applied research project [B] with an industrial partner focussing on improving the performance of heat transfer fluids by addition of nanoparticles (so called nanofluids). Several experimental setups were developed in frame of these projects. The most significant is a heat exchanger loop allowing to study the performance of various heat transfer fluids.

Besides research closely connected with the research topics of the four laboratories, numerous mathematical models in continuum mechanics and thermomechanics of solids and interaction of porous solids and fluids have been developed. These models are generally described by systems of nonlinear partial differential equations or inequalities formulated in a thermodynamically consistent way and mathematically analysed with the aim to prove rigorously existence of their solutions and devise efficient numerical strategies for their approximation implementable on computers. Prof. Roubíček developed variational methods for steady-state Darcy/Fick flow in swollen and poroelastic solids [12]. Existence of steady states in elastic media at small strains with diffusion of a solvent or fluid due to Fick's or Darcy's laws was proved by combining usage of variational methods. Maximally-dissipative local solutions to rate-independent systems and application to damage and delamination problems were studied [16]. Applications of such solutions were illustrated on specific examples from continuum mechanics at small strains involving inelastic processes in a bulk or on a surface, namely damage and delamination. Seismic waves and earthquakes in a global monolithic model [23]. The philosophy that a single “monolithic” model can “asymptotically” replace and couple in a simple way several specialized models relevant on various Earth layers was presented and rigorously justified for special situations. Geophysical models of heat and fluid flow in damageable poro-elastic continua [27] were studied. Thermodynamically based formulation included entropy balance and an explicit global energy balance.

Selected articles in journals:

[1] Vinš, Václav, Fransen, M. A. L. J., Hykl, Jiří, Hrubý, Jan. *Surface Tension of Supercooled Water Determined by Using a Counterpressure Capillary Rise Method*. Journal of Physical Chemistry B. 2015, 119(17), 5567-5575.

[2] Vinš, Václav, Hošek, Jan, Hykl, Jiří, Hrubý, Jan. *Surface Tension of Supercooled Water: Inflection Point-Free Course down to 250 K Confirmed Using a Horizontal Capillary Tube*. Journal of Chemical and Engineering Data. 2017, 62(11), 3823-3832.

[3] Blahut, Aleš, Hykl, Jiří, Peukert, Pavel, Vinš, Václav, Hrubý, Jan. *Relative density and isobaric expansivity of cold and supercooled heavy water from 254 to 298 K and up to 100 MPa*. Journal of Chemical Physics. 2019, 151(3), 034505.

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[6] Součková, Monika, Klomfar, Jaroslav, Pátek, Jaroslav. *Surface tension and 0.1 MPa density data for 1-Cn-3-methylimidazolium iodides with n=3, 4, and 6, validated using a parachor and group contribution model*. Journal of Chemical Thermodynamics. 2015, 83 52-60.
[7] Trávníček, Zdeněk, Vít, T. *Impingement heat/mass transfer to hybrid synthetic jets and other reversible pulsating jets*. International Journal of Heat and Mass Transfer. 2015, 85, 473-487.
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[9] Tesař, Václav. *High-frequency fluidic oscillator*. Sensors and Actuators A - Physical. 2015, 234, 158-167.
[10] Kordík, Jozef, Trávníček, Zdeněk, Pavelka, Miroslav. *Energetic efficiencies of synthetic and hybrid synthetic jet actuators driven by electrodynamic transducers*. Experimental Thermal and Fluid Science. 2015,69, 119-126.
[11] Pátek, Jaroslav, Součková, Monika, Klomfar, Jaroslav. *Generation of Recommendable Values for the Surface Tension of Water Using a Nonparametric Regression*. Journal of Chemical and Engineering Data. 2016, 61(2), 928-935.
[12] Roubíček, Tomáš. *Variational methods for steady-state Darcy/Fick flow in swollen and poroelastic solids*. ZAMM-Zeitschrift fur Angewandte Mathematik und Mechanik. 2017, 97(8), 990-1002.
[13] Celný, David, Vinš, Václav, Hrubý, Jan. *Modelling of planar and spherical phase interfaces for multicomponent systems using density gradient theory*. Fluid Phase Equilibria. 2019, 483, 70-83.
[14] Fransen, M. A. L. J., Hrubý, Jan, Smeulders, D. M. J., Dongen, M. E. H. *On the effect of pressure and carrier gas on homogeneous water nucleation*. Journal of Chemical Physics. 2015, 142(16), 164307_1-164307_7.
[15] Trávníček, Zdeněk, Broučková, Zuzana, Kordík, Jozef, Vít, T. *Visualization of synthetic jet formation in air*. Journal of Visualization. 2015, 18(4), 595-609.
[16] Roubíček, Tomáš. *Maximally-dissipative local solutions to rate-independent systems and application to damage and delamination problems*. Nonlinear Analysis: Theory, Methods & Applications. 2015, 113, 33-50.
[17] Součková, Monika, Klomfar, Jaroslav, Pátek, Jaroslav. *Surface tension and 0.1 MPa density of 1-alkyl-3-methylimidazolium tetrafluoroborates in a homologous series perspective*. Journal of Chemical Thermodynamics. 2016, 100, 79-88.
[18] Kordík, Jozef, Trávníček, Zdeněk. *Optimal diameter of nozzles of synthetic jet actuators based on electrodynamic transducers*. Experimental Thermal and Fluid Science. 2017, 86, 281-294.
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[20] Planková, Barbora, Vinš, Václav, Hrubý, Jan. *Predictions of homogeneous nucleation rates for n-alkanes accounting for the diffuse phase interface and capillary waves*. Journal of Chemical Physics. 2017, 147(16), 164702.
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[23] Roubíček, Tomáš. *Seismic waves and earthquakes in a global monolithic model*. Continuum Mechanics and Thermodynamics. 2018, 30(4), 709-729.
[24] Vinš, Václav, Hykl, Jiří, Hrubý, Jan. *Surface tension of seawater at low temperatures including supercooled region down to – 25 °C*. Marine Chemistry. 2019, 213, 13-23.
[25] Kordík, Jozef, Trávníček, Zdeněk. *Integral Quantities of Axisymmetric Synthetic Jets Evaluated from a Direct Jet Thrust Measurement*. Flow Turbulence and Combustion. 2019, 103(3), 827-844.
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[29] Tesař, Václav, Kordík, Jozef. *Energy storage in macro-capsules for thermal comfort garments*. Journal of Energy Storage 25 (2019)100842

Patents:

[30] Trávníček, Zdeněk - Broučková, Zuzana. *The method and the device for cooling of cylindrical objects by means of the cooling fluid jet*. 2017, Pat. No. 306 506, http://spisy.upv.cz/Patents/FullDocuments/306/306506.pdf
[31] Tesař, Václav. *Fluidic oscillator*. 2016. Pat. No. 306064, http://spisy.upv.cz/Patents/FullDocuments/306/306064.pdf
[32] Tesař, Václav - Šonský, Jiří. *Method of fluid distribution in dependence on electrical control signal and apparatus for making the same*. 2015. Pat.No. 305352, http://spisy.upv.cz/Patents/FullDocuments/305/305352.pdf
[33] Trávníček, Zdeněk - Vít, Tomáš - Hrubý, Jan. *Bladeless steam miniturbine*. 2016. Pat. No. 306049, http://spisy.upv.cz/Patents/FullDocuments/306/306049.pdf
[34] Tesař, Václav. *Sensor for sensing particles or substances carried by a fluid*. 2016. Pat. No. 305767, http://spisy.upv.cz/Patents/FullDocuments/305/305767.pdf
[35] Šonský, Jiří - Tesař, Václav. *A method and a device for forming metal products by gradual addition of small droplets of molten metal*. 2017. Pat. No. 307134, http://isdv.upv.cz/doc/FullFiles/Patents/FullDocuments/307/307134.pdf.

Projects:

Abbreviations:

CAS – Czech Academy of Sciences,

CSF – Czech Science Foundation (GACR),

MoE – Ministry of Education, Youth and Sports of the Czech Republic,

NF – Norway Funds,

TACR – Technology Agency of the Czech Republic.

Principal investigator M. Čenský:

[A] GA17-08218S (CSF, 2017–2019) Materials for thermal energy storage> Thermophysical characterization for design of thermal batteries

Principal investigator J. Hrubý:

[B] TH03020313 (TACR, 2018–2020) Application of nano-additives for enhancement of heat and cold transfer of thermal fluids

[C] EF16_019/0000753 (MoE, project partner, 2018–2022) Research Centre of Low Carbon Energy Technologies (Bio-CCS/U)

[D] 8J18FR008 (MoE, 2018–2020) Joint French-Czech research of supercooled aqueous systems.

[E] 2016–2017 (MoE, INGO II LG15040) Representation of Czech scientists in governing bodies of the International Association for the Properties of Water and Steam in 2016-2017

[F] GA16-02647S (CSF, 2016–2018) Properties of water and seawater in metastable states. Experiment, molecular simulation, and thermodynamic modeling.

[G] TA04011656 (TACR, project partner, 2014–2016) Development of a high-speed orbital gears with flexible satellite pins

[H] 7F14466 (NF/MoE, 2014–2017) Phase Transitions in CCS systems

[I] LG – INGO (MoE, 2013–2015) Representation of Czech scientists in governing bodies of the International Association for the Properties of Water and Steam (IAPWS)

[J] GAP101/11/1593 (CSF, 2011–2015) Research of non-equilibrium steam condensation – a new approach

Principal investigator J. Pátek:

[K] GA13-00145S (CSF, 2013-2017) Experimental research and modelling of thermodynamic properties of new ionic liquids.

Principal investigator Z. Trávníček:

[L] GA16-16596S (CSF, 2016–2018) Optimization of pulsatile jet actuation in fluid mechanics

[M] GA14-08888S (CSF, 2014–2016) Control of flow fields by means of fluid oscillation

Principal investigator V. Vinš:

[N] GA19-05696S (CSF, 2019–2021) Properties of water-based heat transfer fluids under extreme conditions

[O] GA15-07129Y (CSF, 2015–2017) Surface tension of water and aqueous mixtures at equilibrium and metastable states

[P] M100761201 (CAS, 2012–2015) Phase equilibria of gas hydrates modeled with the reference equations of state – a theoretical basis for future CCS and gas transport technologies

Research activity and characterisation of the main scientific results

1. *Laboratory of Vibrodiagnostics and Nonlinear Dynamics* (LVND)

Head: *Dr. Luděk Pešek*

Non-linear dynamics laboratory has been dealing with fundamental and applied research in the areas of: structural dynamics, fluid-structure interactions (FSI) and damping technologies. The structural research includes mainly rotordynamics, such as bladed wheels and gear-box dynamics. The FSI research is mainly focused on the fluid induced vibration in turbomachinery. The damping research aims at passive damping of hard rubbers and dry-friction applications.

The results achieved in the solved projects in the last period (2015-2019):

In the grant project GACR No: 16-04546S the FSI research group was focused mainly on flow induced vibration in periodic bodies e.g. steam turbine and especially the flutter in the steam turbine blade. The research was carried out by numerical modeling and the experimental analysis. For numerical modeling a reduced order aeroelastic model (ROAM) tool is developed for fast analysis of classical flutter. A mesh free fluid solver is developed for fast estimation of unsteady aerodynamics loading and to estimate the aerodynamic damping in 2D and 3D blade cascades. The damping is estimated with the traveling wave mode (TWM) method. The unsteady incompressible flow field is modeled using Panel method based on boundary element method. The structural part is modeled with a non-linear beam element based on FEM solver. Both solvers are coupled to perform aeroelastic simulations. The results were validated with experiments on the turbine blade cascade. The proposed methodology estimates aerodynamic damping with acceptable accuracy for the aeroelastic analysis of the cascade. Moreover, present ROAM shows significant reduction in computational time.

The test cascade with 5 flat plates has been designed for experimental study of FSI problems. The 2 boundary plates were steady and the 3 middle plates were periodically excited by electrodynamic exciters with prescribed amplitude, frequency and phase. Algorithm for harmonic excitation with a phase shift of the plates in the cascade was developed in SIMULINK program for the control system dSPACE. The aeroelastic behaviour of the cascade was studied in collaboration with the department D1 in a wind tunnel at different Reynolds numbers. PIV optical method was used for the flow velocity field analysis. The aeroelastic coupling was the most dominant at forward wave propagation but the most destabilizing effect of the coupling was detected at backward wave propagation due to phase lag of the relative velocity motion and aerodynamic forces with respect to the motion of the reference (middle) blade. The experimental data were valuable for validation of the in-house developed numerical aeroelastic codes.

For determination of critical and post-critical behaviour of self-excited vibration in the blade cascade, the Van der Pol model was proposed. Advantage of this theoretical model is the conversion of negative damping into positive one after the amplitude of self-excited oscillations exceeds prescribed limits. Therefore, to study the interaction of forced and self-excited vibration of blade cascade under flutter we proposed two types of Van der Pol aerodynamic self-excitations. As case studies the different blade systems (bundles, whole wheels) with viscous-elastic or dry-friction damping in the blades shroud, delayed harmonic force excitation and the Van der Pol aerodynamic self-excitation were analyzed. This research was focused on the evaluation of the post-critical dynamic properties of the rotational periodical structures and self-excited vibration suppression by different types of structural damping.

- Půst, L., Pešek, L. Blades forced vibration under aero-elastic excitation modeled by Van der Pol. International Journal of Bifurcation and Chaos. 2017, 27(11),
- Půst, L., Pešek, L., Byrtus, M. Modelling of flutter running waves in turbine blades cascade. Journal of Sound and Vibration. 2018, 436, 286-294

Computational modelling of turbine blades and bladed disks with inter-blade dry-friction damping was studied. Friction effects in blade couplings can be used as a source of passive damping. To describe the nonlinear influence of friction couplings on dynamic behaviour of blades, tie-boss couplings was chosen. To show temporal and spatial variability of contact states during one period of oscillation, the 3D FE models with surface to surface contact by the Augmented Lagrangian method were studied. Solving a full FE model with a large number of nonlinear coupling conditions in discretized contact surfaces is computationally demanding and part of computations was ascertained by HPCs (IT4Innovation Centre). Therefore, the dynamics of a bladed disc with tie-boss couplings was also solved by semi-analytical models, i.e. having a reduced number of DOFs, contact "surface to surface" simplified to one-point contact that moves on the contact surface. Non-linear effect of friction couplings on the dynamic behaviour of the system was studied at different excitation amplitudes. For validation of the models an extensive experimental research of bladed systems with dry-friction coupling was performed. The physical models of blade bundles and blade wheel model were designed, fabricated, equipped by sensors and dynamically tested.

- Pešek, L., Hajžman, M., Půst, L., Zeman, V., Byrtus, M., Brůha, J. Experimental and numerical investigation of friction element dissipative effects in blade shrouding. Nonlinear Dynamics. 2015, 79(3), 1711-1726.

The research on dry friction vibration damping of turbine bladed cascades was published in the chapter of Springer book. The main emphasis herein was the solution of damping effects of dry friction contacts in tie-bosses and shrouds. Friction is modeled herein from phenomenological view. The numerical models, i.e. discrete analytical, reduced and FE, used in our research of non-linear dynamic behaviour, of the blade cascades and bladed wheel are discussed. Dynamics states, such as resonant vibration or free attenuation are considered. The detail dynamic analysis of non-linear behaviour of these systems due to dry-friction contacts is presented for discrete analytical model with the stick-slip friction contact. Travelling wave vibration mode, the dynamic responses of the wheel to nozzle excitation and self-excitation are studied.

- Pešek, L., Půst, L., Šnábl, P., Bula, V., Hajžman, M., Byrtus, M. Dry-friction damping in vibration systems, theory and application to the blade disc assembly. In: J.J. Carlos, ed. Nonlinear Structural Dynamics and Damping. Mechanisms and Machine Science 69. Springer, 2019, 169-259, https://doi.org/10.1007/978-3-030-13317-7_6.

Since traditional CFD-CSD tools are computationally very expensive and required large computational power to simulate the FSI problems, in cooperation with department D4 (grant project GA19-02288J) we develop and apply robust methods of reduced-order modeling for tasks of FSI in large dynamic systems, e.g. wind turbines, helicopter, aircraft, stream turbine.

The boundary element (BE) based panel method (PM) is used to model flow field around bodies. Since we deal with the problem of the dominant resonant vibration of the blades and bladed disks, modal reduction method was used, and the modal properties of the system are accurately preserved. In addition, the numerical modal model can be validated directly by experimental modal analysis. Loose coupling method is used to solve the coupled fluid-structure multiphasic problems. Flow and structural equation are solved independently and they exchange data in pre-set time steps in time marching FSI simulations.

APPLIED RESEARCH – COLLABORATION WITH INDUSTRIAL COMPANIES

A) *Turbine producer Doosan Skoda Power, a.s.*

TACR NCK no. TN1000007 –WP1.07 Development of blade resistive against flutter
The FSI research group has started to participate on applied research dealing with the flutter problem in the turbomachinery. Reduced order flow solver and the aeroelastic solver will be developed for this purpose.

B) *Gear-box producer Wikov Gear, s.r.o.*

TACR no. TA04011656 Research and development of new type of high-speed planetary gear unit with the "flexible pin" technology to support the planet wheels enabling the transmission of high outputs (collaboration with department D2)

Numerical dynamical models of planetary gearbox with four satellites and standing planet carrier were developed. The strongly non-linear model of with four satellites on the flexible pins was developed in MATLAB/Simulink. Due to internal dynamic loads and external forces and moments acting on the gear box, the contacts between the teeth mesh profiles can brake during dynamic deformations. This can cause impact effects in the toothing which can cause further dynamic loading of the whole system. This effect was analyzed for various design parameters. For calculations of spectral properties of four-planet gearing box Wikov a linear model of gear-box with four satellites and standing planet carrier was developed.

Experimental analysis of elastic pins of four-planet gear-box with flexible pins designed and manufactured by Wikov Gear was performed. Measurement was carried out at a test facility at Wikov Gear. With the use of standard bearings of the planets, maximum speeds of 8500 rpm and with the floating ring bearings a speed of 14500 rpm were achieved. The methodology of measurement was proposed. The analysis was focused on evaluation of significant resonances of oscillation of planet pins for attuning parameters and validation of the numerical models.

The high-speed light nonlinear parametric systems with minimum dimensions and masses are very sensitive to their parameters. Therefore, theoretical research of the dynamic analysis of gear planetary systems plays a significant role in their development. The analytical solution leads to complicated systems of integro-differential equations or to complicated simulation models in MATLAB/Simulink. Therefore, the transfer branch of split power flow of planetary system with six degrees of freedom was studied and the bifurcation resonance characteristics and formation of ambiguity of characteristics of relative motions in gear meshes were analyzed.

- Hortel, M., Škuderová, A., Houfek, M.. Linear time heteronymous damping in nonlinear parametric systems. Applied Mathematical Modelling. 2016, 40(23-24.

C) *Railway wheel producer BONATRANS GROUP a.s., Bohumín*

TAČR DELTA no. TF06000020 Transfer of smart and innovated damping technology into the suppression of vibration and noise for rail resilience wheels and vehicle motor mounts (collaboration with National Cheng Kung University, Tainan City, Tchaj-wan).

The project is aimed at implementation of smart and innovative damping technologies into the railway wheels: **a)** new compounds are to be proposed for production of damping rubber segments higher resistant to fatigue and environmental influences for rubber-damped railway wheels; **b)** shape optimization of damping friction ring for monoblock wheels should be designed with uniform distribution of contact pressure along the whole circumference of the wheel.

a) Rubber-like materials for railway wheels with different elastic, damping and thermo-mechanical properties are used as resilient machine elements. For hard rubbers (Shore >50), unlike conventional materials under dynamic loading, a nonlinear time-varying behavior occurs due to the rate and size of straining, temperature, aging etc. Thermal together with mechanical time-variable loadings belong to one of the main causes of their degradation. Therefore, we designed and built a torsional test rig in the temperature chamber for dynamic experiments on rubber samples. The hyper-viscous-elastic dynamic behavior of hard rubbers was evaluated for different harmonic loads (up to 30% strain). From the strain-stress hysteresis curves and the dependence of dissipation on deformation energy we proposed model of hyper-elastic proportional damping of hard rubber coming from the analogy with linear proportional damping.

The methodology of the complex modulus estimation of pre-pressed rubber segments laying between the disk and the rim of rubber-damped railway wheel was proposed and applied on the real case. Since in the vicinity of eigenfrequencies, their dependence to Young modulus is quasilinear, the modulus can be found effectively by the gradient method. The similar behaviour showed itself also for dependence of the modal damping constant on the damping coefficient. The ascertained results of tuned rubber material constants of the railway rubber segments are very valuable for prediction of modal behaviour of the resilient wheels.

- Šulc, P., Pešek, L., Bula, V., Cibulka, J., Boháč, T., Tašek, H. Pre-stressed rubber material constant estimation for resilient wheel application. Advances in Engineering Software. 2017, 113, 76-83.

b) For optimization of monoblock wheels damping by friction rings, new non-circular shape of the ring was proposed (utility model granted). The new ring design was based on beam model calculations where uniform distribution of contact pressure along the whole circumference of the wheel was prescribed.

The methodology for evaluation of dry-friction effect of damping ring on railway wheel dynamics was proposed. From the frequency transfer functions of MIMO analysis, the split double eigen-frequencies and their corresponding damping ratios were successfully identified. For higher amplitudes of excitation when non-linear behavior of the wheel due to damping ring was more pronounced, the SIMO analysis with sweep excitation was found as the most suitable for evaluation of dry-friction effect of the ring.

2. *Laboratory of Modelling of Multiphysical Problems* (LMMP)

Head: *Dr. Vojtěch Radolf*

The Laboratory is engaged in the development of methods for studying problems of the interaction of flowing fluids and deformable bodies and their experimental verification in aerodynamic tunnels and on special experimental stand developed for modelling of aeroelastic and vibroacoustic interactions in biomechanics of human voice. The vibration and acoustic characteristics, aeroelastic stability limits and post flutter regimes of the systems are studied. Attention is given to the self-oscillations of the vocal folds excited by airflow and to the acoustic pressure modified by the frequency-modal characteristics of the human vocal tract during phonation.

The research in 2015-2019 was performed within the following grants of the Czech Science Foundation chaired or co-chaired by the scientists of the Laboratory:

- GAČR P101/11/0207 Coupled problems of fluid and solid mechanics - nonlinear aeroelasticity (2011-2015)
- GAČR P101/12/1306 Biomechanical modeling of human voice production - way to artificial vocal folds (2012-2015)
- GA13-34632S Increasing the level of computational modeling of the behaviour of the ceramic head for total hip joint endoprosthesis (2013-2015)
- GAČR P101/13-10527S Subsonic flutter analysis of elastically supported airfoils using interferometry and CFD (2013-2015)
- GA16-01246S Computational and experimental modelling of self-induced vibrations of vocal folds and influence of their impairments on human voice (2016-2018)
- GA19-04477S Modelling and measurements of fluid-structure-acoustic interactions in biomechanics of human voice production (2019-2021)

Finite element modeling - FEM

The most important results achieved in FE modelling were in development of new numerical solvers for simulation:

a) fluid structure interaction (FSI) in nonlinear aeroelasticity of airfoils like the flutter instability and the post flutter regimes after losing the stability of the system taking into account turbulence and large vibration amplitudes.

b) flow induced vibrations of an elastic continuum vibrating in viscous flow in a channel. In this case, the applications were focused mainly into the biomechanics of human voice but they can be spread to many other fields of FSI problems.

FEM – aeroelasticity of airfoils

Between the best results obtained in years 2015-2019 belongs the developed FE method for numerical simulation of turbulent flow around vibrating airfoil with large amplitudes, which is based on the Reynolds averaged Navier–Stokes (RANS) equations that was applied on solution of gust aeroelastic responses of the airfoil. The in–house software was successfully tested by comparison with the results from literature obtained by an available CFD code and from a low fidelity model.

Another unique FE numerical simulation deals with flutter and post-flutter regimes related to self-oscillations and limit cycle oscillations (LCO) of an airfoil with three degrees of freedom vibrating with large amplitudes (up to ±40 degrees in rotation of a flap) in a viscous turbulent flow described by the RANS equations.

The new original implementation of the stabilized FE method taking into account laminar–turbulence transition of the flow on the airfoil surface was developed and successfully applied on the FSI problem of flow induced vibrations when the airfoil was loaded by a sudden gust. The results indicate better physical relevance of the transition flow model than the laminar or the turbulent models.

- Sváček, P., Horáček, J. On mathematical modeling of fluid-structure interactions with nonlinear effects: Finite element approximations of gust response. Journal of Computational and Applied Mathematics. 2015, 273, 394-403.
- Feistauer, M., Horáček, J., Sváček, P. Numerical simulation of airfoil vibrations induced by turbulent flow. Communications in Computational Physics. 2015, 17(1), 146-188.
- Sváček, P., Horáček, J. Numerical simulation of aeroelastic response of an airfoil in flow with laminar-turbulence transition. Applied Mathematics and Computation. 2015, 267, 28-41.

FEM – FSI problems in FE modeling of human voice

FSI in voice modelling included the elastic vocal folds (VF) and the viscous fluid flow in the glottal channel modelled by the incompressible Navier-Stokes equations in the ALE (Arbitrary Lagrangian-Eulerian) form. Such problems were discretized by the FE method applied both to the structure as well as to the flow, where the residual based stabilization methods were used. The strong coupling was used for FSI solution.

A special attention was paid to the application of a completely new inlet boundary condition using a penalization approach which enables to optimize the inlet boundary condition related to a physical reality by changing the penalty parameter in the interval between two extremes and to treat the complete closure of the channel. The boundary condition gives reliable results related to flutter analysis of the system and physically real values of pressure and flow velocities when the channel is nearly closing during the vocal folds vibration.

The novelty was the application of the discontinuous Galerkin method (DGM) to the solution of viscous compressible flow with low Mach number. The Navier–Stokes equations were discretized by the DGM in space, and in time either by the backward difference formula (BDF) or the DGM. The resulting technique is called the space-time DGM. The goal of the analysis was to prove that the obtained results are comparable with simulations of incompressible viscous flow. The developed FE-based numerical solution of the interaction of compressible viscous flow with the linearly elastic VF structure was compared to the nonlinear St. Venant-Kirchhoff elasticity model. For the elasticity problem, the BDF in time and the DGM in space were used. The numerical simulations of the flow-induced VF vibration showed that it is more adequate to use the nonlinear elasticity model.

The elliptical trajectories of the VF motion, excited by the subglottic pressure numerically simulated by self-oscillations of a two-degree of freedom VF model, and computed from the developed 3D FE computer model of the VF, closely resemble the trajectories measured on

VF in excised larynges. Also numerical simulations of the empirical eigenfunctions were in good agreement with the published experiments performed on human VF. The model was greatly improved considering another layer modeling the space filled with liquid.

Similar 3D FE modelling showed that an expansion of the acoustic side cavities in the human vocal tract (VT) can contribute to forming a complex singer's/speaker's formant cluster and increase the radiated acoustic power in the frequency range 3–5 kHz. The results show that the formant clustering in operatic singing is more complex phenomenon than originally thought.

- Sváček, P., Horáček, J. Finite element approximation of flow induced vibrations of human vocal folds model: Effects of inflow boundary conditions and the length of subglottal and supraglottal channel on phonation onset. Applied Mathematics and Computation. 2018, 319, 178-194.
- Vampola, T., Horáček, J., Laukkanen, A.M., Švec, J.G. Human vocal tract resonances and the corresponding mode shapes investigated by 3D modelling based on CT measurement. Logopedics Phoniatrics Vocology. 2015, 40(1), 14-23
- Vampola, T., Horáček, J., Švec, J.G. Modeling the influence of piriform sinuses and valleculae on the vocal tract resonances and antiresonances. Acta Acustica United with Acustica. 2015, 101(3), 594-602.
- Vampola, T., Horáček, J., Klepáček, I. Computer simulation of mucosal waves on vibrating human vocal folds. Biocybernetics and Biomedical Engineering. 2016, 36(3), 451-465.

EXPERIMENTS – aeroelasticity of airfoils in cooperation with the Department D1

The flow-induced vibration of a NACA 0015 airfoil model with 2 degrees of freedom was investigated in a high-speed wind tunnel using motion and pressure sensors on the airfoil and synchronized high-speed Schlieren visualizations of the unsteady flow field at Reynolds numbers (1.8–5.7) 10^5. With a relatively low pitch to plunge natural frequency ratio and zero initial incidence angle, the model was highly susceptible to dynamic stall instability with the peak-to-peak pitch amplitude reaching up to 90°.

- Šidlof, P., Vlček, V., Štěpán, M. Experimental investigation of flow induced vibration of a pitch-plunge NACA 0015 airfoil under deep dynamic stall. Journal of Fluids and Structures. 2016, 67, 48-59.
- Kozánek, J., Vlček, V., Zolotarev, I.. The new airfoil model NACA0015, modal analysis and flutter properties. Applied Mathematical Modelling. 2017, 46, 698-706.

EXPERIMENTS – in vitro modeling of phonation and voice measurements in humans

Unique experimental modeling studies were performed on an especially developed 1:1 scaled model of human phonation. It was shown that the VF self-oscillations could be strongly influenced by interaction with acoustic resonances of the human VT in case when the VT is prolonged by the so-called resonance tube used in voice therapy methods. This was demonstrated by constructing the relationships of subglottal pressure variation in time versus glottal area variation forming time oriented loops. It was shown that a part of the airflow energy required for phonation is substituted by the acoustic energy, utilizing the first acoustic resonance which is near the frequency of the VF self-sustained vibrations.

Similar in vivo measurements confirmed a considerable influence of soft tissues in the human VT on the first resonance frequency. The results confirm that yielding walls must be considered in computer modelling of the semi-occluded human VT. This was explained by an acoustic-structural interaction of the VT with a mechanical low-frequency resonance of the soft tissue in the larynx.

The novel mathematical model of acoustic-structural interaction confirmed the conclusions of experiments that the vibration of the laryngeal tissues during water voice therapy can be substantially supported by a low acoustic-mechanic resonance of the vocal tract, because it was shown that this resonance for phonation through the tube into water is in the frequency range of bubbling. The frequency intervals for bubbling and the mechanic resonance overlap, so a strong vibration of the larynx can arise if both frequencies merge.

Mechanical stress loads the human vocal folds (VFs) due to their collisions. This stress is the reason for VF tissue damage causing nodules or polyps. It was the reason for our several studies focused on impact stress (IS) investigation in phonation.

A VF replica and a model of VT for vowel [u:] were used and the impact stress (IS) between self-oscillating VFs was measured for [u:] and for VT prolonged by a tube immersed in water. IS measured in the range of subglottic pressure, which corresponded to humans, was higher for [u:] than for the tube in water. The results suggest that IS is not likely to increase harmfully in water resistance voice therapy.

Our experimental and computer modeling study of glottal closing velocity during phonation showed that the IS between the colliding vocal folds should not be evaluated from the maximum velocity of the glottal closing because the velocity of the closing diminishes just before the glottal closure. This phenomenon, which can be caused by an air cushion effect in the fast narrowing glottal gap, was demonstrated by results of measurements: a/ by high speed camera in a human, b/ in the lab model for the vowel [u:] phonation and c/ using a three-mass computer model employing a Hertz model of impact force. The results suggest that the IS in voice is lower than originally thought.w.

The performed laboratory experiments confirmed that the phonation characteristics of the developed 1:1 scaled vocal folds model fillable by liquid are in the range of physiological parameters of humans and adjustable for men and women voices. The results are useful not only for future development of the human vocal folds prosthesis but also for experimental verification of computational models and studies which are not possible to realize in humans. The team of the laboratory was engaged in development of self-oscillating human vocal folds prosthesis, which resulted in the joint patent called "*A vocal cord substitution and a method of tuning the vocal cord substitution"* obtained in 2016 in cooperation with the Faculty of Mechanical Engineering, CTU Prague, 1st Medical Faculty of the Charles University and the Institute of Macromolecular Chemistry of the Czech Academy of Sciences. The results of this group were awarded by the Grant Agency of the Czech Republic as one of the three best results established in 2015.

- Radolf, V., Horáček, J., Dlask, P., Otčenášek, Z., Geneid, A., Laukkanen, A.M. Measurement and mathematical simulation of acoustic characteristics of an artificially lengthened vocal tract. Journal of Sound and Vibration. 2016, 366, 556-570.
- Horáček, J., Radolf, V., Laukkanen, A.M. Low frequency mechanical resonance of the vocal tract in vocal exercises that apply tubes. Biomedical Signal Processing and Control. 2017, 37, 39-49.
- Horáček, J., Radolf, V., Laukkanen, A.M. Impact stress in water resistance voice therapy: A physical modeling study. Journal of Voice. 2019, 33(4), 490-496.
- Horáček, J., Radolf, V., Laukkanen, A.M. Experimental and computational modeling of the effects of voice therapy using tubes. Journal of Speech Language and Hearing Research. 2019, 62, 2227-2244.

PROBLEMS OF BIOMECHANICS OF HUMAN REPLACEMENTS

a) Increasing of the hip joint replacements reliability. The aim of this problem was to realize a computation of failure probability of the total hip joint endoprosthesis ceramic head with macro- and microscopic shape deviations of the conical contact surfaces during gait process. There were two steps to solve: 1. Calculations of the stress states in the ceramic heads (with shape deviations of the contact cone areas) during the gait process. 2. Calculations of the ceramic head's reliability which require the material parameters of the used ceramic material.

   Analyses of the results of computational FE model show that the greatest impact on the stress and failure probability of the head during gait process has the size and relative position of the micro shape deviations on the conical surface of the head and stem. Failure probability of the ceramic head increases with increasing size of the shape deviations. It is therefore necessary to calculate the failure probability for specific shape deviations and position of the head relative to the stem.

b) Increasing of the reliability of total replacement of the trapeziometacarpal joint. The problem is *in vivo* peeling of the DLC microlayers from surface of the joint made of the Co-Cr-Mo alloy. This problem was solved using computational modelling. The extreme tensile stress was found in the region of the joint where the peeling of the DLC microlayers was detected. The result was the shape modifications of the implant of the joint.

CARDIAC CELL BIOPHYSICS

The research was focused on exploration of the effects of ethanol on membrane transport system and electromechanical activity of cardiomyocytes. The effects of clinically relevant concentrations of ethanol on ionic membrane currents, action potential and cellular contraction were analyzed in the models of rat and human ventricular cardiomyocytes. The model of rat ventricular cardiomyocyte was also used to investigate the effect of differences in distribution of sodium-calcium exchanger between the tubular and surface cell membrane on cellular electromechanical activity. Subsequently, the impact of transmural differences in excitation-contraction delay and contraction velocity of cardiomyocytes on isovolumic contraction of the heart was studied by means of a new 3D FE model of human left ventricle developed in co-operation with the Technical University Brno.

- Pásek, M., Bébarová, M., Christé, G., Šimurdová, M., Šimurda, J. Acute effects of ethanol on action potential and intracellular Ca2+ transient in cardiac ventricular cells: a simulation study. Medical & Biological Engineering & Computing. 2016, 54(5), 753-762.

3. *Laboratory of rotational laser vibrometry* (LRLV)

Head: *Dr. Pavel Procházka*

The Laboratory was established in 2015 under the support of the EU project "Laboratory of the Rotational Vibrometry" No. CZ.2.16/3.1.00/21359 of the Operational Programme Prague Competitiveness. The determination of the Laboratory is the research and development of non-contact vibration diagnostic systems of rotating blades of high power turbomachines, compressors and fans. The equipment of the Laboratory consists of a rotary model bladed wheel with an electric motor drive; a vacuum chamber of the rotating wheel eliminating aerodynamic forces and friction heating; an electromagnetic vibration exciting system; a non-contact tip-timing measurement system of circumferential displacements of the blades; a calibrated strain-gauge system with a slip-ring transmission; a Laser Scanning Vibrometer Polytec PSV-500 with a derotator; and a reference Vibrometer Polytec OFV-5000. The measurement system is equipped with eight pairs of electromagnets for a computer controlled vibration excitation in the axial and radial directions. The excitation can be either harmonic or impulse. The whole model wheel, including sensors and electromagnets, is covered by a shield made of pressure-resistant glass. Two vacuum pumps decrease the air pressure in this chamber, so that conditions near to vacuum can be created. An important advantage of the blade vibration measurement is the usage of two measuring methods: Blade Tip Timing and Laser Doppler Vibrometry, which allow independent data evaluation. Moreover, two opposite blades are equipped with strain gauges providing additional information about blade straining during rotation. Maximal speed of the wheel is 7,000 rpm. The Laboratory is unique in the Europe. Its features predispose the utilization of the research results in power industry and engineering.

The Laboratory solved the project Vibrodiagnostics of rotating blades of rotary machines in power engineering; programme VP03 - Effective energy conversion and storage, Strategy of the Academy of Sciences AV21. The aim of this project was to interconnect the scientific fields of electrical engineering, mechatronics, mechanics and mathematical statistics for the development of vibrodiagnostic systems of rotating blades with an initial focus on reliability and efficiency of low-pressure steam turbines. A mathematical model was developed to optimize sensing vibration and stationary deflections of rotating turbine blades. Methods have been developed for statistical evaluation of blade vibration shapes determined from experimental data.

Special magnetoresistive sensors have been developed for measurement vibrations of turbomachines during rotation. The aim was to increase the sensitivity, accuracy and frequency range of these non-contact vibration sensors. A number of top results have been achieved in this respect. For example, these sensors are able to detect 10 μm rotating blade deflections at a peripheral speed of 700 m/s. Also unique is the frequency bandwidth, which extends not only to high frequencies above 300 kHz, but also covers the DC band. Thus, the sensors can be used statically to measure a number of significant static turbine characteristics. Many of these principles have therefore been protected as a utility models or patents.

- Procházka, P. Methods and Facilities for Calibration of Noncontact Blade Vibration Diagnostic Systems. IEEE Transactions on Instrumentation and Measurement. 2018, 67(10), 2345-2352,
- Procházka, P. Impulse Exciter of Rotating Blades with an Increased Excitation Force. IEEE Transactions on Instrumentation and Measurement. 2019, 68(1), 300-302),
- Procházka, P. Electromagnetic Simulator of Rotating Machine Blades for Noncontact Sensor Dynamic Testing. IEEE Transactions on Instrumentation and Measurement. 2018, 67(6), 1506-1508.
- Procházka, P., Vaněk, F. Operational Measurement of Stationary Characteristics and Positions of Shrouded Steam Turbine Blades. IEEE Transactions on Instrumentation and Measurement. 2016, 65(5), 1079-1086.

The Laboratory is part of a consortium solving the project "National Center of Competence Cybernetics and Artificial Intelligence", ID TN01000024 of the Technology Agency of the Czech Republic. The solved sub-project "Robotic Operations in Hazardous Environment and Intelligent Maintenance" is realized through cooperation with companies. In this project, the Laboratory investigates measurement methods and intelligent sensors for sensing vibrations of the blades of rotating machines at remote sites. Companies in Vietnam and South Africa have already shown interest in these sensors.

Methods and program functionalities have been developed for the calculation of advanced blade vibration characteristics from experimental data: frequency analysis of the instantaneous blade vibrations, statistical overviews of dynamic and static characteristics, residual lifetime and graphical presentation of results. The prototype of the vibrodiagnostic device was realized and verified on the model test wheel, in the test rig Doosan Skoda and also on real steam turbines. The system developed in the Laboratory was used in cooperation with Doosan Skoda and West Bohemian University at the combined gas-steam power plant Pocerady on a turbine 280 MW for monitoring vibrations of blades 1220 mm. Measuring was completed after three years of faultless operation. The developed Blade Tip Timing system was used to measure vibration on a 35 MW condensation steam turbine in Martinique, where it was in operation for two years.

Currently (2019 -2021), the Laboratory solves the project EU H2020 "Batista - Blade Tip Timing System Validator", ID 862034, Call Clean Sky 2. The consortium set up for this project has EMTD (Coordinator - GB) and the University of Manchester (GB) as further members. SAB (Safran Aero Boosters - BE) is engaged in the project as a supervisor. The aim of the project is theoretical and experimental research for validation of systems based on the Blade Tip Timing method.

The laboratory had a high rate of applied outputs connected with development of sensors and magnetic excitation of bladed wheels protected by the Czech Industrial Property Office, namely 4 patents granted, 1 utility model granted and 2 patents are pending.

4. *Laboratory of Modelling and Identification of Dynamic and Mechatronic Systems* (LMID)

Head: *Dr. Jan Kozánek*

The Laboratory is engaged in the identification and tuning of complicated and mechatronic dynamic systems, the development of mathematical and physical modelling methods for these systems, and their optimisation. The mathematical models are considered to be linear with the corresponding spectral and modal characteristics, weak and stronger nonlinearities, and applications in the dynamics of machines with an emphasis on rotational machines with both classic and contactless bearings (e.g. energy storage systems focusing on flywheel technologies using radial and axial superconducting bearings), on vibration stability and especially on the magnetorheological squeeze film damping devices for vibration suppression of rotors.

Self-excited oscillations of the airfoil profile NACA0015 in subsonic flow were investigated in aerodynamic tunnel within Grant GA13-10527S. Especially, frequency-modal and flutter characteristics, and the identification of the start of flutter and limits of the aeroelastic stability were studied. The identified eigenvalues and eigenmodes for zero flow velocity were compared with measured flutter properties (the flutter frequency, the modes of vibration and the time evolution of the displacements) of the airfoil.

- Kozánek, J., Vlček, V., Zolotarev, I. The new airfoil model NACA0015, modal analysis and flutter properties. Applied Mathematical Modelling. 2017, 46, 698-706.

The magnetorheological squeeze film damping devices for vibration suppression of rotors were studied within Grant GA15-06621S. It's about solutions of a complex interaction between coupled mechanical, hydraulic, magnetic and electric phenomena. The mathematical models (with bilinear materials affected by a magnetic field) were proposed and numerically verified for a wide range of the rotor operating speeds. During the solution it was obtained a number of knowledge about the nonlinear effects, time delays, and complex influences of the electromagnetic phenomena occurring in magnetorheological damping devices used in the vibration attenuation of rotors.

- Zapoměl, J., Ferfecki, P., Kozánek, J. Modelling of magnetorheological squeeze film dampers for vibration suppression of rigid rotors. International Journal of Mechanical Sciences. 2017, 127, 191-197.
- Ferfecki, P., Zapoměl, J., Kozánek, J. Analysis of the vibration attenuation of rotors supported by magnetorheological squeeze film dampers as a multiphysical finite element problem. Advances in Engineering Software. 2017, 104, 1-11.
- Zapoměl, J., Ferfecki, P., Kozánek, J. The mathematical model for analysis of attenuation of nonlinear vibration of rigid rotors influenced by electromagnetic effects. Journal of Sound and Vibration. 2019, 443, 168-177.

The parametric identification in mechanical engineering and approximate identification of dynamical systems were investigated and presented as chapter in Springer Proceedings in Mathematics & Statistics - Dynamical Systems in Theoretical Perspective 2018 (Awrejcewicz, J.), p. 217-234. Usually, as the input data of the parametric identification methods in the frequency domain, the corresponding pairs of the “unit harmonic force excitation”—“steady state harmonic response” are considered. This new proposition deals with approximate identification of linear dynamical systems by time response on unknown initial displacement (or velocity) with the help of the Fourier transform.

Identification of dynamic properties of tone-wood have been carried out In cooperation with Prague Musical Academy, Depart. of Acoustics for the comparison with the FE models. Dynamic experiments were based on the impulse excitation and the steady state harmonic response. Frequency transfer function fitting identification method determined complex eigenfrequencies and damping.

Aspects of energy storage systems focusing on flywheel technologies were studied in the project of the Czech Academy of Sciences “Strategy AV21”, programme “Efficient Energy

Transformation and Storage". Vibration stability of a vertical flywheel lifted by permanent magnetic rings were investigated by numerical experiments. The steady state response of the flywheel on the unbalance excitation is calculated by means of the trigonometric collocation method and its stability is evaluated by application of the Floquet theorem.

Research activity and characterisation of the main scientific results

The Department D4 together with the CeNDYNMAT centre deal with theoretical, numerical and experimental research of *(i)* wave propagation in solids and advanced materials, *(ii)* development of phenomenological models in metal plasticity, and *(iii)* non-destructive testing and characterization of materials and structures. Owing to the interdisciplinary character of the D4, its research topics range from physical and material science to computational mechanics and mechanical engineering. The main results, including the most important references, are classified into the following topics. Individual D4 laboratories that participated in the output are mentioned. At the end of this chapter, all grant projects supported from public funds from national as well as EU sources and three general contracts with the State Office for Nuclear Safety (SÚJB) in the period 2015-2019 are listed.

Wave phenomena in solids and advanced materials: analytical, numerical and experimental approaches

performed by ***Laboratory of Computational Solid Mechanics*** *and* ***Laboratory of Non-Destructive Testing***

Analytical, numerical and experimental studies of stress wave processes in solids have got a long-time tradition in the Department D4. In *analytical* methods, the subsurface characteristics of the surface waves in various composite materials have been investigated. Further, the analytical solution of wave motion in a thick cylindrical rod undergoing longitudinal impact has been derived and the results have been verified numerically. This task is a perfect benchmark test for novel numerical methods for the solution of wave propagation problems and impact-contact problems. Further, the response of a two-layered medium to an impulse loading by an analytical approach has been studied and compared with the results of the finite volume method (FVM) and the finite element method (FEM). The analytical solution used Laplace and Fourier transforms. The accuracy of the verification of the results of analytical solutions has been analysed. In the next step, the analytical solution has been generalized to the problem of a multi-layered 2D medium with special orthotropic properties and used for approximate modelling of non-stationary waves in a functionally graded medium of different types. This is the beginning of the work on wave propagation in general heterogeneous and anisotropic media.

In *numerical* modelling, the dispersion properties of the FEM and isogeometric analysis (IGA) have been studied. The latter represents a higher-order version of FEM employing Non-Uniform Rational B-Splines (NURBS) as basis functions. The temporal-spatial dispersion relationships have been derived for explicit and implicit time integration, where the suitable mesh and time step size have been recommended for wave problem analysis. Simultaneously, improvement of current FEM contact-impact procedures has been accomplished. An original three dimensional algorithm based on the pre-discretization penalty method has been modified to consider bipenalty treatment of contact constraints including implementation of self-contact conditions. In wave propagation in heterogeneous media, a special numerical approach has been developed based on the decomposition of longitudinal and shear waves, and pull-back time interpolation. In this case, one can integrate accurately all wave-fronts with minimum dispersion pollution. This approach has been extended into domain decomposition computations, where each subdomain has a different time step. Next, the wave propagation in layered structures has been studied and applied for porose fluid-saturated materials and for auxetic structures. Finally, advanced numerical methods have been applied for structural dynamics. First, IGA analysis has been performed to investigate the accuracy and convergence rate in linear free vibration problems. A novel approach for direct inverse mass matrix has been developed and tested in transient problems in structural dynamics. The final inverse mass matrix is sparse, has the same structure as the consistent mass matrix and preserves the total mass of the structures. The methodology has been verified for linear and higher-order FEM including IGA analysis. It can significantly increase the performance of explicit analysis in connection with the mass scaling and tailoring.

In the *experimental* study, wave propagation in various materials such as metals, plastics, ceramics and biological materials has been studied. Their dynamic behaviour consisting of identification of parameters of constitutive relationships including strain-rate effects were evaluated as well. Various experimental equipment has been used and developed, such as the Taylor test, Brasil disc test, split Hopkinson pressure bars, and others. Special attention has been paid to study attenuative, dissipative and fracture properties of several materials of interest.

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Development and implementation of advanced computational models in phenomenological plasticity and creep

performed by ***Laboratory of Thermomechanics of Materials*** *and* ***Laboratory of Material Diagnostics***

This research activity covers theoretical and experimental research in phenomenological plasticity and includes all crucial sub-activities required for an independent research, i.e., models development, implementation, calibration, validation, and development of experimental methods in metal plasticity. In general, theoretical and experimental research of metal plasticity is crucial for Department D4 together with the CeNDYNMAT centre. It is the main subject of cooperation with several foreign universities in USA and the Republic of China (Taiwan).

Several advanced models for metal plasticity were proposed and enhanced. The models reflect current experimental observations, e.g., isotropic, kinematic, and directional distortional hardening. Namely the directional distortional hardening mechanism is quite important, since it is likely responsible for complex phenomena observed in cyclic plasticity and ratcheting. The yield surface convexity is studied in detail, as it is necessary for the integration stability. Also, some attention has been paid to the thermodynamic consistency. Finally, these models generalize von Mises yield criterion and employ an associative flow rule.

Plasticity models are implemented in the in-house FEM code PMD (Package for Machine Design) and in the proprietary FEM code Abaqus via UMAT interface. Both codes are written in Fortran computer language, and critical parts of the code are parallelized and vectorized. Several standard integration techniques are used, though the explicit integration dominates. Due to convexity of the yield surface, stability of the integration algorithms is not affected.

For industrial application of the models developed, calibration algorithms are crucial. Current calibration algorithms are defined in terms of an optimization problem for models parameters, though some explicit methods based on closed form solutions and suitable for simple models were developed as well. The optimization algorithms use the simplex method and the gradient descent method and are implemented in Matlab and Fortran language.

Calibrated models are validated on a wide collection of experimental data. Although there are some attempts to calibrate on complex geometries using FEM simulations, our research still addresses uniform stress states, e.g., uniaxial and biaxial stress-state. Following the department development plan, a brand new biaxial hydraulically operated testing system by Instron company was purchased in 2018. The system is suitable for numerous experiments in metal plasticity with the capabilities of other forms of mechanical testing. The system is fully programmable and allows establishing a real time feedback and a real time evaluation of measured data. Current experiments address the detection of distorted yield surfaces, ratcheting, and fatigue. The biaxial stress state is achieved in tubular thin-walled specimens. Strains are measured by biaxial extensometer and by strain gages. The methodology of detection of yield surfaces was designed in a close collaboration with the Northern Arizona University and the National Cheng Kung University.

Another important issue is the development of constitutive creep models for numerical FEM calculations. Recently, complex model describing creep behaviour under variable stress conditions during primary and secondary creep stages was developed by Kloc et al. in the Institute of Physics of Materials CAS, Brno. The model can handle transient effects on the stress changes, as well as low-stress creep behaviour. The constitutive equation was built using the relevant creep data for P-91-type steel, but it can be applied to the creep behaviour of most structural materials. The proposed creep material model including transient effects was implemented in the finite element code PMD. The material model together with numerical implementation was verified by means of uniaxial stress loadings and torsion tests. Next, complex creep probabilistic exponential model with damage designed in the 1980s by Bína et al. in SVUM Běchovice was successfully applied in creep analysis of high pressure steam turbine casing manufacturer company Doosan Škoda Power, Pilsen. The output was the evaluation of residual deformations at time 10,000 and 200,000 hours in selected points of divided plane of turbine casing including comparison with measurement and prediction of the ANSYS program where the Norton-Bailey creep model was used.

Also, some attention was paid to advanced models for soil plasticity and soil mechanics. Several concepts were established and analysed in this field. A new element of fabric anisotropy was introduced in a constitutive model for sands. By comparing simulations with the results of centrifuge testing of the Boundary Value Problems (BVP), it is shown to have a very significant effect on the outcome of the bearing capacity of the footing foundation. The approach can be considered a paradigm of how one must go about addressing BVP based on element level constitutive calibration.

Further, some materials require a zero purely elastic range in inelastic constitutive modelling, which results in an incrementally and implicitly non-linear constitutive law. The numerical implementation of such law does not converge if done explicitly, thus, its implicit implementation was formulated for the first time in literature. The procedure was applied to a model for granular material, but it is general enough to constitute the paradigm for any future application to other materials, e.g., artificial graphite.

Finally, the sufficient conditions for reaching and maintaining Critical State in granular mechanics were studied and shown to be incomplete by specially designed numerical experiments by means of the Discrete Element Method. The incompleteness was removed by adding one more sufficient and necessary condition involving fabric within the newly developed Anisotropic Critical State Theory. The impact will be that of revamping the fundamental paradigm of Critical State Theory that lies on the basis of every acceptable granular mechanics theory today.

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Influence of the T-stress on crack growth on experimental (macro) and atomistic level in metallic materials; Quantum modelling computations

*performed by **Laboratory of Computational Solid Mechanics** and **Laboratory of Material Diagnostics***

The research aimed to find out the influence of T-stress, temperature and sample geometry in 3D bcc iron crystals on the ductile-brittle transition using atomistic simulations via molecular dynamics (MD). Comparison of continuum predictions with 3D atomistic simulations of the effect of T-stress, namely its sign on brittle-ductile behaviour of cracks in bcc iron specimens at different temperatures (0, 300 K and 600 K) has been done. Fracture experiments on Single Edge Notched specimens made of bcc iron have been performed. Theoretical and numerical predictions of crack behaviour under mode I are in a good agreement with realized fracture experiments. Deformation processes (emission of blunting dislocations, twinning, crack deflections) at the cracks of different lengths have been studied. Based on the observation, it can be concluded that the effect of the T-stress is sensitive to: crack length, the orientation of the available slip systems at the crack, and further to the sign of the T-stress, temperature and loading rate or strain rate. The used in-house MD code has been updated concerning the required computations. In the coupling of FEM and MD domains, we have applied the bridging scale method and a new bridging approach based on the penalty-like method.

Next, the IGA analysis was implemented and applied to the nonlinear eigenvalue problems in electronic structure calculations. The external charge density as a "boundary condition" in a generalized sense has been utilized. A new efficient approach for the evaluation of Hellmann-Feynman forces within non-local pseudopotentials for applications in multiscale modelling of fracture of iron specimens has been proposed. The model clusters containing 30-40 atoms have been analysed and the Hellmann-Feynman forces have been evaluated for various deformations so that the parameters of the force-interaction potentials could be derived.

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Acoustic emission (AE) source localization and identification in complicated materials and structures

*performed by **Laboratory of Non-Destructive Testing***

Acoustic Emission (AE) method is widely used for non-destructive evaluation and identification of damage in materials and structures. We designed new algorithms to verify the AE source location possibilities. Basic algorithm computes the shortest paths of elastic waves propagation in structures of complicated shape. It provides data evaluation in problematic areas according to particular sensor placement, and enables collecting representative data to train Artificial Neural Networks (ANN) in their application to AE source location. So-called maps of source location sensitivity, similarity and ambiguity are obtainable even for discontinuous or anisotropic bodies.

By using simple devices with sophisticated programming, AE activity can be evaluated on-line and in more details than by traditional AE analysers. It was successfully proved during the loading tests of titanium alloys for medical implants in a frame of broad international cooperation. Similar procedure was also used for diagnostics of bearings in rotated machines using convolutional ANN. The continuous AE data recorded during endurance tests of washer parts were used to simulate critical rolling contact fatigue of the bearings. Simple AE parameters, e.g., the mean frequency or RMS of the signal were sufficient to detect early stages of the bearing defects. New method of continuous AE analysis, supported by convolutional ANN, may be used as an integral part of online Structural Health Monitoring (SHM) system. Most precise AE source location results obtained by Time reversal method are described in the next paragraph--Time reversal ultrasonic signal processing used in nondestructive evaluation of materials and structures.

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Structural Health Monitoring and Condition Monitoring supported with ultrasonic NDT methods (AE, NEWS, Guided Waves)

*performed by **Laboratory of Non-Destructive Testing** and **Laboratory of Computational Solid Mechanics***

Structural Health Monitoring (SHM) becomes an important emerging technology, improving reliability and safety of highly stressed structures by supporting their effective maintenance and by predicting lifetime. It deals with the development and implementation of technologies and systems where monitoring, inspection, damage assessment and residual life prediction become an integral part of 'smart' structures. The use of SHM systems has the potential to provide greater confidence in the integrity of a structure. Based on previous experiences, the development of a small complex SHM system was initiated with the aim to reduce whole life costs and to provide additional safety measures. It was desirable to apply SHM on structures for which failure would have catastrophic results, such as nuclear power plants. Commonly, regular inspections are conducted using Nondestructive Testing and Evaluation to ascertain whether the structure is damaged. To replace periodic inspections on nuclear power plants by a continuous monitoring of highly stressed parts, we prepared a new project on SHM applied to the Technology Agency of the Czech Republic called “Innovative methods for nuclear plant safety evaluation based on SHM technologies and related procedures – NEMENUS (NEw MEthods for NUclear Safety)”. The project, supported by the State Office for Nuclear Safety (SÚJB), has been approved for years 2018 to 2022. The main task of the project is to develop and physically build a representative model of the SHM system, and provide it with supporting software. The complex SHM system functionality will be tested and demonstrated on model samples representing various structural changes and degradation phenomena. Based on thorough literature review, the complex SHM model was designed while using different sensors for various NDT/E methods, namely ultrasonic methods such as AE, NEWS, GWI (Guided Wave Inspection), and also optical cables with FBG (Fiber Bragg Gratings). Various static and dynamic loads will stimulate symptoms of damage and defects activity on small models. Structural health data extracted from NDE measurements will be transferred to the host SHM control processor and to a developed digital twin, which will allow prediction of damage progress. All research experiences acquired during the previously solved projects will be utilized in solving NEMENUS tasks along with broad international cooperation.

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Time reversal (TR) ultrasonic signal processing used in nondestructive evaluation of materials and structures

performed by ***Laboratory of Non-Destructive Testing*** *and* ***Laboratory of Computational Solid Mechanics***

The AE source location methods based on time reversal signal processing were further developed and used to solve extremely difficult problems in ultrasonic non-destructive testing (NDT) connected with wave dispersion, extraneous noise, etc. TR procedures were proved to be useful for better location of abrupt (burst) and continuous AE sources, and also for damages and cracks identification by nonlinear elastic wave spectroscopy (NEWS - TR) and other methods suited for use in Structural Health Monitoring (SHM). The most challenging task of the solved CSF project (2017-2019) was the signal transfer from a real physical body to its "digital twin". A lot of TR experiments ranging from small aluminium samples to large steam pipeline were accomplished to verify robustness of the TR procedure. AE signals recorded in an operating nuclear power plant were used as a source simulating extraneous noise subsequently cleaned up by TR, enhancing signal to noise ratio. For the planar source location of random continuous signal sources with precision of about 1-2 mm we used cross-correlation between just two sensors. Big effort was devoted to the development of relevant FEM methods for elastic wave propagation modelling with respect to TR. Factors affecting TR signal reconstruction quality, such as temperature or shape changes, were experimentally studied and theoretically described. Results helped to transfer acoustic emission signal onto a similar, remote, real or numerical model, where they can be better interpreted. The Image Source Method (ISM), also referred as a method of mirrored sources, was used as a ray tracing approximation. Using TR, it was possible to localize AE sources and partially reconstruct their source function. Another important result was a newly designed TR-based reference-free procedure for in situ calibration of AE and ultrasonic transducers.

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Combined noninvasive mechanical-ultrasonic diagnostics of biological tissues and composite materials

performed by ***Laboratory of Non-Destructive Testing***

Human skin tissue represents an anisotropic bio-polymer with complex mechanical (viscoelastic) behaviour and exhibits highly nonlinear and hysteretic memory effects. Knowledge of such mechanical properties of human skin is of great interest in plastic surgery, dermatology, cosmetics, and in related fields. Experimental in vivo properties of the skin were noninvasively investigated by measurements of ultrasound propagation speed along the skin in various directions. From these measurements, elastic moduli and their anisotropy were evaluated. Statistical testing was used to reveal the influence of several parameters related to the volunteer on the results, e.g. position on forearm, age, humidity, electrical admittance, etc. Also the influences of the used excitation parameters were studied (mechanical loading, ultrasound frequency and amplitude, etc.). The anisotropy of human skin was evaluated from directional dependence of elastic wave velocity related to complex elastic modules. The method exploits originally designed flexible multi-directional circular probe with built-in piezoelectric ultrasonic transducer array. Spectral properties of signals propagating in different directions were used to characterize directional-dependent nonlinear behaviour of human skin. Nonlinear properties of the skin are further examined by NEWS-TR techniques. The method was, similarly to human skin, also utilized in industrial applications for characterization of mechanical anisotropy of composites used in aerospace industry. The nonlinear anisotropic properties of such materials combined with the characteristic of this method enabled detection of impact damage inside composites. The main advantage of the developed method is its fast, local, and easy-to-use application on various materials and with respect to their instantaneous state.

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Expert support of the State Office for Nuclear Safety (SÚJB) in the field of independent assessment of flaws evaluation in welded components for Czech nuclear plants

*performed by **Laboratory of Computational Solid Mechanics**, **Laboratory of Thermomechanics of Materials** and **Laboratory of Non-Destructive Testing***

Department D4 participated in expert assessments for the **State Office for Nuclear Safety (SÚJB)**, in particular in the field of numerical evaluations of defects in welded components in Czech nuclear power plants (NPP). The assessments were elaborated for the methodology for evaluation of defects indications, found in heterogeneous welds in operating NPPs, as prepared under the umbrella of the Association of Mechanical Engineers (A.S.I.). Another example is the elaboration of a study on “weld overlay” (WOL) for repairs of heterogeneous welded components in NPPs under “stress corrosion cracking”. The study was followed up by an assessment of a standardizing technological document, which was prepared also under A.S.I. The document contains both obligatory rules, and recommendations for the application of WOL in Czech NPPs.

Next example of D4 expertise for SÚJB is the calculation of the critical and the maximum acceptable flaw in heterogeneous welds, used in the emergency power supply nozzle of steam generator EDU - on the basis of methodologies R6, BS 7910:2005, and API 579-1/ASME FFS-1. Further elaborations related to the assessment of CEZ computation methodology for feed water spraying in steam generators, under a postulated feed-water pipe rupture, and to the CEZ methodology for measurement and evaluation of vibrations in NPP components by portable diagnostic instruments. The objective was setting acceptance criteria for operational vibrations in piping systems (this task was carried out in cooperation with D3 department).

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2. Foreign Internship Support for Researchers from the Institute of Thermomechanics of CAS, MEYS, project No EF16_027/0008500, (2018–2021)
3. Modeling the Mechanics of Multiaxial Ratcheting, United States Department of Defense, project No W911NF-19-1-0040, (2019–2021)
4. Image of viscoelastic properties of human skin by time reversal ultrasonic spectroscopy NEWS, project PLET–2 in the regional activity "Cosmetic Valley" in the French region Val de Loire (2016–2019)
5. Modelling of acoustic wave propagation in strongly heterogeneous media; multi-scale numerical and analytical approaches, CSF, project No GAP101/12/2315, (2012–2016)
6. Advanced phenomenological models of plasticity and their application to life assessment of machine components, CSF, project No GA15-20666S, (2015–2017)
7. Modelling of acoustic wave propagation in strongly heterogeneous media; multi-scale numerical and analytical approaches, CSF, project No GAP101/12/2315, (2012–2016)
8. Homogenization and multi-scale computational modelling of flow and nonlinear interactions in porous smart structures, CSF, project No GA16-03823S, (2016–2018)
9. Time reversal ultrasonic signal processing used in nondestructive evaluation of materials and structures, CSF, project No GA17-22615S, (2017–2019)
10. Influence of Complex and Cyclic Loading Modes on Lifetime of Machine Parts Made by Additive Manufacturing, CSF, project No GA19-03282S, (2019–2021)
11. Dynamic and nonlinear behaviour of smart structures; modelling and optimization, CSF, project No GA19-04956S, (2019–2021)
12. Robust reduced-order modeling of fluid-structure interaction problems, CSF, project No GA19-02288J, (2019–2020)
13. Nonlinear interaction of elastic waves with a single crack, CSF, project No GA19-14237S, (2019–2021)
14. Development, validation and implementation of metal plasticity constitutive models with kinematic and directional distortional hardening, MEYS project No LH14018, (2014–2016)
15. Advanced Phenomenological Models of Plasticity and Phase Transformations in Modern Engineering Materials, MEYS, project No LTAUSA18199, (2019–2022)

16. Research and development of new type of high-speed planetary gear unit with the "flexible pin" technology to support the planet wheels enabling the transmission of high outputs, TACR, project No TA04011656, (2014–2017)
17. The development of accurate rifle with a composite hybrid barrel, TACR, project No TH01010772, (2015–2017)
18. Development of new technologies for the manufacture of advanced tools and components, TACR, project No TH02010026, (2017–2019)
19. Innovative methods for nuclear plant safety evaluation based on SHM technologies and related procedures-NEMENUS (NEw MEthods for NUclear Safety), TACR, project No TH01010772, (2018–2022)
20. Thin coats deposition – advanced tools and innovative technologies, MIT, project No EG15_019/0004451, (2015–2019)
21. National Competence Center – Cybernetics and Artificial Intelligence, TACR, project No TN01000024, (2019–2020)
22. National centre of competence for Materials, Advanced Technologies, Coatings and their Applications, TACR, project No TN01000038, (2019–2020)
23. Independent assessment of technical documentation for flaws evaluation in welded components for Czech nuclear plants, SÚJB, general contract No 16/01/0094-15/2016, (2016)
24. Independent assessment of flaws evaluation in welded components for Czech nuclear plants, SÚJB, general contract No 17/03/0322-7/2017, (2017–2018)
25. Independent assessment of implementation of technical requirements for pipelines in Czech nuclear power plants, SÚJB, general contract No 03/190034-5/2019, (2019–2020)

Research activity and characterisation of the main scientific results

The main research activities can be divided into three groups: **i)** development of new laser-ultrasonic devices, done as a core research of the department, **ii)** application of these devices to specific materials science problems, always done in broad collaborations with team developing new materials, and **iii)** theoretical and numerical modelling of behavior of the studied materials. The first group resulted in several new experimental set-ups and development of laser-ultrasonics methodology, the second and the third group resulted in numerous journal publications. In the following overview, newly developed devices are first introduced, with a list of material topics each device was applied to given. Then, the materials science topics are listed, both those studied experimentally and theoretically, with the most relevant publications given for each output.

i) Development of new laser-ultrasonic devices

Resonant ultrasound spectroscopy (RUS) for long-term measurements at elevated temperatures

A new laser-RUS experimental arrangement was designed and built, including a temperature chamber for long-term measurements at elevated temperatures. The motivation for this device came from collaborations with metallurgy-oriented team. The idea was to enable in-situ observations of elastic constants evolution during the ageing and annealing processes, in order to monitor the diffusion-driven transitions (precipitation, dissolution, omega-transitions) during these processes. The new device is able to hold stable temperature of up to 650°C for several days or even weeks (one month was the maximum time used up to now), which are typical ageing times for example for several technologically important titanium alloys.

This device was so far applied for measurements on: several metastable beta-Ti alloys, finely grained metals prepared by severe plastic deformation, cold-sprayed materials, NiTiHf high-temperature shape memory alloys, and 3D printed light metals.

Resonant ultrasound spectroscopy in nitrogen vapours

In order to allow studying low-temperature behaviors of metallic materials, a new RUS setup was designed and constructed, enabling RUS measurements down to 80 K, using a nitrogen vapour-based cryostat. Unlike in all other RUS devices, where low-pressure nitrogen is used as a medium for thermal coupling between the sample and the heater/cooler, here the use of low-pressure helium is required, which makes the device more demanding as far as the design and operation conditions are concerned. The motivation for this device came from collaboration with solid state physics-oriented teams, where elastic constants at very low temperatures play an important role.

This device was so far applied for measurements on: CoCrNi-based Heusler alloys exhibiting re-entrant austenite phase at temperatures ~ 100 K, metastable titanium alloys undergoing a beta-to-omega transition upon cooling, and NiTiHf shape memory alloys in which the transition temperatures are shifted down by H-phase precipitation.

Temperature resolved Brillouin Spectroscopy (BS) device

A tandem Fabry-Perot interferometer bought in 2015 was used for design and construction of an experimental set-up for BS. This device enables measurements of elastic constants of transparent or translucent materials by Brillouin scattering of light passing through the material. In 2019, the BS set-up was upgraded by a He-cryostat, enabling measurements down to 12 K.

This device was so far applied for measurements on: unfilled tungsten-bronze crystals, single crystals of rare-earth scandates, thin epitaxial perovskite films.

Transient Grating Spectroscopy (TGS) with rotational-positioning stages

The TGS method is an all-optical method that can be utilized for local measurements surface acoustic wave (SAW) velocity in anisotropic materials. This method has been developed by the team since approximately 2010. This new experimental arrangement enables rotations, positioning and (small-range) temperature control of the sample, which significantly enhances the applicability of the TGS method. The device also enables measurements with three different SAW wavelengths (20 μm, 10μm and 5μm), which can be utilized for characterization of dispersion curves in thin surface films.

This device was so far applied for measurements on: Thin NiTi and NiMnGa films, Fe-Si, CuAlNi and NiFeGaCo single crystals, NiTi polycrystals and Ti15Mo single crystals

Line-source/point-receiver (LSPS) device for SAW measurements

The LSPS experimental set-up was designed and built in order to enable measurements of SW velocities under uniaxial prestress. The motivation came from the collaboration with teams developing alloys with overcritical stress-strain behaviors. The device is equipped by a small, in-house built testing machine mounted on a rotational stage, such that full stress induced anisotropy of SAWs can be assessed.

This device was so far applied for measurements on: FePd single crystals with overcritical behavior, NiFeGaCo single crystals and NiTi polycrystals in R-phase.

ii) Applications of ultrasonic methods to advanced materials

Characterization of temperature-induced processes in finely grained metals by resonant ultrasound spectroscopy

The contact-less resonant ultrasound spectroscopy enables to detect small changes in structure of materials due to temperature evolution, as these changes induce measurable shifts of mechanical resonances of samples of these materials in the ultrasonic frequency range. Within a collaboration with the Faculty of Nuclear Sciences and Physical Engineering Czech Technical University in Prague and the Faculty of Mathematics and Physics, Charles University, this approach was applied onto two classes of materials: a machinable aluminium alloy AA6262 and superplastic magnesium alloys. In the first case the resonant ultrasound spectroscopy was used to detect the melting of small embedded particles with Pb and Sn, which are crucial for the machinability of this alloy, in the second case for analysis of grain boundary sliding in dependence on the grain size. Subsequently, the same methodology was used for cold-sprayed materials.

- Nejezchlebová, J., Seiner, H., Ševčík, M., Landa, M., Karlík, M. Ultrasonic detection of ductile-to-brittle transitions in free-cutting aluminum alloys (2015) NDT and E International, 69, pp. 40-47.
- Koller, M., Sedlák, P., Seiner, H., Ševčík, M., Landa, M., Stráská, J., Janeček, M. An ultrasonic internal friction study of ultrafine-grained AZ31 magnesium alloy (2015) Journal of Materials Science, 50 (2), pp. 808-818.
- Janovská, M., Minárik, P., Sedlák, P., Seiner, H., Knapek, M., Chmelík, F., Janeček, M., Landa, M. Elasticity and internal friction of magnesium alloys at room and elevated temperatures (2018) Journal of Materials Science, 53 (11), pp. 8545-8553
- Seiner, H., Cizek, J., Sedlák, P., Huang, R., Cupera, J., Dlouhy, I., Landa, M. Elastic moduli and elastic anisotropy of cold sprayed metallic coatings (2016) Surface and Coatings Technology, 291, pp. 342-347.

Ultrasound characterization of graphene nanoplatelets-based materials

Within a collaboration with the Institute of Ceramics and Glass CSIC (Madrid, Spain) and Florida International University (Miami, FL, USA), spark plasma sintered (SPSed) materials were analysed, consisting either of a mixture silicon nitride and graphene nanoplatelets, or of pure consolidated graphene nanoplatelets. These materials exhibit unique anisotropic properties, especially as far as the thermal and electrical conductivity, acoustic damping and tribologic characteristics are concerned. In both cases, the directional dependence of the elastic moduli were determined and discussed in relation with the microstructure of the material.

- Seiner, H., Ramirez, C., Koller, M., Sedlák, P., Landa, M., Miranzo, P., Belmonte, M., Osendi, M.I. Elastic properties of silicon nitride ceramics reinforced with graphene nanofillers (2015) Materials and Design, 87, pp. 675-680.
- Koller, M., Seiner, H., Landa, M., Nieto, A., Agarwal, A. Anisotropic Elastic and Acoustic Properties of Bulk Graphene Nanoplatelets Consolidated by Spark Plasma Sintering (2015) Acta Physica Polonica A, 128(4), pp. 670-674.

Determination of elastic moduli of thin micro- and nanostructured layers

Within a bilateral collaboration with the Israeli Institute of Technology (Technion, Haifa), a research on mechanical properties of few micrometers thick sputtered Al and NiTi layers was carried out, both promising candidates for applications in micromechanics. By using a mathematical model, the resonant spectra of free elastic vibrations of substrates with samples of these layers were inversely analysed, which enabled determination of elastic moduli of these layers. For the NiTi alloy, the evolution of Young's modulus with temperature in the vicinity of the transition temperatures was studied, for Al layers the correlation between the Young's modulus and porosity was analyzed. The same approach was also applied to thin layers of nanoporous semiconductors, for which also a study of the relation between elasticity and internal nanoarchitecture was carried out.

- Thomasová, M., Sedlák, P., Seiner, H., Janovská, M., Kabla, M., Shilo, D., Landa, M. Young's moduli of sputter-deposited NiTi films determined by resonant ultrasound spectroscopy: Austenite, R-phase, and martensite (2015) Scripta Materialia, 101, pp. 24-27.
- Ben-David, E., Landa, M., Janovská, M., Seiner, H., Gutman, O., Tepper-Faran, T., Shilo, D. The effect of grain and pore sizes on the mechanical behavior of thin Al films deposited under different conditions (2015) Acta Materialia, 87, pp. 321-331.
- Janovská, M., Sedlák, P., Kruisová, A., Seiner, H., Landa, M., Grym, J. Elastic constants of nanoporous III-V semiconductors (2015) Journal of Physics D: Applied Physics, 48 (24), art. no. 245102.

Studying omega-transitions in metastable titanium alloys by means of ultrasound

Within a collaboration with Charles University (Prague) and the Ufa Technical University (Russia), the formation of omega-particles in beta-titanium alloys was analyzed. It was shown that even a very small volume fraction of omega-particles in the beta-matrix leads to a pronounced increase of elastic moduli. The research was carried out both for thermally-induced omega-transitions in single crystals and for stress-induced omega-transitions in polycrystals processed by severe plastic deformation.

- Nejezchlebová, J., Janovská, M., Seiner, H., Sedlák, P., Landa, M., Šmilauerová, J., Stráský, J., Harcuba, P., Janeček, M. The effect of athermal and isothermal ω phase particles on elasticity of β-Ti single crystals (2016) Acta Materialia, 110, pp. 185-191.
- Václavová, K., Stráský, J., Polyakova, V., Strásk á, J., Nejezchlebová, J., Seiner, H., Semenova, I., Janeček, M. Microhardness and microstructure evolution of ultra-fine grained Ti-15Mo and TIMETAL LCB alloys prepared by high pressure torsion (2017) Materials Science and Engineering A, 682, pp. 220-228.
- Nejezchlebová, J., Seiner, H., Sedlák, P., Landa, M., Šmilauerová, J., Aeby-Gautier, E., Denand, B., Dehmas, M., Appolaire, B. On the complementarity between resistivity measurement and ultrasonic measurement for in-situ characterization of phase transitions in Ti-alloys (2018) Journal of Alloys and Compounds, 762, pp. 868-872.
- Nejezchlebová, J., Janovská, M., Sedlák, P., Šmilauerová, J., Stráský, J., Janeček, M., Seiner, H.

- Elastic constants of β-Ti15Mo (2019) Journal of Alloys and Compounds, 792, pp. 960-967.

Application of surface ultrasonic waves for detection of martensitic phase transitions

The possibility of utilizing the changes of surface acoustic wave velocity as sensitive indicators of structural changes in martensitically transforming materials was explored. Within long-term collaborations with the Israeli Institute of Technology (Technion, Haifa) and the Osaka University (Japan), this approach was successfully applied to detect the thermally induced transitions in thin NiTi layers as well as stress-induced transitions in FePd single crystals.

- Grabec, T., Sedlák, P., Stoklasová, P., Thomasová, M., Shilo, D., Kabla, M., Seiner, H., Landa, M. In situ characterization of local elastic properties of thin shape memory films by surface acoustic waves (2016) Smart Materials and Structures, 25 (12), art. no. 127002.
- Seiner, H., Stoklasová, P., Sedlák, P., Ševčík, M., Janovská, M., Landa, M., Fukuda, T., Yamaguchi, T., Kakeshita, T. Evolution of soft-phonon modes in Fe-Pd shape memory alloy under large elastic-like strains (2016) Acta Materialia, 105, pp. 182-188.

Laser-Ultrasonic characterization of low temperature phases of shape memory alloys

Within the collaboration with the Institute of Physics CAS and the VSB-Technical University of Ostrava, elastic properties of polycrystalline NiTi and NiTiCu shape memory alloys were studied by ultrasonic measurements. It was revealed that these alloys can exhibit significant elastic anisotropy due to reorientation of martensitic variants, and that this anisotropy depends of the pseudoplastic straining history of the material. It was observed that Young's modulus in the direction oriented along the applied uniaxial compression significantly increases.
In addition, properties of ferromagnetic shape memory alloys were investigated by ultrasonic methods with the aim to analyze the soft phonon structure in the low-temperature phases (martensites). The results are in good agreement with theoretical ab-initio predictions and confirm that the non-modulated martensite of the NiMnGa alloy exhibits strong elastic anisotropy with shear instability related to the soft acoustic phonons mediating the reverse transition.

- Thomasová, M., Seiner, H., Sedlák, P., Frost, M., Ševčík, M., Szurman, I., Kocich, R., Drahokoupil, J., Šittner, P., Landa, M. Evolution of macroscopic elastic moduli of martensitic polycrystalline NiTi and NiTiCu shape memory alloys with pseudoplastic straining (2017) Acta Materialia, 123, pp. 146-156.
- Sedlák, P., Seiner, H., Bodnárová, L., Heczko, O., Landa, M. Elastic constants of non-modulated Ni-Mn-Ga martensite (2017) Scripta Materialia, 136, pp. 20-23.

Newly designed materials - light-weight ferromagnetic composites

The D5 team contributed to the development of a new class of metallic materials – light-weight ferromagnetic metallic composites. This research was carried out within the CSF AdMat Centre of Excellence project. The mixtures of Co-Ni-Al and α-Ti powders were compacted by SPS, which resulted in fully dense ferromagnetic materials with decreased mass density and interesting mechanical properties for potential applications.
The contribution of the team was in ultrasonic characterization of the prepared composites by resonant ultrasound spectroscopy, providing elastic constants and internal friction parameters for various volume fractions of Co-Ni-Al and α-Ti, both at the room temperature and at elevated temperatures.

- Koller, M., Chráska, T., Cinert, J., Heczko, O., Kopeček, J., Landa, M., Mušálek, R., Rameš, M., Seiner, H., Stráský, J., Janeček, M. Mechanical and magnetic properties of semi-Heusler/light-metal composites consolidated by spark plasma sintering (2017) Materials and Design, 126, pp. 351-357.
- Kopeček, J., Bartha, K., Mušálek, R., Pala, Z., Chráska, T., Beran, P., Ryukhtin, V., Strunz, P., Nováková, J., Stráský, J., Novák, P., Heczko, O., Landa, M., Seiner, H., Janeček, M.

Structural characterization of semi-heusler/light metal composites prepared by spark plasma sintering (2018) Scientific Reports, 8 (1), art. no. 11133.

Phononic properties of 3D-printed periodic ceramic micro-scaffolds

Acoustic properties of periodic ceramic micro-scaffolds were studied in collaboration with the Institute of Ceramics and Glass ICV-CSIC Madrid, Spain, and the Harvard University, USA. The transmission of longitudinal ultrasonic waves through scaffolds of tetragonal and hexagonal microlattices was measured. It was observed that the wave propagation in these structures exhibits well-detectable acoustic band structures. The bandgaps at relatively high frequencies were shown to be in close agreement with the predictions of numerical models, especially for tetragonal scaffolds. Further analysis was focused on hexagonal scaffolds (energy focusing phenomena) and design and development of scaffolds from MAX-phase ceramics.

- Kruisová, A., Ševčík, M., Seiner, H., Sedlák, P., Román-Manso, B., Miranzo, P., Belmonte, M., Landa, M. Ultrasonic bandgaps in 3D-printed periodic ceramic microlattices (2018) Ultrasonics, 82, pp. 91-100.
- Koller, M., Kruisová, A., Seiner, H., Sedlák, P., Román-Manso, B., Miranzo, P., Belmonte, M., Landa, M. Anisotropic elasticity of ceramic micro-scaffolds fabricated by robocasting (2018) Acta Physica Polonica A, 134 (3), pp. 799-803.
- Belmonte, M., Koller, M., Moyano, J.J., Seiner, H., Miranzo, P., Osendi, M.I., González-Julián, J. Multifunctional 3D-Printed Cellular MAX-Phase Architectures (2019) Advanced Materials Technologies, 4 (9), art. no. 1900375.

iii) Modelling of advanced materials

Formation of periodic structures in single crystals of shape memory alloys.

Within a collaboration with the Israeli Institute of Technology Technion (Haifa), the Julius-Maxmilian University in Wuerzburg (Germany) and the RWTH University in Aachen (Germany), a theoretical research on formation of periodic structures (twinned and nanotwinned) structures was carried out for single crystals of two shape memory alloys: Cu-Al-Ni and Ni-Mn-Ga. In the first case, the effect of the formation of twinning laminates on the stress-strain behaviour of a single crystal was studied, in the second case an analysis of nanotwin formation in so-called modulated phases was given, and the relation between these structures and the intermartensitic transitions was discussed.

- Benešová, B., Frost, M., Kampschulte, M., Melcher, C., Sedlák, P., Seiner, H. Incommensurateness in nanotwinning models of modulated martensites (2015) Physical Review B - Condensed Matter and Materials Physics, 92 (18), art. no. 180101
- Faran, E., Seiner, H., Landa, M., Shilo, D. The effects of microstructure on crackling noise during martensitic transformation in Cu-Al-Ni (2015) Applied Physics Letters, 107 (17), art. no. 171601.

Numerical models of inelastic processes in shape memory alloys

Within a long-term collaboration with the Institute of Physics CAS, RWTH Aachen (Germany), and ESRF Grenoble (France) numerical models of inelastic straining processes in polycrystalline shape memory alloys and their localization were developed. By use of finite element methods, these models were applied for various geometries and loading modes. The comparison of the model predictions with results of 3D X-ray diffraction tomography were published in the prestigious journal Science.

- Sedmák, P., Pilch, J., Heller, L., Kopeček, J., Wright, J., Sedlák, P., Frost, M., Šittner, P. Grain-resolved analysis of localized deformation in nickel-titanium wire under tensile load (2016) Science, 353 (6299), pp. 559-562.
- Frost, M., Sedlák, P., Kadeřávek, L., Heller, L., Šittner, P. Modeling of mechanical response of NiTi shape memory alloy subjected to combined thermal and non-proportional

mechanical loading: A case study on helical spring actuator (2016) Journal of Intelligent Material Systems and Structures, 27 (14), pp. 1927-1938.
- Frost, M., Benešová, B., Sedlák, P. A microscopically motivated constitutive model for shape memory alloys: Formulation, analysis and computations (2016) Mathematics and Mechanics of Solids, 21 (3), pp. 358-382.

Theoretical models of transformation-plasticity coupling

Within a collaboration with the Institute of Physics CAS and the Nuclear Physics Institute CAS, theoretical models of interaction between martensitic transition fronts and dislocation slip-based plasticity were developed. Several lengthscales (from atomistic to polycrystalline) and several loading regimes (from low-temperature/low-stress to high-temperature/stress above the yield point) were considered. The developed models were able to explain correctly several intriguing phenomena, for example the asymmetry between forward and reverse transition, as far as the plastic strains are concerned, or the reverse transition appearing upon loading at high temperatures.

- Heller, L., Šittner, P., Sedlák, P., Seiner, H., Tyc, O., Kadeřávek, L., Sedmák, P., Vronka, M. Beyond the strain recoverability of martensitic transformation in NiTi (2019) International Journal of Plasticity, 116, pp. 232-264.
- Heller, L., Seiner, H., Šittner, P., Sedlák, P., Tyc, O., Kadeřávek, L. On the plastic deformation accompanying cyclic martensitic transformation in thermomechanically loaded NiTi (2018) International Journal of Plasticity, 111, pp. 53-71.
- Šittner, P., Sedlák, P., Seiner, H., Sedmák, P., Pilch, J., Delville, R., Heller, L., Kadeřávek, L. On the coupling between martensitic transformation and plasticity in NiTi: Experiments and continuum based modelling (2018) Progress in Materials Science, 98, pp. 249-298.

Modelling of wave scattering in complex polycrystalline media

Within a collaboration with ReceNDT GmbH Linz, Austria (Johannes Kepler University spin-off), numerical simulations of wave front interaction with grains and grain boundaries were carried out. The focus was laid on surface acoustic waves and their scattering-induced attenuation in polycrystalline metals. Semianalytic approaches were applied, which led to enhanced robustness and significant decrease of computational time.

- Ryzy, M., Grabec, T., Österreicher, J.A., Hettich, M., Veres, I.A. Measurement of coherent surface acoustic wave attenuation in polycrystalline aluminum (2018) AIP Advances, 8 (12), art. no. 125019.
- Ryzy, M., Grabec, T., Sedlák, P., Veres, I.A. Influence of grain morphology on ultrasonic wave attenuation in polycrystalline media with statistically equiaxed grains (2018) Journal of the Acoustical Society of America, 143 (1), pp. 219-229.

Identification and analysis of rarely observed microstructures in shape memory alloys

Within a broad international collaboration, geometrically ordered microstructures appearing in low temperature phases of shape memory alloys were studied by mathematical theory of martensitic microstructures. The focus was laid on exotic and/or rarely observed microstructures, such as branching twins in bent single crystals, non-conventional (i.e., irrational) twins in modulated structures, and elastically stressed interfacial regions observed by sub-surface X-ray measurements.

- Chulist, R., Straka, L., Seiner, H., Sozinov, A., Schell, N., Tokarski, T. Branching of {110) twin boundaries in five-layered Ni-Mn-Ga bent single crystals (2019) Materials and Design, 171, art. no. 107703
- Seiner, H., Chulist, R., Maziarz, W., Sozinov, A., Heczko, O., Straka, L. Non-conventional twins in five-layer modulated Ni-Mn-Ga martensite (2019) Scripta Materialia, 162, pp. 497-502.

- Bucsek, A., Seiner, H., Simons, H., Yildirim, C., Cook, P., Chumlyakov, Y., Detlefs, C., Stebner, A.P. Sub-surface measurements of the austenite microstructure in response to martensitic phase transformation (2019) Acta Materialia, 179, pp. 273-286.

The research in all above listed areas was supported by several **grant projects**. These where:

1. Multidisciplinary research center of advanced materials AdMat, Czech Science Foundation, project No. 14-36566G, 2014-2018
2. Experimentally justified multiscale modelling of shape memory alloys, Czech Science Foundation, project No. 14-15264S, 2014-2016
3. Evaluation of Elastic Properties of Materials Processed by Severe Plastic Deformation, Czech Science Foundation, project No. 13-13616S, 2016-2019
4. Fluid Acoustics in Periodic Micro-Architectures,Czech Science Foundation, project No. 17-01618S, 2016-2019
5. Architectured metallic materials designed for cold spray kinetization, Czech Science Foundation, project No. 17-13573S, 2016-2019
6. Understanding modulated structures in Heusler alloys, Czech Science Foundation, project No. 17-00062S, 2016-2019
7. Tailoring elasticity of Ti-based alloys by thermally and stress induced phase transformations, Czech Science Foundation, project No. 17-04871S, 2016-2019
8. Localization phenomena in shape memory alloys: experiments & modelling, Czech Science Foundation, project No. 18-03834S, 2018-today
9. Mathematical modelling of ferromagnetic shape memory alloys, DAAD Czech-German bilateral mobility project (with RWTH Aachen), project No. 1411, 2014-2015
10. Development of characterization methods for materials for energy harvesting, Czech Academy of Sciences, Programme Strategy 21, project No. 909029, 2019 (one year)

Research activity and characterisation of the main scientific results

The major research achievements obtained in the research areas covered by the Department are briefly described below.

Laboratory of Dynamics of Electrical Machines and Drives

Result: *Electrical Machines with Multi-Phase and Combined Stator Windings*

Members of Research Team Involved: *L. Schreier, M. Chomát, J. Bendl*

In the observed period, the attention was paid to AC multi-phase electric machines. These machines are used in practical applications due to several advantages they have contrary to three-phase machines. The operation of multi-phase machines is less noisy. These machines can have better efficiency and are more resistant to faults. The attention has been paid to five- and six-phase machines and machines with the combined winding. It has been shown that in the case of multi-phase machines, the attention must be paid, besides to the final (fundamental) spatial wave, also to higher spatial harmonics, which can have a considerably negative influence mainly on the currents and the torque of these machines. For analysing the situation in these machines, the method of space vectors and symmetrical components of instantaneous values of currents and voltages has been used. The method makes it possible to effectively and relatively simply take into consideration the higher spatial waves of the current layer, magnetic inductance and the flux in the yoke. It has been shown that the attention must be paid to higher spatial waves mainly during the unsuitable way of feeding by asymmetrical voltage and in the case of the loss of one or more stator windings due to the fault in the feeding source (in most applications …the frequency converter) or during the fault in the electric machine itself. By means of the mentioned method, mathematical models of the chosen types of machines have been produced and their numerical models have been set up. By means of these models, the properties of the considered machines have been examined both in the steady and various transient and fault states. For examining the operation of multi-phase machines, a method has been developed that makes it possible to respect the loss of particular stator windings and that is based on the possibility to consider the loss of some of the windings by connecting the suitably chosen auxiliary impedances between the terminals of this winding and the terminals of the voltage source. The attention has been paid to six- and five-phase machines, though the mentioned method makes it possible to analyse AC machines with an arbitrary number of phases. Methods of controlling these machines have been proposed. These methods make it possible to feed five- and six-phase machines in such a way that higher spatial waves do not arise and their undesirable effects both in steady and emergency operations during the loss of one- or multi-phase winding are limited. In the case of synchronous machines with permanent magnets, the influence of the shape of magnets on the rise of higher spatial harmonics has been analysed and conditions of the arrangement of magnets in such a way that the undesirable third spatial wave of the flux in the yoke is suppressed have been set up. Also proposed has been the suitable arrangement of the combined winding.

All theoretical conclusions have been verified by experimental measurements. The measurements have confirmed a very good agreement between the theoretical conclusions and the measured waveforms of the observed quantities, e.g. currents and torque of the examined machines. The analysis of faults of the rotor cage winding that represent a multi-phase system has started. For this analysis, the findings and experience gained during the analysis of machines with a higher number of stator phases have been used.

Participation of Research Team

The result was achieved entirely by the members of the research team of the Department.

Main Outcomes

- Chomát, M., Schreier, L., Bendl, J. Analysis of magnetic field distribution in induction machine with combined star-delta stator winding. *The Journal of Engineering.* 2019, 2019(17), 4369-4374. ISSN 2051-3305.
- Schreier, L., Bendl, J., Chomát, M. Analysis of influence of third spatial harmonic on currents and torque of multi-phase synchronous machine with permanent magnets. *Electrical Engineering.* 2018, 100(3), 2095-2102. ISSN 0948-7921.
- Schreier, L., Bendl, J., Chomát, M. Comparison of properties of two basic variants of combined star-delta stator winding of induction machines. *Electrical Engineering.* 2018, 100(3), 2155-2164. ISSN 0948-7921.
- Schreier, L., Bendl, J., Chomát, M. Novel Arrangement of Combined Star-Delta Stator Winding Aimed at Reduction of Copper Usage in Electric Machine. *Maszyny elektryczne - Zeszyty Problemowe.* 2018, 119(3), 117-122. ISSN 0239-3646.
- Schreier, L., Bendl, J., Chomát, M. Analysis of Properties of Induction Machine with Combined Parallel Star-Delta Stator Winding. *Maszyny elektryczne - Zeszyty Problemowe.* 2017, 113(1), 147-153. ISSN 0239-3646.
- Schreier, L., Bendl, J., Chomát, M. Effect of combined stator winding on reduction of higher spatial harmonics in induction machine. *Electrical Engineering.* 2017, 99(1), 161-169. ISSN 0948-7921.
- Schreier, L., Bendl, J., Chomát, M. Operation of five-phase induction motor after loss of one phase of feeding source. *Electrical Engineering.* 2017, 99(1), 9-18. ISSN 0948-7921.
- Schreier, L., Bendl, J., Chomát, M. Analysis of induction machines with combined stator windings. *Acta Technica CSAV.* 2015, 60(2), 155-171. ISSN 0001-7043.
- Schreier, L., Bendl, J., Chomát, M. Effect of higher spatial harmonics on properties of six-phase induction machine fed by unbalanced voltages. *Electrical Engineering.* 2015, 97(2), 155-164. ISSN 0948-7921.

Laboratory of Power Electronics

Result: *Direct and Predictive Power Control Methods for Grid-Connected Converters in B4 and B6 Configurations*

Members of Research Team Involved: *V. Valouch, J. Škramlík, P. Šimek, M. Bejvl*

The object of the analysis was control methods of the positive and negative sequences of the current of a grid connected converter during voltage faults and/or reference changes in order to assure a proper exchange of active and reactive powers without power ripple, to mitigate harmonic distortion of grid currents, and to control grid phase current and power peaks. The MPC (Model Predictive Control) presents a lot of advantages: it is a type of the feedforward control with small number of parameters to be tuned, usual nonlinearities and constraints can be included into the strategy, it is characterized by high dynamics, and also various demands on controlled object behaviour can be laid and balanced each other. The MPC solves at every switching interval the problem of an optimal control in a finite prediction horizon on the basis of measured and/or estimated system variables. The MPC has becoming very popular in power electronics applications nowadays. Depending on which variables are assumed as system control variables we may classify two main concepts of the MPC. Specifically, in the field of the power electronics these two main control principles are: 1) the control variables are the commutation instants between different converter states; 2) the control variables are all possible converter states. In all the cases we try to minimize the value of an objective (cost) function. The developed control techniques enable to assure an exchange of active and reactive powers between the grid-connected converter and the grid, without power and currents ripples, and makes a control of grid phase current peaks possible at the same time.

Participation of Research Team

The research was done in co-operation with the Faculty of Electrical Engineering, Czech Technical University in Prague.

Main Outcomes

- Lettl, J., Šimek, P., Valouch, V. Compensation of Disturbed Load Currents Using Active Power Filter and Generalized Non-active Power Theory. In: *Progress in Electromagnetics Research Symposium*. Prague: Electromagnetics Academy, 2015, s. 2500-2505. ISSN 1559-9450.
- Valouch, V., Bejvl, M., Šimek, P., Škramlík, J. Power Control of Grid-Connected Converters Under Unbalanced Voltage Conditions. *IEEE Transactions on Industrial Electronics.* 2015, 62(7), 4241-4248. ISSN 0278-0046.
- Valouch, V., Šimek, P., Škramlík, J. Analytical Closed-Form Solution of Current Responses of Four-Switch Converter Connected to Three-Phase Unbalanced Grid. In: *Proceedings of the 2015 International Conference on Electrical Drives and Power Electronics (EDPE)*. Košice: Technical University of Košice, 2015, s. 25-29. ISBN 978-1-4673-7376-0. E-ISSN 1339-3944.
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Result: *Modern Phase and Frequency Locked Loops for Electronic Power Converters*

Members of Research Team Involved: *V. Valouch, J. Škramlík, P. Šimek*

The synchronization methods belong mainly to two main categories: Phase Locked Loop (PLL) and Frequency Locked Loop (FLL) strategies. A basic closed loop three-phase synchronization technique is the SRF-PLL (Synchronous Reference Frame-PLL). This basic simple technique has some disadvantages that may be mitigated by different proper modifications of the technique. A novel FLL technique has been developed that incorporates advantages of the common filtering techniques, and uses also a PJD (Phase Jump Detector). The PJD cuts the tight bond between the estimated frequency and phase of the voltage vector, specifically in case of phase jumps. Experimental results provided by this new method confirm the quality of the method.

Participation of Research Team

The research was done in co-operation with the Faculty of Electrical Engineering, Czech Technical University in Prague.

Main Outcomes

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- Šimek, P., Škramlík, J., Valouch, V. A frequency locked loop strategy for synchronization of inverters used in distributed energy sources. *International Journal of Electrical Power & Energy Systems.* 2019, 107(May), 120-130. ISSN 0142-0615.
- Šimek, P., Valouch, V. Cascaded delayed signal cancellation based pre-filtering technique to improve frequency locked loop for grid synchronization. In: Dudrik, J., Fedák, V., Kyslan, K., Matuško, J., eds. *International Conference on Electical Drives and Power Electronics*. Nový Smokovec: KoREMA, 2019, s. 391-396, č. článku 8883930. ISBN 978-1-7281-0388-4. ISSN 1339-3944.

Result: *Development of Control for Large Industrial Drives*

Members of Research Team Involved: *P. Kokeš, R. Semerád*

The IT was a subcontractor of power drive contracts for processing industry and for mining industry. The development carried out in the Institute can be divided into several parts. The system software for EmadynF, which is a controller produced by company Elektrotechnika, a.s. and acts as a slave device in the Ethercat network, was substantially improved. The previous system software was rewritten and much new functionality was added, e.g. implementation of File over Ethercat (FoE) communication protocol, new Service Data Objects (SDO) for transfer and manipulation of control data, for application parameters loading and for diagnostic data logging. The Master-Slave software interfaces for control of three applications were proposed and implemented.

The application software for induction motor (AM) variable speed drives with vector control of motor torque was developed. These drives of power up to 4.1MW were fed from medium-voltage (MV) 7-level inverters. At first, the sensorless control algorithm was proposed for these drives, i.e. the drives were able to start and run without speed sensors, but finally so called sensorless catching algorithm had to be implemented, i.e. the motor feeding could be started not only at zero speed but the rotor could rotate up to nominal speed (in one rotational direction and after AM de-excitation only).

The application software for synchronous motor (SM) drives with vector control of motor torque was created. These 1.8MW and 5.8MW drives were fed from indirect frequency converters consisting of the MV 7-level Active Front-End (AFE) and MV 7-level inverter. The sophisticated control algorithm was used to eliminate some motor parameters fluctuations. An enormous effort was made to decrease an unwanted 12-order motor torque component causing mechanical vibrations. At first, resonant controllers were used to eliminate higher-order components either in stator currents or in the speed loopback. The novel numerical SM model, which utilizes so called winding functions and enables to respect the spatial arrangement of slots and windings, was created in the end. In this model the 12-order torque component was directly calculated and used for its feedforward compensation. Finding up to 12 constants of the model required a lot of measurement on the real motors.

The AFE control software had to be modified to meet national standards and requirements for back influence of MV grid-connected converters. After simulations the AFE switching frequency and AFE input filter were optimized and the algorithm eliminating low-order frequencies was made up. The DC-link voltage was also kept on its minimum according to the immediate motor operating mode, which enabled decreasing power losses in the inverter.

All these algorithms were simulated in Matlab, implemented into EmadynF, tested on the laboratory model in the Institute and we also provided support for drives commissioning.

Participation of Research Team

The research was done under a collaborative project with company Elektrotechnika, a.s.

Main Outcomes

- Kokeš, P., Adam, Z. Palaser Project - Back Effect of AFE Converter on Supply Grid Voltage (In Czech). Praha: Institute of Thermomechanics CAS, 2017. 17 s. Z-1575/17.
- Kokeš, P. G2 Project - Software Interface for Actuating Main Drive via Ethercat Network, Version 2 (In Czech). Praha: Institute of Thermomechanics CAS, 2016. 17 s. T-525/16.
- Kokeš, P. System Software of EmadynF Controller, Software Interface for Events Logging via EtherCAT Network (In Czech). Praha: Institute of Thermomechanics CAS, 2015. 10 s. T-523/15.
- Kokeš, P. Palaser Project - Software Interface for Actuating AFE Converter via Ethercat Network (In Czech). Praha: Institute of Thermomechanics CAS, 2015. 12 s. T-521/15.
- Kokeš, P. Palaser Project - Software Interface for Drive Control via Ethercat Network, ver.2 (In Czech). Praha: Institute of Thermomechanics CAS, 2015. 16 s. T-520/15.
- Kokeš, P. G2 Project - Software Interface for Actuating Main Drive via Ethercat Network (In Czech). Praha: Institute of Thermomechanics CAS, 2015. 18 s. T-518/15.
- Pavelka, J., Šimek, J., Kobrle, P., Kokeš, P. Cause of mechanical vibrations of Palašer synchronous motors and its removal (In Czech). Česká elektrotechnická společnost ČSVTS, 2019. ISBN ISBN 978-80-02-02860-4. In: *XXXVI. Celostátní konference o elektrických pohonech*. Plzeň: ÚOS Elektrické pohony, 2019, s. 1-21. ISBN 978-80-02-02860-4.
- Pavelka, J., Šimek, J., Kobrle, P., Kokeš, P. The Cause of Mechanical Vibration of Palašer Synchronous Motors and its Removal (In Czech). *Elektro.* 2019, 29(11), 6-9. ISSN 1210-0889.
- Pavelka, J., Šimek, J., Kobrle, P., Kokeš, P. The Cause of Mechanical Vibration of Palasher Synchronous Motors and its Removal. *Transactions on Electrical Engineering.* 2019, 8(4), 68-73. E-ISSN 1805-3386.

Result: *Advanced electrical equipment of traction substations*

Members of Research Team Involved: *P. Kokeš, R. Semerád, P. Šimek, M. Bejvl, J. Janovec*

The power frequency converter for 25 kV AC traction substations is under development. Using this converter, the reactive power consumption from the grid will be eliminated, the energy consumption from the grid will be symmetrized, higher harmonics generated by the traction vehicles should be filtered, and regenerative energy of braking vehicles will be utilized better.

Computer models for MMC (Modular Multilevel Converter) power conditioner was created and tested. Modulation and balancing principles of MMC were studied, analysed and chosen for implementation in new Ethercat-based control system. A low voltage laboratory model, which all the required functionalities will be verified on, was designed and is being built up.

Participation of Research Team

The research was done in co-operation with Elektrotechnika, a.s.

Associated Grant and Collaborative Projects

Grant of Technology Agency of the Czech Republic TH03020265.

Main Outcomes

- Research reports of IT CAS no. Z-1606/19 - Lowest Level of Inverter FB-MMC Control and no. Z-1601/19 – Possibilities of Compensation and Symetrization of Current in Traction.

Laboratory of Electrophysics

Result: *Temperature Measurements in Non-Stationary Thermal Plasma with high temporal resolution.*

Members of Research Team Involved: *J. Hlína, J. Šonský, J. Gruber*

Progress in technologies utilizing plasma torches is closely connected with the development of new approaches aiming at realistic description of the conditions in thermal plasmas. Our research has set up a new approach to the diagnostics of physical parameters, especially of temperature, in thermal plasma jets using tomographic methods with high temporal resolution. These methods offer new possibilities in optical diagnostics of asymmetric and non-stationary thermal plasmas. Temperature measurements present a special problem of the diagnostics of such plasmas and need careful consideration regarding the particular gas properties and the choice of a proper spectral range for measurements. An approach, based on measuring the optical emission of plasma in wide spectral intervals, has to be adopted to ensure a sufficiently strong signal for fast optical recording. The measurement system and evaluation methods were entirely developed at our laboratory. The solution involved construction of a unique optical system for multi-directional measurement of plasma radiation working with array detectors composed of optical fibers and photodiodes, and the development of evaluation methods based on MATLAB procedures. The method was extended to air plasma, which is close to technological applications of air plasma cutting torches. The investigations have brought new findings on short-time and spatial characteristics of temperature fields and instabilities involved.

Participation of Research Team

The principal experimental part of the research was carried out in the Department. The theoretical part, consisting of computations of the plasma radiation in various spectral intervals depending on the plasma composition, temperature and thickness, was carried out at the Laboratoire Plasma et Conversion d'Energie, a common laboratory of the CNRS, Institut National Polytechnique of Toulouse, and the University Paul Sabatier of Toulouse, France.

Associated Grant and Collaborative Projects

Program of Internal Support of International Collaboration by the Czech Acad. Sci.: M100761202

Main Outcomes

- Hlína, J., Šonský, J., Gruber, J., Cressault, Y. Fast tomographic measurements of temperature in an air plasma cutting torch. *Journal of Physics D-Applied Physics.* 2016, 49(10), 105202. ISSN 0022-3727.
- Hlína, J., Šonský, J., Gruber, J. Tomographic Measurements of Temperature Fluctuations in an Air Plasma Cutting Torch. *Plasma Chemistry and Plasma Processing.* 2017, 37(3), 689-699. ISSN 0272-4324.

Result: *Physical Mechanisms of Fluid Polyamorphism*

Members of Research Team Involved: *M. Duška*

We use the theory of phase transitions and the concept of two competing interconvertible amorphous structures to develop a generic phenomenological approach. It succeeds in unifying all, apparently unrelated, cases of fluid polyamorphism with and without phase separation, from the liquid-liquid transition in supercooled water and silicon to superfluid helium and polymerized sulfur. Our approach generically describes the phase behavior and thermodynamic anomalies typically observed in polyamorphic materials. Our results mark a paradigm shift that significantly broadens fluid polyamorphism from its original narrow scope to a cross-disciplinary field that addresses a wide class of systems and phenomena with the interconversion of alternative molecular or supramolecular states.

Participation of Research Team

The research was done in co-operation with the Institute for Physical Science and Technology, University of Maryland, USA, and the International Association for the Properties of Water and Steam (IAPWS)

Associated Grant and Collaborative Projects

Young Scientist IAPWS Fellowship (http://www.iapws.org/)

Main Outcomes

- Anisimov, M. A., Duška, M., Caupin, F., Amrhein, L. E., Rosenbaum, A., Sadus, R. J. Thermodynamics of Fluid Polyamorphism. *Physical Review X.* 2018, 8(1), 011004. ISSN 2160-3308.

Result: *Aerosol synthesis of metallic nanoparticles by spark discharge*

Members of Research Team Involved: *T. Němec, J. Šonský, J. Gruber*

Spark evaporation is a simple and efficient way to synthesize metallic nanoparticles in the gas phase. A spark discharge generator (SDG) has been developed in-house consisting of a spark evaporation chamber and a high-voltage pulsed power supply. This multi-disciplinary research area has been newly established in the department in 2016 utilizing and combining the knowledge in the areas of nucleation phenomena, plasma discharges, and hydrogen fuel cells gained by members of the research team during their research career. The SDG setup allows us to synthesize sub-10-nm particles from conductive source materials (metals, semiconductors, carbon) in a controlled atmosphere resulting into samples of very high-purity, narrow size distribution and controlable composition. Direct deposition of the nanopowder from the gas phase leads to formation of highly-porous functional layers with a high specific surface that can be used for example as electrodes for low-temperature hydrogen fuel cells in case of platinum nanoparticles or platinum nanoalloys. We studied platinum nanoparticles generated in two different atmospheres (inert vs. oxidizing) resulting in various crystalline or amorphous structures. A special feature of the SDG setup was the use of unipolar spark discharges resulting in a preferential evaporation of a single electrode. The SDG process has been monitored by high-speed camera showing the temporal and spatial development of the spark discharge event and its cathode hot spots. Another diagnostic tool for the spark discharge is optical spectroscopy, which gives us information about the composition of the plasma channel. The structure and morphology of the SDG nanomaterials were analyzed by TEM, SEM, and XRD. Contacts with other institutions working in the fields of nanoparticle characterization and hydrogen fuel cells have been established:

- Institute of Physics, Czech Academy of Sciences
- Nuclear Research Institute in Řež
- Centrum výzkumu Řež
- Institute of Chemical Technology in Prague

- New Technologies – Research Centre, University of West Bohemia
- VSB - Technical University of Ostrava

Membership of the institute in HYTEP – Czech Hydrogen Technology Platform has been renewed in relation with these research activities.

Participation of Research Team

The spark discharge generator has been developed in-house. The generated nanomaterials have been analyzed by TEM, SEM, XRD in cooperation with the Department of Material Analysis at the Institute of Physics, Czech Academy of Sciences. The catalytic properties of the SDG nanomaterials in a hydrogen fuel cell were characterized in collaboration with the Green Energy and Environment Laboratories, Industrial Technology Research Institute, Taiwan. Discussions with Nuclear Research Institute in Řež, Centrum výzkumu Řež, and Institute of Chemical Technology in Prague led to grant applications to the Technology Agency of the Czech Republic.

Associated Grant and Collaborative Projects

Strategy AV21 – 3. Efficient Energy Conversion and Storage: 2017 High-power spark discharge generator for fine powder synthesis, 2018 Hydrogen fuel cell laboratory test stand, 2019 Catalyst layer deposition using SDG nanomaterials.

International cooperation program between CAS (call 19/2019) and South and Southeast Asia countries 2019 - participation at *S&T JFS Networking Event (Nanotechnology), Surakarta*

TAČR grant applications TM01000018, TK03030021

Main Outcomes

- Němec, T., Šonský, J., Gruber, J., de Prado, E., Kupčík, J., Klementová, M. Platinum and platinum oxide nanoparticles generated by unipolar spark discharge. *Journal of Aerosol Science.* 2020, 141(March), 105502. ISSN 0021-8502.
- Němec, T., Šonský, J., Klementová, M. Catalytic nanoparticle synthesis by spark discharge. In: Bouzek, K., ed. *HydrogenDays 2018. Book of Abstracts*. Prague: Česká vodíková technologická platforma, 2018, s. 1-1. ISBN 978-80-907264-0-6.
- Gruber, J., Šonský, J., Němec, T. Metallic Nanoparticle Synthesis by Spark Discharge for Energy Applications. In: *S&T JFS Networking Event (Nanotechnology)*. 2019.
- Patent application PV 2017-460

Result: *Design of magnetically pseudolevitated flywheels*

Members of Research Team Involved: J. Šonský, J. Gruber, V. Tesař

One of the possibilities of storing energy is utilizing flywheels. Although energy density of such solution is lower than e.g. rechargeable batteries, the advantages of such solution are simplicity, zero toxicity, stability over large number of frequent charge-discharge cycles and longevity. We have been developing magnetically levitated flywheels which work in room temperature conditions, eliminating the need for cryogenics. By using only permanent magnets and HAL-sensor controlled feedback stabilization by electromagnets, we achieved very low power consumption for stabilization of the levitation.

Participation of Research Team

The research, design and development of the magnetically levitated flywheels were done in our department as well as analysis of their operating characteristics.

Main Outcomes

- Šonský, J., Tesař, V. Design of a stabilized flywheel unit for efficient energy storage. *Journal of Energy Storage.* 2019, 24, 100765. ISSN 2352-152X.
- Šonský, J. *Setrvačníková soustava skladování energie*. IT CAS, 2019. Patent no. or utility model no. or industrial design no.: 307872. Date of the patent acceptance: 29.05.2019.

Result: *Plasma generated by cumulative detonation in a combustion chamber*

Members of Research Team Involved: J. Šonský, J. Gruber, V. Tesař

Combustion processes in present-day engineering applications are of the deflagration type. This limits achievable values of thermodynamic parameters, such as the highest reached temperature and the corresponding degree of gas ionization. Increase of these parameter values and reaching the thermal plasma state would allow number of potentially useful combustion applications to be improved like propulsion or electricity generation.

We have developed and constructed a combustion chamber with detonation-type combustion that can reach, by cumulative implosion of the detonation wave, extreme temperatures of generated thermal plasma. Part of the energy deliberated by combustion process is concentrated in small volume by implosion of the detonation wave, creating thermal plasma with high velocity, which can be directly converted to electrical energy due to high electrical conductivity of the plasma by means of magneto-hydro dynamics. More advanced solutions using magneto-cumulative conversion to avoid extremely high external magnetic field for effective conversion of resulting plasma kinetic energy to useful electricity were theoretically designed and patented.

Participation of Research Team

The research, design and development of the magnetocumultive generator were done in our department by Jiří Šonský, with the help of prof. Václav Tesař, especially with publications and patenting, and analysis of experimental data concerning plasma dynamics were performed by Jan Gruber. Spectroscopic measurements were done in collaboration with Alan Mašláni from Institute of Plasma Physics.

Main Outcomes

- Šonský, J., Tesař, V. Generating Plasma by Cumulative Detonation in a Combustion Chamber. *International Journal of Aerospace Engineering.* 2019, 2019(2019), 4612383. ISSN 1687-5966.
- Šonský, J., Tesař, V., Gruber, J., Mašláni, A. Implosive Thermal Plasma Source for Energy Conversion. *Plasma Physics and Technology.* 2017, 4(1), 87-90. ISSN 2336-2626.
- Tesař, V., Šonský, J. No-moving-part commutation of gas flows in generating plasma by cumulative detonations (survey). *Energy.* 2018, 157(August), 493-502. ISSN 0360-5442.
- Patent application PV-2017-117