Topics of dissertation thesis

Study program: P0413D270001 – MANAGEMENT OF INDUSTRIAL SYSTEMS
Study program: P0712D130003 – CHEMICAL AND ENVIRONMENTAL ENGINEERING
Study program: P0713D070002 – THERMAL ENGINEERING AND FUELS IN INDUSTRY
Study program: P0715D130002 – CHEMICAL METALLURGY
Study program: P0715D270007 – METALLURGICAL TECHNOLOGY
Study program: P0719D270003 – NANOTECHNOLOGY
Study program: P0788D270004 – MATERIAL SCIENCE AND ENGINEERING

Study program: P0413D270001 - MANAGEMENT OF INDUSTRIAL SYSTEMS

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Petr Besta, Ph.D.	Modern technology of iron and steel production in the context of increasing the economic efficiency of processes	Environmental requirements affect all production areas. The topic of the doctoral thesis focuses on advanced technologies of iron and steel production. Both the technological area and the impact on the environment will be examined.
2	prof. Ing. Petr Besta, Ph.D.	Use of the concept Industry 4.0 in the industrial conditions of the Czech Republic	The increasing of the process efficiency through the use of the Industry 4.0 concept. Analysis of the current concept used within the Czech Republic. Generating a methodology for increasing the effectiveness of implementation.
3	prof. Ing. Jiří Plura, CSc.	Development of methods of products and processes quality planning	Quality planning processes fundamentally affect the resulting product quality and therefore customer satisfaction and organizational competitiveness. Their success can be greatly improved by using appropriate quality planning methods. The solution to this topic will be based on a detailed analysis of appropriate product and process quality planning methods. The identified methods will be systematized according to partial quality planning processes. The current level of individual methods processing will be analyzed and opportunities for improvement will be identified. On the basis of identified opportunities and defined priorities, suggestions will be processed to improve selected methods and the ways of their using.
4	prof. Ing. Jiří Plura, CSc.	Development of approaches to risk and opportunity management in the context of Quality 4.0 concept	Risk-based thinking is an integral part of all approaches to building and developing modern quality management systems, which confirms the inclusion of this issue among the requirements of the ČSN EN ISO 9001 standard and a other industry standards. The goal of the process of considering risks and opportunities is to eliminate the most significant risks or, conversely, to strengthen the most significant opportunities. This establishes a basis for increasing the effectiveness of the quality management system, achieving improved results and preventing negative effects. The success of this process depends on the ability to identify all significant risks, properly evaluate them and take effective actions to address the risks or opportunities. The solution to the mentioned topic will be based on a detailed research and analysis of existing approaches to risk management. The current level of their development will be analyzed and opportunities for their improvement will be identified in the context of the emerging concept of Quality 4.0, especially with regard to the conditions and opportunities related to this concept. On the basis of identified opportunities and defined priorities, suggestions will be processed to improve selected approaches to risk management and the ways of their using.

5	doc. Ing. Šárka Vilamová, Ph.D.	Price dumping of metallurgical products as unfair competition	Metallurgy is historically a very important industrial area, which has its own specifics, but even in this industrial sector we will not avoid unlawful conduct of competing entrepreneurs, aiming to harm or eliminate competition in the market and thus increase their profits. The aim of the dissertation will be to clarify the issue of unfair competition in the field of metallurgical products with a particular focus on price dumping.
6	prof. Ing. Darja Noskievičová, CSc.	Fault management in modern production systems	The modern production systems, produced more and more complex products, are based on very complex cyber-physical systems (CPS) that consist of physical components and cyber elements and their interactions. This complexity evocates higher probability of faults of the production systems, their elements, and products, too. It means that also complexity of fault detection rises in such conditions. Analysis of cyber-physical attack vulnerabilities of quality control tools must be incorporated into analyses. The dissertation will be devoted to analysis of effective fault management system as a part of predictive quality management system, its requirements and structure and its proposal.
7	prof. Ing. Darja Noskievičová, CSc.	Sustainability of digital transformation	The entire digital transformation is based on at least two pillars on the consumer side: Internet access with a fixed price and infinite energy at a reasonable price. The dissertation will be focused on analysis of limitations of today´s trend of digital transformation and smart factories building especially in the light of present energy crisis and possible solutions.

Study program: P0712D130003 - CHEMICAL AND ENVIRONMENTAL ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Vlastimil Matějka, Ph.D.	Photocatalytically active materials in building industry	The topic of doctoral thesis is focused on the utilization of photocatalytically active materials (photocatalysts) in building industry. Photocatalysts are used in the field of photocatalytic cleaning of water and air and thus contribute to elimination of contaminants in living environment. Application of the photocatalyts in building industry for air purification is promising with respect to the fact that the surfaces of building are in direct contact with surrounding atmosphere. Building materials based on latent hydraulic materials, for example metallurgical slags, represents still not widely used alternative to common building materials based on Portland cement. Application of photocatalytically active materials in the mixtures of latent hydraulic materials, or deposited on their surfaces, could further increase the utility value of the resulting products. The aim of the work is to propose and prepare suitable photocatalysts and verify their applicability and functionality in the mixtures of alkali activated latent hydraulic materials. Part of the work will be also focused on the description of the effect of photocatalyst on hydration processes. As the output of the work the formulation of the mixture including selected: i) latent hydraulic material, ii) alkali activator and iii) selected photocatalyst will be proposed with emphasize to acquire the optimal ratio between photocatalytic performance and mechanical properties. The indication of possible specific application of developed material will be proposed as well.
2	prof. Ing. Lucie Obalová, Ph.D.	Catalytic destruction of nitrogen containing pollutants	Nitrogen oxides (N2O, NO, NO2) and NH3 are significant pollutants. Many current technologies for reducing these substances in waste gases are economically demanding or require the presence of a reducing agent (ammonia, urea, hydrocarbons) that can lead to emissions of other pollutants (ammonia slip). It is therefore desirable to develop and test new methods for reducing emissions of these components. The main task will be an experimental study of catalytic degradation of nitrogen oxides without the use of a reducing agent and/or oxidation of NH3 on catalysts containing selected transition metals and a description of the physical-chemical properties of catalysts by available analytical techniques (chemical analysis, X-ray diffraction, physical nitrogen sorption, temperature-programmed desorption and reduction, etc.). The aim of the thesis will be to assess the effectiveness and stability of the materials studied, to clarify the mechanism of ongoing reactions and the relationships between the

			properties of catalysts and their activity and selectivity, and to optimize the method of catalyst preparation.
3	prof. Ing. Lucie Obalová, Ph.D.	Possibilities of anaerobic co-fermentation of biowaste or energy biomass with waste or purposefully grown algae biomass	Algae appear to be a promising source of biomass for the production of biofuels. Algae can be anaerobically decomposed relatively easily to produce biogas and fertilizer, but the high-water content reduces the overall efficiency of the process. The possibilities and processes of obtaining algae biomass will be studied, for example with the use of waste gases from industrial processes. The processes of pretreatment of the green mass of algae with the aim of increased degradability in the process of anaerobic digestion will be described. The theoretical advantages and disadvantages of co-fermentation of algae with biowaste or conventional energy biomass will be evaluated. At least one experiment of continuous algae biomass production with subsequent processing by anaerobic digestion will be carried out. Batch digestion tests will verify the kinetics of biogas production from algae. (Semi)continuous processes will verify the co-fermentation of algae with selected types of biowaste or energy biomass. If possible, the (semi)continuous mono-fermentation of algae will also be verified. The practical applicability and benefits of algae co-processing in biogas stations will be evaluated.
4	prof. Ing. Lucie Obalová, Ph.D.	Application in anaerobic digestion of chemically modified biochar and pyro-oil generated from digestate	Zero-waste approach coupling anaerobic digestion and pyrolysis requires the transformation of the organic matter contained in the digestion solid effluent via pyrolysis to valuable products. The products consist of a pyro-oil including an enriched-in-organics water phase that can be valorized for biogas generation and a solid material (“biochar”) which can be potentially used in several applications e.g. bioremediation, gas cleaning, soil amelioration or as additive in anaerobic digestion. Biochar deriving from biomass pyrolysis has been reported to have a positive effect on anaerobic methane generation. Biochar produced from the solids of the effluent of anaerobic digestion appeared to have lower efficiency. The research during PhD study aims to close the cycle between the two processes by

			initially valorizing the water-phase of pyrolysis oil in biogas production and secondly find appropriate pathways of pretreatment, mainly chemical, for the digestate-derived char to optimize the catalytic activity in an anaerobic digestion system. Laboratory experiments of pyrolysis of separated digestate solids and experiments of its application to laboratory fermenters will be carried out.
5	prof. Ing. Lucie Obalová, Ph.D.	Removal of persistent pollutants from sewage sludge during their various technological processing with the aim of further utilization of sludge in agriculture	The doctoral thesis will be focused on the degradation efficiency of persistent pollutants present in sewage sludge during various further processing of the sludge. It includes technologies used or potentially usable in wastewater treatment plants (sanitization, drying, heat treatment, etc.). The work will be focused on monitoring the persistent pollutants in the sewage sludge followed by the verification of the effect of individual technologies on the decrease in concentration or transformation of the persistent pollutants (especially drugs and other organic compounds).
6	prof. Ing. Lucie Obalová, Ph.D.	Waste-based photocatalytic reactions for pollutants degradation	Different steps of research will include finding and modifying wastes as the catchment of the reaction (e.g. brick waste, floor ceramic waste, tile wastes, etc); selecting emerging pollutants; examination and optimization of different features effects on removal percentage based on Response Surface Methodology techniques; evaluation of degradation kinetic and equilibrium by classical models and experimental practices; application of machine learning computations for smartening the process; creating a lab-scale setup (column) for the continuous reaction assessment in optimum conditions which are obtained from batch lab scale examinations; mass transfer modeling; evaluation of Circular Economy and Integrated Solid Waste Management as managerial insights because of using wastes.
7	prof. Ing. Lucie Obalová, Ph.D.	Removal of persistent pollutants from sewage sludge during their various technological processing with the aim of further utilization of sludge in agriculture	The doctoral thesis will be focused on the degradation efficiency of persistent pollutants present in sewage sludge during various further processing of the sludge. It includes technologies used or potentially usable in wastewater treatment plants (sanitization, drying, heat treatment, etc.). The work will be focused on monitoring the persistent pollutants in the sewage sludge followed by the verification of the effect of individual technologies on the decrease in concentration or transformation of the persistent pollutants (especially drugs and other organic compounds).

8	prof. Ing. Kamila Kočí, Ph.D.	Heterojunction photocatalysts for photocatalytic generation of hydrogen	Heterojunction photocatalysts allow to influence the efficiency of the photocatalytic reactions by effective electron–hole pairs separation and permit absorption of incident light to form electron-hole pairs in the solar spectral region. The work will focus on fundamental research on novel heterojunction photocatalysts for photocatalytic hydrogen generation from aqueous solutions of alcohols or other organic compounds. The aim of the work will be a comprehensive analysis of the relationship between the preparation of heterojunction photocatalysts, their physico-chemical properties and photocatalytic activity for hydrogen generation.
9	prof. Ing. Kamila Kočí, Ph.D.	Photocatalytic reactions for environmental protection	Photocatalytic processes are particularly promising for the cleaning of air contaminated by pollutants. By using sunlight they can work even without fossil fuels. One of the key factors influencing the efficiency of photocatalytic reaction is a suitable choice semiconductor photocatalyst that is not only satisfying the energy band gap, but especially desirable position of the valence and conduction bands enabling the successful progress of the process. The main goal of the work is to describe the fundamental facet of the effects on the activity of prepared materials in the photocatalytic reduction of CO2 and to clarify the relationship between the activity, selectivity and stability of materials and their physico-chemical properties. A trainer´s workplace is completely equipped for this job.
10	prof. Ing. Petr Praus, Ph.D.	Nanocomposites of MXenes for photocatalytic reactions	MXenes are new and not yet fully explored two-dimensional nanomaterials based on carbides and/or nitrides of transition metals. In 2011, Ti3C2 was synthesized for the first time and since then it has been working on the synthesis of MXenes of various metals. Their physicochemical properties can be significantly influenced by their functionalization with various elements and chemical groups, e.g., due to their electrical conductivity. Photocatalytic reactions are one of little described possibilities of using MXenes. The synthesis and properties of MXenes and their nanocomposites with selected semiconductor materials will be investigated. The resulting nanocomposites will be characterized by common methods and further used for photocatalytic reactions, such as the decomposition of selected organic substances and the generation of hydrogen. New findings are expected not only in terms of the properties of new composite nanomaterials, but also in terms of heterogeneous photocatalysis.

11	prof. Ing. Daniela Plachá, Ph.D.	Preparation of polymer membranes for gas and vapor separation	The dissertation will be focused on the preparation of robust and effective thin-film polymer nanocomposite membranes suitable for the separation of gases and vapors in industrial applications. The prepared membranes will be tested for obtaining and purifying hydrogen and for the separation and regeneration of volatile organic substances and other hydrocarbons. As part of the dissertation, the student will be focused on the preparation of polymer nanocomposites in the form of a thin film, including the selection of suitable polymers and nanofillers, as well as on the study of its physico-chemical, structural and mechanical properties, and subsequently will also test the transport of selected gases. The construction of apparatus for separation processes will also be part of the work.
12	prof. Ing. Petr Praus, Ph.D.	Hybrid composite nanomaterials for photocatalytic applications	Hybrid composite nanomaterials (HCN) of the adsorbent-semiconductor photocatalyst type are multifunctional materials with adsorption and photocatalytic properties. The synergy between these phenomena leads to the emergence of highly efficient hybrid photocatalysts that have higher photocatalytic activity and higher selectivity for the desired types of reactions. The interface created between the two materials can facilitate the transfer of substances from the adsorption centres to the surface of the semiconductor and vice versa. Attention will be focused mainly on metal-free carbon nanomaterials with minimal risk to the environment. In this doctoral thesis, various HCNs will be synthesized and characterized, and their photocatalytic properties will be tested using environmentally significant substances.

Study program: P0713D070002 - THERMAL ENGINEERING AND FUELS IN INDUSTRY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Vlastimil Matějka, Ph.D.	The intensification of the separation of the magnetic phases reached on iron presented in slags from steel production	The slags that originate during the steel production processes are reached in iron, which is presented in different phases. Some of these phases have magnetic properties and can be magnetically separated and the resulting magnetic phase can be used in the process of iron production. The thesis is focused on the searching of the optimum process for the isolation of the magnetically active phases from metallurgical slags. The experiments will include the treatment of the slags using selected milling techniques, flotation, and magnetic separation. In the course of the experiments the magnetic and non-magnetic phases will be achieved and the emphasis will be also placed on the searching of the application possibilities for both fractions. Obtained samples will be characterized using the methods of chemical and phase analysis, the morphology of the particles will be studied using microscopy techniques.
2	prof. Ing. Dagmar Juchelková, Ph.D.	Product optimizing for the thermochemical conversion of biomass/waste into bioenergy	The doctoral thesis will be devoted to the possibilities of thermochemical conversion of biomass and waste for the production of electricity and heat. Special attention will be paid to the appropriate composition of the input raw material and the intensification of the conversion process
3	doc. Ing. Adéla Macháčková, Ph.D.	Features of heat exchange intensification in heat exchangers	The intensification of heat exchange in heat exchangers has an impact on its efficiency, design and reliability when are used in a given technology.The topic of the work is therefore primarily based on the preparation, design and verification of specially prepared surfaces - heat transfer surfaces of heat exchangers so as to increase the thermal parameters (e.g. heat transfer coefficient) and at the same time to comply with the hydrodynamic parameters of the heat transfer medium flow. Unique thermal devices prepared by different technological processes (e.g. diffusion welding) will be investigated.
4	doc. Ing. Adéla Macháčková, Ph.D.	Verification of operating parameters of heat exchanger surfaces of cooling circuits for power plant energy systems	The energy system here is defined as a system of combined energy generation in both conventional and nuclear power plants. The energy systems taking place on a given heat exchanger surfaces use two separate media, which are dynamically changing systems with adequate heat fluxes. The circulation of the media ensures an optimal, economical and trouble-free condition of the power plant as a complex. Therefore, it is important to examine such a energy system, to observe and record its operating parameters and to predict possible future non-integrity and problems on the basis of these parameters. Thus, the topic of this thesis is focused on monitoring the operating characteristics of dynamic systems, especially non-stationary thermal processes with prediction of future situations.

Study program: P0715D130002 - CHEMICAL METALLURGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Kateřina Skotnicová, Ph.D.	Binder systems for diamond grinding tools	The dissertation will focus on the design, preparation and complex characterization of new binder systems based on non-ferrous metals for the diamond grinding tools sintered along the boundaries of diamond grains. Diffusion processes and phase transformations in the systems as Cu-Sn-Ti, Cu-Sn-Co, etc., taking place during the sintering process will be studied in detail. The findings will lead to the development of innovative diamond grinding tools for machining products such as cemented carbides and glass, which will have improved performance, especially lower resistance in machining, improved self-sharpening properties and increased dimensional stability. The structural characteristics, chemical and phase composition of the prepared composite materials will be investigated using scanning electron microscopy, energy-dispersive X-ray spectroscopy, thermal analysis, XRPD, etc.
2	doc. Ing. Lenka Řeháčková, Ph.D.	Rheological properties of silicate melts and their modeling by artificial neural networks	Adequate slag fluidity is crucial for stable iron production. During this process, crystallization of the slag can occur, accompanied by an increase in its viscosity. The aim of this dissertation is to investigate the influence of the slag composition on the temperature dependence of viscosity. The prepared oxide systems will differ in the content of MgO, B_2O3, TiO_2, Na_2O, CaF_2, FeO, and Fe_2O_3. The measurements will be carried out using an Anton Paar FRS 1600 high-temperature rheometer and will be supplemented by a series of "ex situ" analyses such as electron microscopy and energy-dispersive X-ray microanalysis and X-ray diffraction analysis. The measured temperature dependencies of dynamic viscosity, viscosity and flow curves will be fitted to current models for multicomponent oxide systems, including modeling using artificial neural networks.
3	doc. Ing. Vlastimil Matějka, Ph.D.	Synthesis and physicochemical characterization of iron oxides nanocomposites with carbon coatings: FexOy/C used as electrode materials in batteries and supercapacitors	The main aim of the doctoral thesis is to develop cost-effective methods of preparation of nanocrystalline iron oxides and their nanocomposites with carbon coatings: FexOy/C of the appropriate structural and electrochemical properties, which find an application as the electrode materials in batteries and supercapacitors. The materials will be synthesized i.e. using modified sol-gel methods, co-precipitation, hydrothermal or combustion methods. Some part of this research work will be focused to create nanocomposites with carbon coatings, i.e. with MWCNT, rGO or g-C3N4. All the synthesized electrode materials will be extensively characterized using several complementary techniques. The crystal structure of the electrode materials will be analyzed by X-ray powder diffraction combined with Raman spectroscopy techniques, the particle size and morphology will be studied by SEM, TEM, HRTEM. Additionally, BET measurements will be used to control the specific surface area

			and porosity of the synthesized materials. Electrochemical measurements will be performed on the electrode's prepared from the synthesized materials.
4	doc. Ing. Vlastimil Matějka, Ph.D.	The influence of the cooling rate on the amorphous character of metallurgical slags	The main aim of the doctoral thesis is the research focused on the indication of the effect of the cooling rate of molten slags on the formation of the amorphous phase. Blast furnace, steel furnace, and ladle furnace slags will be studied. The chemical composition of the slags will be studied using X-ray fluorescence analysis, and the phase composition will be studied using X-ray diffraction method. The slags will be analysed using the method of simultaneous thermal analysis with the aim of revealing the phase transformations during the heating up to the temperatures of liquidus. Melted slags will be further cooled down with predefined cooling rates and the resulting samples of the slags will be analysed using X-ray diffraction analysis to reveal the effect of the cooling rate on the phase transitions, especially on the content of the amorphous phase. With this approach, the optimum cooling rate, which ensures the amorphous character of given slag will be identified. The chemical composition of the slags, which will not spontaneously form a sufficient amount of the amorphous phase even at the highest cooling rates, will be modified by the addition of selected compounds. To reveal the effect of the modification of the chemical composition of the slags, these modified slags will be subjected again to thermal analysis, followed by X-ray diffraction studies of the resulting products. In a theoretical line, the experiments will be supported with the modelling of the phase transitions with the help of appropriate software, for example ThermoCalc.
5	doc. RNDr. Bruno Kostura, Ph.D.	Study of chemical and physico-chemical processes of processing metallurgical waste focused on circular utilization of waste.	The work will be focused on a comprehensive study of chemical and physico-chemical processes of processing selected solid metallurgical wastes, such as various types of sludge and dust. Mainly hydrometallurgical and pyrometallurgical methods of treatment of these materials will be tested, focusing on the separation of accompanying metals, especially lead and zinc. A detailed chemical and phase analysis of both the original and modified materials, as well as the obtained separates, will be performed. The electrochemical and possibly magnetic properties of the obtained materials will also be studied, all with a focus on their further use. Furthermore, the possibilities of including other types of waste of suitable composition in separation processes will be studied. Elemental analysis of the investigated materials will be performed using the XRFS method, information about their internal structure and phase changes will be provided by X-ray diffraction, SEM analysis, FTIR and Raman spectroscopy. Information on the behavior of materials exposed to temperature regimes will be provided by TG and DTA. Among the electrochemical methods, chronocoulometry and cyclic voltammetry will be used.

6	prof. Ing. Jana Dobrovská, CSc.	Kinetic study of transformation processes of selected metal systems	The applicability of materials depends on their final properties, which are determined primarily by the structure of the material. The resulting structure is also affected by the kinetics of ongoing processes in their preparation. Fe-based materials will be selected for kinetic studies.Experimental thermo-analytical curves measured for various heating/cooling rates using a Setaram SETSYS 18TM simultaneous TG/DTA/DSC/TMA analyzer (20 to 1750 ° C) will be used to study the kinetics and determine kinetic parameters (especially activation energy) of phase transitions. The kinetics of processes during material heating/cooling will be described using selected kinetic models, the selection of a suitable model is a difficult task and requires a good knowledge of the structure of the material and the processes taking place during heating/cooling. The program Thermokinetics SW Kinetics NEO and various types of offered models will be used for kinetic analyzes.
7	prof. Ing. Jana Seidlerová, CSc.	Preparation of slag modification for xenobiotics removal	The topic is focused on preparation and characterization of modified or activated slags that could be used to remove inorganic or organic pollutants. The prepared materials will be tested to use the removal of selected pollutants or groups of pollutants. Modern sophisticated methods of analytical, phase and structural analysis etc. will be used for testing. The determined experimental results will be fitted by suitable physic-chemical models.
8	prof. Ing. Jana Seidlerová, CSc.	Study of organic pollutants formation in recycling processes of metallurgical waste	Metallurgical wastes are an important source of iron. However, their recycling is associated with specific problems, including the generation of gaseous pollutants. The work is focused on the study of gaseous pollutants formation depending on the type of both the recycling process and the processed waste under laboratory conditions. Knowledge of the mechanisms and causes of gaseous pollutants formation could contribute to preventing their occurrence.
9	doc. Mgr. Lucie Bartoňová, Ph.D.	Evaluation of utilization perspectives of industrial wastes	Annually, industrial enterprises produce vast amounts of industrial wastes all over the world. Therefore, further technological utilization of these wastes is a global concern because it not only provides value-added products but also mitigates serious waste disposal problems and, at the same time, facilitates saving natural resources. Industrial wastes exhibit different chemical and physical characteristics depending on their industrial origin and the composition of parent raw materials. For this reason, an optimal utilization approach must be proposed with the view of origin and characteristics of individual waste. To address the aforementioned challenges, the main objective will be to explore the possibilities of utilization of various waste materials and/or their fractions and critical evaluation of corresponding advantages and drawbacks related to their characteristics.

10	prof. Ing. Bedřich Smetana, Ph.D.	Study and development of materials for heat storage and transport technologies	Thesis is focused on the study and development of innovative materials in solid and liquid phase for thermal energy storage, transport and conversion (TESm - Thermal Energy Storage materials and HTF – Heat Transfer Fluids). Aim of the study is obtaining of modified and new stable progressive materials usable in technological applications (e.g. in the field of CSP - Concentrated Solar Power technologies and in other technological fields) with the pottential of more efficient energy storage, transport and conversion. Modification of known and development of new materials with their study will be realised for low (bellow 550 °C) and high (above 550 °C) temperature applications. Experimental study of materials will be realised mainly with use of thermal analysis (TA) and calorimetric methods: DTA, 3D DSC, TG, TG/DTA, TG/DSC a Dilatometry. Theoretical study will be realised also. The subject matter is thermophysical, thermodynamical and kinetic behaviour – properties (behaviour) study of synthesised materials – relation between chemical and phase composition and resulting properties.
11	prof. Ing. Bedřich Smetana, Ph.D.	Development and study of metal hydrides for chemical energy storage and utilization in the field of hydrogen technologies	The substance of thesis is a complex systematic experimental and theoretical research in the field of thermophysical, thermodynamical and kinetic behaviour of Ca(Co)-Mg-Ni based systems and their hydrides in wide temperature region. Metallographic, microanalytical and electronmicroscopy analyses (SEM, TEM, EDS, WDS, EBSD) will be performed to obtain specified aims. Further key experimental study will be realized using methods of thermal analysis (TG, TG/DTA, TG/DSC with MS, High Pressure DSC and DILATOMETRY). Theoretical study will be performed using thermodynamic modelling by Calphad method. The aim of research is development of new materials for hydrogen storage/release and new knowledge regarding thermophysical, thermodynamical and kinetic behaviour of studied systems, description of relations between studied properties (phase transition temperatures, specific heats, CTE, density,…) and chemical, phase composition and structure in wide temperature region. The research subject is also the study of equilibrium phase diagrams and hydrogen sorption process necessary for utilisation in the field of hydrogen technologies.
12	prof. Ing. Bedřich Smetana, Ph.D.	Study of thermophysical properties of advanced materials based on Fe-C-Mo-Ni-Cr with use of thermal analysis methods	Thesis is focused on experimental and theoretical study of thermophysical behaviour of Advanced alloys by precisely defined conditions. Object of the study are systems in solid and liquid phase (in melt) based on Fe-C-Mo-Ni-Cr, which are important also for technollogical purpose. Study will be realised mainly with use of thermal analysis methods: DTA, DSC, dilatometry and excelent experimental systems. The relation between chemical composition, phase composition and structural constituents of studied systems and thermophysical properties is one of the work aims. Experimental results will be supported by results obtained with use of thermodynamical SW Thermo-Calc, JMatPro, IDS, possibly with SW Dictra. Creation of own thermophysical and thermodynamical database is assumed.

			Further aim of the work is the development of methodology of thermophysical properties of materials studied in solid and liquid phase.

Study program: P0715D270007 - METALLURGICAL TECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Ivo Schindler, CSc.	Optimization simulation of hot bulk forming by alternating compression in two directions	Physical simulations of many forming technologies are often significantly limited when a large cumulative strain is required. In these cases, multiple deformations by uniaxial compression or plain strain compression test do not, in principle, sufficiently satisfy the given requirement. This problem is solved by the MAXStrain II mobile exchange unit (unique in the Czech Republic), connected to the Gleeble 3800-GTC simulator, which can handle up to 80 compressions (passes), alternately in two mutually perpendicular directions. It is possible to program various time and temperature regimes of individual passes with different magnitude and rate of strain, or the course of final cooling. An original method of calculating the equivalent strain in individual compressions was developed, which can be advantageously used in simulations of many intensive bulk forming processes, such as continuous rolling, drop forging and free forging. Through the simulation parameters, it is possible to influence the resulting (ultra)fine-grained structure and mechanical properties of the sample, the evaluation of which is effective due to the relatively even strain distribution. The topic of the PhD thesis is formulated in general and assumes the application of the methodology to the selected type of forming technology in combination with specific materials examined (i.e. alloys of non-ferrous metals, steels or metal matrix composites).
2	prof. Ing. Markéta Tkadlečková, Ph.D.	Development of a simulation of the continuous casting process of steel billets	The dissertation aims to develop a simulation of the continuous casting process of steel billets in ProCAST software. The work will focus on the development of geometry preparation, computational mesh, calculation definition, all depending on the expected results. Attention will also be focused on the possibility of defining electromagnetic mixing using a UDF. The results should provide information about the flow in the mould, the solidification character of the continuously cast billet and volume defects.
3	doc. Ing. Silvie Brožová, Ph.D.	Technological, economic and ecological possibilities of extraction of selected heavy metals from industrial wastes	Metallurgy generates large quantities of metal-bearing waste. Deposition on heaps poses an ecological risk to the environment. The metals contained in the waste represent an economically significant source of secondary raw material. The work will also include the energy benefits of recycling. The aim of the work will be to assess the possibilities of recycling metallurgical waste.

4	doc. Ing. Pavlína Pustějovská, Ph.D.	Study of the possibility of testing fine-grained iron-bearing materials	The doctoral thesis will focus on the study of the possibility of testing fine-grained iron-bearing materials and waste. Design of a method and sampling of selected iron-bearing materials and waste. Gain new knowledge by testing prepared samples. Interpretation of the experimentally determined reduction characteristics for real operating conditions. Application of a kinetic model to predict the course of a blast furnace process using manufactured samples. The goal will be to verify the procedures associated with the appropriate treatment of fine-grained iron-bearing waste materials that could be used as part of the charge in metallurgical aggregates.
5	doc. Ing. Petr Lichý, Ph.D.	Study of binder systems of moulding mixtures for the production of cast metallic foams	The dissertation will focus on the use of binder systems (both inorganic and organic) of moulding mixtures for the preparation of porous metallic materials. Metallic foams can have different distributions of internal cavities, which then influence their final properties and applications. The moulding mixtures will thus be evaluated mainly in terms of properties such as: strength, storability, wear resistance, colapsibility, etc. For the future use of these materials, it will also be crucial to evaluate their environmental friendliness.
6	doc. Ing. Ivo Szurman, Ph.D.	Metallurgical aspects of the preparation of special CCA alloys.	The basis of the dissertation will be the preparation of selected special CCA alloys with the use of vacuum induction melting method. Alloying with a small amount of other elements with the aim of modifying the microstructural characteristics is also assumed. One of the main tasks will be monitoring the metallurgical micropurity of the prepared material. The prepared materials will also be subjected to thermomechanical processing and their microstructural and basic mechanical characteristics will be evaluated using standard methods.
7	doc. Ing. Radim Kocich, Ph.D.	The study of possibillities for composites production by technologies based on plastic deformation	Thesis should be focused on theoretical as well as experimental evaluation of composite materials preparation. Each production technology will be evaluated in view of structure as well as properties changes of composites. Among others computer simulations will be used in order to predict material behavior. Obtained values will be compared with the results arisen from numerical predictions.
8	doc. Ing. Radim Kocich, Ph.D.	Analysis of the influence of intensive plastic deformation on structure and properties of selected bio-applicable titanium alloys	Titanium alloys are at present preferred in medicine especially due to their favourable properties. They have a wide range of application, from dentistry to orthopaedics. Nevertheless, each type of application demands slightly different properties of the given product, which goes hand in hand with variations in structure. The dissertation work will be focused on characterization of selected titanium based alloys subjected to the influence of intensive plastic deformation. Plastic deformation will be imparted into the processed materials via conventional, as well as unconventional forming technologies. The emphasis of the work will be on the analysis of mechanical properties and structure changes related to the particular applied deformation technology. Besides, verification of the influence of

			deformation ratio and the method of imposing the strain into the material on deformation parameters is planned to be performed.
9	doc. Ing. Radim Kocich, Ph.D.	Design and development of data assembling methodology for rheological law valid for very high strain rates	The aim of these thesis would be in the design and development of methodology leading to achievement of data necessary for chosen mathematical models assembling that describe deformation behavior of chosen materials in broader range of temperatures. For these purposes will be part of work carried out on equipment enabling realization of high speed deformation tests. These aims would be reached also by numerical simulation based on FEM software utilization. Besides, interest will be paid also on the application of newly developed modules aiming to description of phenomenon accompanying these forming processes from view of structure development.
10	doc. Ing. Radim Kocich, Ph.D.	The possibilities of forming methods application in ODS materials with higher thermal resistance manufacturing	The aim of these thesis would be in the study of effectiveness of chosen forming processes in view of their suitability for compact bulk materials. Besides, interest will be paid on the grain refinement effectivity or more precisely on final properties. Among others, conventional as well as unconventional forming methods will be studied. Main attention would be paid on monitoring of mechanical properties in particular under higher temperatures. The focus will be devoted also to the possibility to spread these manufacturing methods into commercial scale.

Study program: P0719D270003 – NANOTECHNOLOGY

No.	Supervisor	Title of dissertation thesis	Annotation
1	prof. Ing. Daniela Plachá, Ph.D.	Study of adsorption properties of 2D nanomaterials	As part of the dissertation, the interactions of organic molecules with the surface of 2D nanomaterials will be studied. The surface of these materials spontaneously reacts with molecules present in the environment, which affects their further storage and processing, as their properties are significantly affected, e.g. wettability, adhesion, electrochemical properties and also the adsorption properties themselves. Selected organic substances and 2D materials, their mutual interactions and changes in properties will be studied in the thesis. Experimental results will be compared with theoretical calculations of molecular calculations and simulations.
2	prof. Ing. Daniela Plachá, Ph.D.	Study of properties of sorbents based on carbon foam	As part of the dissertation, chemical modifications of carbon foam will be performed using various nanoparticles to improve sorption or catalytic properties leading to effective removal of inorganic and organic pollutants from water and air. Nanoporous carbon foams will be prepared from natural substances and subsequently modified and characterized in terms of physicochemical, structural and sorption properties. The dissertation will be developed in close collaboration with Northumbria University, Newcastle upon Tyne, UK.
3	prof. Ing. Daniela Plachá, Ph.D.	Preparation of polymer nanocomposites with antimicrobial effects	As part of the dissertation, polymeric biocompatible nanocomposites with antimicrobial effects with a wide range of applications will be prepared, eg for the preparation of support scaffolds for cell growth with the possibility of using 3D printing or for other biomedical applications. The use of various nanofillers, optimization of material composition and subsequently physicochemical, structural, mechanical, antimicrobial, and cytotoxic properties of prepared materials will be studied. Based on the identified properties, suitable applications will be designed and tested. The dissertation will be prepared in cooperation with ICTP / CSIC in Madrid.

4	doc. Dr. Mgr. Kamil Postava	Mueller matrix polarimetry and microscopy of Twisted light	Nowdays, the progress in wavefront modification have enabled complex classes of Twisted Light which carry spin and orbital angular momentum, offering new tools for light-matter interaction, imaging, detection, communication, and security holograms applications. Spin angular momentum (SAM) arises when the electric field vector traces a helical path with propagation, and takes the values of $\pm\hbar$ per photon, depending on the polarization handedness (i.e., right- or left-hand circular polarization). Orbital angular momentum (OAM) is the phenomena, where the wavefront carries a phase singularity. This is typically realized when the wavefront has helical form producing a one-dimensional (1D) phase singularity - a line of undefined phase (and zero intensity) along the optical path. In this case, the Poynting vector precesses around the phase singularity and producing a donut-like intensity profile, also known as an optical vortex. The proposed Ph.D. thesis is focused on study of metasurface structures for generation of OAM Twisted light. For the numerical modelling, the CST Microwave studio (or COMSOL multipsysics) will be used. The modeled structure will be developed by UV laser direct write optical litography. Methods of Mueller matrix spectroscopy and polarimetric microscopy will be used for optical characterization of the fabricated OEM structures.
5	doc. Dr. Mgr. Kamil Postava	Ultrafast properties of spin lasers with periodic gratings: Novel concepts in data transfer technology	Spin-lasers are semiconductor devices in which recombinations of spin-polarized electrons in active region (quantum wells and dots) lead to emission of circularly-polarized photons. The possibility of using and modulate spin-polarized electrons together with including low-dimensional nanostructures (periodical gratings, quantum wells, quantum dots) opens new horizons in modern semiconductor research and information technology. Proposed doctoral thesis will be focused on theoretical and experimental study of steady-state and dynamical effects in such advanced structures together with their optimalization for ultrafast modulation, terahertz generation and secure data transfer. Theoretical models for generation of light from the structures of spin-lasers and thin-film lasers with lateral periodic and aperiodic structures will be applied and generalized. Designed structures will be prepared using technologies at VSB-TUO and foreign collaborating laboratories and their polarization, spectral, and dynamic response will be measured.
6	doc. Dr. Ing. Michal Lesňák	Application of the SPRi method	The subject of our research will be to design biochips for the SPR (surface plasmon resonance) method to measure low concentrations of proteins in solutions. This measurement method can be advantageously used in biochemistry, medicine, pathogen detection in food or military applications. Our method mainly consists of measuring low concentrations of proteins (large organic molecules) in various solutions. Improving the accuracy and speed of measuring low concentrations of proteins in solutions could have a major impact on the quality of medical care provided in hospitals. After discussion with physicians, we decided

			to focus on the detection of ovalbumin, human serum albumin (HSA) in urine and Cystatin-C.
7	doc. Dr. Mgr. Kamil Postava	Advanced diffraction optical structures in security holography	The main target of the thesis is to design new diffracting structures for applications in security holography. The structure will exhibit special colour effects, 3-dimensional animation effects, polarization selectivity, and light capture. The sample structure will be prepared using laser lithography and physical vapor deposition.
8	prof. Ing. Kamila Kočí, Ph.D.	CO_2 transformation to valuable chemicals by photocatalytic processes over highly active materials	The main goal of the work is to describe the fundamental facet of the effects on the activity of prepared materials in the CO_2 transformation and to clarify the relationship between the activity, selectivity and stability of materials and their physico-chemical properties.
9	doc. Dr. Mgr. Kamil Postava	Properties of ultrafast spin-orbit current in magnetic multilayers	Dynamics of spintronic and spin-transport phenomena will be studied using pump-probe technique based on ultrashort pulsed laser beam. The pumped electric pulse will be obtained using Auston switch. Probe beam delayed by optical delay line will inspect magnetic state using magneto-optical effects. Testing structure will be prepared using advance lithography.
10	doc. Dr. Mgr. Kamil Postava	Advanced diffraction optical structures in security holography	The main target of the thesis is to design new diffracting structures for applications in security holography. The structure will exhibit special colour effects, 3-dimensional animation effects, polarization selectivity, and light capture. The sample structure will be prepared using laser lithography and physical vapor deposition.
11	doc. Ing. Jonáš Tokarský, Ph.D.	Molecular simulation of adsorption on nanocomposite adsorbents and adsorbents prepared from natural materials	The subject of the dissertation is to compare different strategies for simulating the adsorption of molecules on materials with complex and/or difficult to define structure (natural phyllosilicates intercalated and surface modified with organic substances, core@shell structures, activated carbon, etc.). Adsorption simulations on large and complex models of adsorbent structures (very time consuming) will be compared with adsorption simulations on simplified models in order to achieve comparable results and find the optimal degree of simplification. The aim of the dissertation is to find simple and fast simulation strategies providing sufficiently accurate results for given types of adsorbents.

12	prof. Ing. Lucie Obalová, Ph.D.	Preparation of heterogeneous catalysts based on transition metal oxides and lanthanides enriched with active species for catalytic oxidation of volatile organic compounds	The doctoral work will bring new knowledge about the effect of preparation and chemical composition of heterogeneous supported catalyst on its physico-chemical properties (micro/structure, acidity, reducibility etc.) and catalytic activity in oxidation of volatile organic compounds (VOCs) often used as solvents in pharmaceutical industry. In the frame of the work the catalyst preparation and chemical composition will be optimized in order to achieve catalyst highest performance from the view of catalytic activity as well as selectivity and durability. The attention will be also dedicated to the description of oxidation mechanism of selected VOCs on the developed heterogeneous catalyst. Within the catalytic experiments the oxidation of dichloromethane, formaldehyde or toluene will be investigated. Student will partially do the experimental work in cooperation with foreign university via the short-term student stays.
13	prof. Ing. Jana Seidlerová, CSc.	Biosynthesis of metal nanoparticles by plant biomass and study of nanoparticles formation	The biological way (bioreduction) is an alternative method for nanoparticles preparation. The main goal of this work will be the preparation of metal or metal oxides nanoparticles by biosynthesis (bioreduction) with plants extracts, identification of phytochemicals and other biomolecules which are participating in the bioreduction process and the clarification of the particular biosynthesis mechanisms.
14	Mark Hermann Rümmeli	Synthesis of novel chemically doped graphene and their application	In this project a hybrid chemical vapor deposition/chemical vapor transport fabrication approach will be implemented for the synthesis of chemically doped graphene with novel elements. For example, Be is predicted to be an exciting doped graphene for electrochemical application, but has yet to be synthesized. The potential of the synthesized doped graphene's in applications will be explored in areas such as gas sensors, CO_2 capture and as active electrode material in ion batteries.
15	Mark Hermann Rümmeli	Electron beam manufacture of doped graphene from electron beams	This project explores the use of different composite polymer/metal-organic films deposited on various substrates and the role of electron beam irradiation with and without heating for its local doped graphitization with precision. Different electron beam conditions and temperatures are to be explored systematically through various characterizations as well as complimentary ex situ synthesis to provide a comprehensive understanding of the underlying graphitization mechanisms.
16	Mark Hermann Rümmeli	Chemical vapor deposition (CVD) of novel substitutional graphene and advanced characterization	This project explores the use of different precursor phases (liquid, solid, gas) for the fabrication of novel metal dopants in graphene. The systematic evaluation of the growth mechanisms will lead to a comprehensive understanding of the growth mechanisms. The work will also involve training and characterizations by aberration corrected transmission electron microscopy and will involve visits to collaborative institutions for training and measurement.

17	Mark Hermann Rümmeli	In situ synthesis and engineering of novel mono and hetero two dimensional materials	In this project a variety of systems will be explored to drive the synthesis and engineering of two dimensional (2D) materials inside a transmission electron microscope (TEM). This will entail the fabrication and engineering of 2D materials using electron beams and heat as well as gas injection in situ in a TEM using custom build TEM specimen holders/reactors. The studies should lead to deep insight to the processes at the atomic scale.
18	prof. RNDr. Richard Dvorský, Ph.D.	Preparation of sorption nanostructures with photocatalytic regeneration	Sorbents for water treatment and air cleaning is necessary to replace after saturation and dispose of the exposed material. More economic is application of photocatalysis for permanent regeneration by dissociation of pollutants directly on the sorption surface. Very economic process would be regeneration by Solar illumination. The sorption material suitable for photocatalytic regeneration has been prepared in our laboratory and further research is focused on increasing of sorption capacity based on patented method of controlled sublimation.
19	doc. Ing. Gražyna Simha Martynková, Ph.D.	Membrane composites with nanofibers for the batteries	The doctoral thesis is focused on the preparation, study and characterization of membrane nanocomposites for parts of batteries, namely flow-through batteries (Redox-flow batteries (RFB) and parts of Li-batteries (LiB), where the membrane is a separator. Nanocomposite membranes will contain carbon nanoparticles and other suitable layered nanomaterials embedded in the matrix to improve membrane properties. Conventional MIVs are of ionic polymers such as sulfonated tetrafluoroethylene polymers with the drawbacks of relatively low ion selectivity and reduced material stability (co with Prof Ramani, WU, USA). The topic of separators in LiB is period where the development of a selective membrane that would extend the cycling life of rechargeable batteries by preventing the formation of unwanted dendrites (in collaboration with dr Slavík, Theion, Germany) By combining advanced technologies together with nanotechnologies, a membrane with stable chemical and thermal properties for specific batteries ity molecular modeling approaches, where optimal physical and structural parameters will be modeled based on the experiment.
20	doc. Ing. Gražyna Simha Martynková, Ph.D.	Nanoporous carbon for bones scaffolds	The thesis is focused on the study and research of meso and nanoporous carbonaceous material with graphitic structure. The preparation of the material is accomplished by carbonization of the macromolecular precursor material and high temperature treatment in an inert atmosphere. Carbonized material is used as scaffold for dental or small bones, and it is densified with biopolymer such as collagen for better biocompatibility and bioceramic for regeneration. The testing of biostability and structural properties will be one of the main goals. The evaluation of biocarbon materials will be characterized using the following methods: porosimetry, XRD, SEM with AFM, XRFS, ICP.

21	doc. Ing. Gražyna Simha Martynková, Ph.D.	Biocompatible hydroxyapatite ceramics and its composites with a biogenic component	The doctoral thesis will focus on the synthesis and preparation of hydroxyapatite ceramics for dental and orthopedic prosthetic use, as well as characterization in terms of structure and chemistry, and evaluation of application parameters. The prepared ceramic via chemical route will be tested for biocompatibility. The aim is to create material with improved mechano-chemical parameters, increased biocompatibility and the possibility of integration with living tissue. The prepared ceramics will be modified with various types of organic substances, especially to increase the antimicrobial and regenerative ability of the final product in the body.
22	doc. Ing. Gražyna Simha Martynková, Ph.D.	Application of nanometal particles in conductive polymers for energy applications	The work is focused on the special topic of incorporating metal nanoparticles into various alternatives of bio-polymer matrices and their copolymers. The composite will be in the form of a thin foil or fiber fabric. A set of nanometals -Ag, Cu and Ti- is homogeneously dispersed in the matrix. Metal nanoparticles are prepared in a bio-sustainable way without toxic substances. The composites will be tested for electrical and mechanical parameters. The characterization of nanocomposites is focused on the morphology of the surface of the composite, dispersion of nanoparticles and changes in the phase composition of individual components. An intensive study of component interactions will be complemented by modeling.
23	doc. Dr. Mgr. Kamil Postava	Optimization and design of metasurface and diffracting surface using artificial intelligence	Metasurfaces and diffracting optical surfaces have a wide potencial in planar imaging optics, polarization devices, metrology, and safety elements. The thesis is focused on parametrizing the structure, calculation of optical response, and structure optimization using genetic algorithms and supercomputer facility.
24	prof. Ing. Jana Seidlerová, CSc.	Stability study of functional nanocomposites	Due to their structural arrangement, clay minerals can be carriers of specific inorganic and organic compounds that can alter their properties. By anchoring molecules on the surface or by intercalation, specific adsorbents or photocatalysts can be prepared. Such a composite must not only have good adsorption, photocatalytic properties, or both adsorption and photocatalytic properties, but must also be stable in each environment. The aim of this work is to prepare a specific nanocomposite and subsequently to observe and describe its behaviour in the environment, to design and validate a method by which stability could be routinely tested.

25	Ing. Dominik Legut, Ph.D.	Heat transfer in advanced nuclear fuels	The uranium, plutonium, and thorium carbides as well as the mixed uranium-plutonium carbides are currently being widely studied for their potential application as fuel for propulsion systems and advanced nuclear fuels in the so-called generation-IV reactors with high operating temperature (to maximize efficiency). The advantage over the uranium/plutonium oxides is in higher thermal conductivity and much shorter time of radiating burned fuel to store before getting to radiation background levels (20-30 years). The goal of this Ph.D. thesis is to understand and determine the rules of Nature how to maximize the transfer of the energy (thermal conductivity) by means of quantum-mechanical and molecular dynamical calculations at the IT4 Innovations on HPC clusters. More info at www.md-esg.eu.
26	Ing. Dominik Legut, Ph.D.	Modelling of THz laser sources	The energy conversion of between various vibration modes are govern by their coupling and the relaxation time of these modes (their mutual scattering). In this PhD work, based on the quantum mechanical simulations of the anharmonic vibrational effects we will shed a light to the principles how to enhance selected vibration modes to generate THz radiation in solids. For this purpose we will utilize the HPC clusters at IT4Innovations with the state of the art codes for anharmonicity treatment and post-processing. More info at www.md-esg.eu
27	Ing. Dominik Legut, Ph.D.	Design of novel materials for thermonuclear reactors	The purpose of this work is to design novel materials for the plasma-to-coolant heat transfer in the thermonuclear fusion reactors. The expected outcome is a set of experimentally confirmed alloys (together with our team at the Institute of Plasma Physics of the Czech Academy of Science in Prague) able to withstand a critical malfunction (Loss-of-coolant Accident) - the conditions comparable to the ones in Sun's core. The student will perform the calculations on the state-of-the-art HPC clusters located at the IT4Innovation National Supercomputing Center. More info at www.md-esg.eu.
28	Ing. Dominik Legut, Ph.D.	Multiscale modeling of coupling phenomena in magnetic material	The objective of this PhD project is to apply advanced modeling approaches and associated numerical tools for a complete fundamental understanding of coupling phenomena in magnetic materials across length scales using HPC clusters located at the IT4Innovation National Supercomputing Center. The project deals with the design of novel permanent magnets with less content or none of the critical and expensive rare earth elements like Nd or Sm. More info at www.md-esg.eu

29	Ing. Dominik Legut, Ph.D.	Modeling thermodynamic properties of liquid-solid interface	The aim of the PhD research is to study the thermal and transport properties of molten salts in the next generation thermonuclear reactors by means of numerical simulations. At the atomistic level, the intrinsic physical properties of crystalline phases of LiF-BeF2 systems will be investigated with ab-initio quantum mechanical calculations. At the nanoscale level, the thermal and transport properties will be studied by large-scale molecular dynamics simulations of the solid-liquid interface between crystalline and molten fluoride salts. The projects aims in general to detemined the eutectic point of two phases and be able to model purely from calculations properties of matter close to melting temperatures.

Study program: P0788D270004 - MATERIAL SCIENCE AND ENGINEERING

No.	Supervisor	Title of dissertation thesis	Annotation
1	doc. Ing. Vlastimil Matějka, Ph.D.	The utilization of the metallurgical slags as the abrasives and fillers	The slags from the metallurgical industry represent valuable by-product. Part of these slags is recycled directly in the place of their origin; other important application area is the building industry. Although the efforts is to utilize the slags in the highest possible level, there is still the part of the slags, which are stored on the landfill. Implementation of the slags as the abrasives and fillers in polymer composites is the other way to increase their material utilization. Within the frame of the PhD thesis the selected metallurgical slags will be tested as the abrasives and fillers in the formulation of Cu-free friction composites. Experimental part of the thesis will be conducted in the collaboration with University of Trento (Italy).
2	doc. Ing. Kateřina Skotnicová, Ph.D.	Preparation of sintered magnets based on Nd-Fe-B with reduced content of rare earth metals	The dissertation will focus on the development of physico-chemical and technological bases for the preparation of sintered magnets based on Nd(R)-Fe-B (R = Nd, Pr, Dy, Tb, Ho) with reduced content of rare earth metals with a variable set of functional parameters for a wide range of applications, i.e. both high magnetic energy and thermostable with high coercive force due to the use of different alloying additives in a matrix alloy. The main research activities will include the study of the effect of principal manufacturing parameters of magnetic materials based on $R_2Fe_{14}B$ intermetallic compound (R = Nd, Pr, Dy, Tb), i.e. conditions of powder material preparation, alloying method, alloying composition, sintering and heat treatment conditions, on forming optimal structural state of main magnetic phase grains. Attention will be paid to the investigation of phase transformations and diffusion processes that occur during the formation of intergranular phases and 2-14-1 phase grains during the mechanical activation and sintering. Structural characteristics, chemical and phase composition will be investigated using scanning electron microscopy, energy dispersion spectrometry, thermal analysis methods, X-ray powder diffraction, Mösbauer spectroscopy, etc. Magnetic properties will be studied using a vibrating sample magnetometer and an automatic hysteresisgraph

3	doc. Ing. Kateřina Skotnicová, Ph.D.	New types of metallic binders based on non-ferrous metals for diamond grinding tools	The dissertation will be focused on the design and complex characterization of new binder systems based on non-ferrous metals for the preparation of diamond grinding tools sintered along the diamond grain boundary. Diamond grinding tools with a metal matrix show good shape retention due to its high strength and stiffness. Therefore, they are mainly applied in precise and ultra-precise grinding processes. The solution will include the design and optimization of the chemical composition of the metal matrix, which will be supported by thermodynamic and phase diagram calculations for multi-component systems using Thermo-Calc and Calphad software, as well as structural and phase analyses, the study of phase transformations and diffusion processes, etc. Knowledge will be obtained about the influence of the chemical composition of the matrix based on non-ferrous metals, the ratio of individual components of the matrix/diamond, pressing pressure, temperature, time and sintering atmosphere on achieving the required strength and functional properties of diamond tools. Structural characteristics, chemical and phase composition will be investigated using scanning electron microscopy, energy dispersive spectrometry, mercury porosimetry, helium pycnometry, methods of thermal analysis, X-ray. diffraction analyses, etc.
4	Ing. Martin Négyesi, Ph.D.	Study of specimen size effect on tensile test results	When examining degradation processes of industrial facilities, the influence of microstructure on mechanical properties is of a high importance. The knowledge of tensile properties is necessary to accurately assess a degree of deterioration and assure the integrity of studied components. Generally, tensile properties are assessed by standardized tensile tests using standard size specimens. However, a caution needs to be paid when transferring data from tensile tests to real size components. Frequently, a lower volume of material is available for testing, so that miniaturized specimens must be manufactured instead of standard size specimens. Then, the size effect needs to be considered. The objective of this study is to examine the influence of specimen size and shape on tensile test results. Materials under test will be commonly used structural steels, as well as other non-ferrous metals such as aluminium or nickel alloys. The emphasis will be put on the effect of microstructural characteristics, especially the grain size. High temperature annealing at various temperatures and times will be applied in order to produce various sizes of grains. Relationships between structural characteristics, specimen size and shape and tensile properties will be searched for. Standardized tensile testing, light optical microscopy and scanning electron microscopy will be employed in the study. The data will be evaluated by the Weibull stress approach coupled with the finite element analysis.

5	Ing. Martin Négyesi, Ph.D.	Influence of adjoining flaws on fracture behaviour of structural components	The fracture behaviour of structural components caused by single flaw can be well predicted nowadays. However, more adjoining flaws are frequently found in structural components. The adjoining flaws interact together and their resulting effect on the fracture behaviour may become stronger. Estimates of the fracture behaviour caused by adjoining flaws still lack sufficient accuracy. Current criteria are either too conservative or, on the other hand, give non-conservative estimates. The aim of this study is to shed more light on the issue of adjoining flaws and contribute to the refinement of the current criteria. Effects of the distribution and sizes of the adjoining flaws on the fracture toughness will be investigated. New fracture criteria will be proposed and parameters with major role on the flaw growth will be identified based on the results of this study. The study will also deal with specimen manufacturing which is challenging and needs a special technique to be employed. Steel plate specimens with surface or through-thickness flaws will be preferentially tested. Specimens will be introduced into tensile and bend testing with monotonic loading. The effect of microstructure on the growth of adjoining flaws will be also treated by employing the fractographic analysis. FEM analyses will be used in order to reduce the number of experiments.
6	prof. RNDr. Radek Zbořil, Ph.D.	The development and chemical modification of new 2D materials based on graphene for applications in energy and catalysis	PhD study will be focused on development of new 2D materials based on chemistry of fluorographene and graphene acid. These new derivatives will act as substrates for the covalent immobilization of single metal atoms and they will be tested in several applications including energy storage, electrocatalysis and heterogeneous catalysis. The specific attention will be devoted to relationship between chemical/structural properties of new 2D systems and their efficiency in energy-related and catalytic technologies. The student will receive the unique expertise in synthesis of new 2D systems combining approaches of materials chemistry and colloidal chemistry, in materials characterization (e.g. HRTEM, XPS, XRD, SEM, AFM) and their testing with the use of electrochemical, chromatographic and spectroscopic techniques.

7	prof. RNDr. Radek Zbořil, Ph.D.	Deposition and chemical routes of materials for the effective transformation of solar energy	PhD study will deal with chemical routes and deposition methods for synthesis of various semiconductors (TiO2, BiVO4, Fe2O3), which are applicable in photocatalysis and photoelectrochemistry including the technologies of direct solar splitting of water (pure hydrogen production) or photoreduction of CO2. The student will receive the expertise in advanced synthesis of layered semiconductors via magnetron sputtering technique and materials characterization with a broad portfolio of characterization techniques (e.g. HRTEM, XPS, XRD, SEM, AFM). The approaches of defect engineering and post-processing chemical insertion of single metal atoms will be applied to enhance the efficiency of solar energy harvesting. The specific attention will be devoted to mechanism of action of new nanomaterials combining experimental approaches and theoretical calculations in collaboration with IT4I.
8	prof. Ing. Bohumír Strnadel, DrSc.	The effect of residual stress on fatigue characteristics in structural steels	The study is focused on investigation of fatigue strength of ferritic-pearlitric steels when residual stress acts in microstructure. This effect is investigated in dependence of various parameters in loading such as stress ratio or stress amplitude.
9	doc. Ing. Soňa Rusnáková, PhD.	Experimental Observation of Composite Structures with Pre-Cured Preforms	The aim of this doctoral topic is to study interface between pre-cured preforms and subsequently cured composite material. Except of multiscale cure process with experimental observation the quality of adhesion will be investigated. The research will be focused on development of interfaced properties between various pre-cured and uncured preforms, to explore the possibilities of increasing adhesion and to real integration of developer pre-cured preform during manufacturing. During manufacturing the focus will be on vacuum infusion technology and autoclave processing. The novel strategy consists on developed knowledge will be formulated and verified on real experimental part.