PROJECTS OF THE INSTITUTE OF MATERIALS SCIENCE

Project Title The effect of microstructure and phase composition on corrosion resistance of hot dip alloys

doc. Ing. Martin Kusý, PhD. Coordinator 01/01/2018 Start Date End Date 31/12/2021 Program VEGA

Annotation The submitted project focuses on the detailed study of microstructure and phase composition of Zn and Al alloy for hot dip coatings. Microstructural characteristics, changes in phase composition, solid solution supersaturation and texture will be analyzed in relation to the resistance of the analyzed corrosion resistant alloys. The alloys will be prepared by rapid solidification processes in bulk, suitable for more complex microstructural analyzes, but also in the form of thin coatings made by dipping in molten alloys. The rapid solidification as an alloy preparation process was chosen because of the similarity with the hot-dipping processes on the continuous production lines. We study in detail the simple system based on the reactive diffusion couple Fe-Zn, which we describe in after equilibrium and nonequilibrium solidification via suitable thermodynamic models using the Calphad method. These will then be used to model the microstructure by the Phase Field method implemented in the Micress program.

Project Title Materials design of high-entropy alloys and their characterization

Coordinator RNDr. Pavol Priputen, PhD. Start Date 01/01/2018

31/12/2021 End Date

Program VEGA

- Annotation
- The goal of the work is to design and prepare series of high-entropy alloys in the form of bulk alloys, as well as thin films and to do basic characterization of their structure, phase constitution and properties. The bulk alloys will be prepared by arc and/or induction melting, while the thin films will be prepared by magnetron sputtering and ion implantation. For structure and phase constitution analysis, electron microscopy, x-ray diffraction, electron diffraction, and energy dispersive x-ray spectroscopy techniques will be used. Among the properties studied, the attention will be focused particularly on mechanical properties (hardness, toughness and strength), chemical properties (corrosion resistance), and physical properties (thermodynamic stability). The project is oriented on fundamental research with regard to practical applicability of the results achieved. Obtained findings will be published in in peer-reviewed journals from CC database and presented at international scientific conferences.

Project Title Research of possibilities of Al-Ti-N based hard coatings thermal oxidation stability enhancement

Coordinator prof. Ing. Ľubomír Čaplovič, PhD. Start Date 01/01/2019 31/12/2021 End Date Program VEGA

Annotation The project is focused on a development and characterization of hard coatings produced for tool materials and characterized with enhanced thermal and oxidation resistance. It is based on the current knowledge in the field of influence of alloying elements such as B, La, V, Ta and W on increasing of Ti-Al-N coatings oxidation resistance. Two technological processes (cathodic arc vacuum and magnetron sputtering) will be involved for depositions of functional coatings and evaluation of alloying elements effect on increasing of thermal resistance and nanostructured morphology of such fabricated coatings. The most advanced analytical techniques, such as HRSEM, HRTEM, EBSD, XRD, PIXE, RBS and tribological tests will be used for coatings characterization. The aim of the project is a development of new advanced coatings designated for tool materials and characterized with excellent tribological and thermal properties

Project Title Determination of optimal cryogenic treatment regime for tool steels

Coordinator prof. Ing. Peter Jurči, PhD. Start date 01/01/2020 End date 31/12/2023

End date 31/12 Programme VEGA

Annotation The projekt is focused to in-depth investigation of phenomena that occur in selected chromium-vanadium ledeburitic tool steel as a result of different regimes of cryogenic treatmnent. Effects of important processing variables like the austenitizing temperature, temperature and duration of sub-zero treatment, and tempering regimes on the microstructure, hardness, flexural strength, fracture toughness, wear performance and corrosion resistance of examined steel will be determined within the project. This would lead to better exploitation of the potential of cryogenic treatment for tool steels. A great number of experimental techniques will be used in the project, which enables to achieve the main scientific goal – to confirm the scientific hypothesis on possible simultaneous enhancement of normally conflicting properties like hardness and wear resistance on the one side, and the toughness on the other side, for selected Cr-V ledeburitic steel by using the cryogenic treatment.

Project Title Physical properties of heavy metal oxide glasses

CoordinatorMgr. Ondrej Bošák, PhD.Start date01/01/2020End date31/12/2022ProgrammeVEGAAnnotationThe project is focused or

ion The project is focused on the study of special glasses designed for applications in photonics and optoelectronics including the central area of the infrared area of the spectrum. New ternary glasses based on TeO2 and Sb2O3 will be prepared on the basis of international cooperation. In the first part, selected physical properties of glasses will be characterized. In the framework of the project solution, effects of changes in the glass composition, observable changes in structure, and the possibilities of rare earth elements doping will be investigated by using electrical and dielectric methods. The next part will examine the influence of technological parameters of glass preparation, possibilities of diagnostics and prediction of achieved quality by monitoring of selected electrical parameters.

Project Title Thermal stabilization of high-temperature superconducting tapes for fault

current limiters

Coordinator Dr.-Ing. Marcela Pekarčíková

Start Date 01/01/2021

End Date 31/12/2024

Program VEGA

- Annotation Additional thermal stabilization is necessary for commercially available hightemperature superconducting tapes, in order to use the tapes in devices for fault current limiting in high-voltage grids. The proposed project is aimed at fabrication of thermally stabilizing composite coating (epoxy resin with ceramic filler), which will act as a sink and absorber of the heat produced in a limiting event. Various materials for thermal stabilization will be tested, with regard to their thermal, physical, and mechanical properties, and their resistance against thermal shocks. Possibilities for improvement of mechanical properties will be investigated by additional reinforcement of the thermal stabilization. The effectivity of the thermal stabilization will be determined for superconducting tapes from various producers, by experimental limiting of fault current. Experiments will be complemented with numerical modelling.
- **Project Title** Research on hybrid manufacturing of the components by means of progressive overlay welding methods

Coordinator Ing. Martin Sahul, PhD. Start Date 01/01/2021

End Date 31/12/2024

Program VEGA

Annotation Additive manufacturing (AM) is a relatively new idea applied to the production of complex metal parts by "layer by layer" method. The project is focused on AM of components using Wire and Arc Additive Manufacturing (WAAM). MIG and CMT overlay welding methods will be used to produce 3D components. Proposed aluminium alloy and austenitic stainless steel will be used as welding materials. During the WAAM process, the parameters of overlay welding will be monitored, molten pool will be online analysed by means of a high-speed camera and the measurement of the temperature fields by thermocouples will be carried out. Light microscopy and mechanical testing will be used to characterize the deposited components. State-of-the-art analytical techniques (SEM, TEM, EBSD, and X-ray diffraction) will be used for more detailed analysis.

| Project title | E-learning and implementation of information technologies in teaching of materials-technology courses | |
|---------------|--|--|
| Coordinator | doc. Ing. Roman Moravčík, PhD. | |
| Start Date | 01/01/2020 | |
| End Date | 31/12/2022 | |
| Program | KEGA | |
| Annotation | The project is focused on the implementation of e-learning in the teaching and examination process in materials-oriented courses such as Materials Science I, Mechanical Testing and Defectoscopy of Materials, Heat Treatment and Surface | |

Treatment of Materials and Thermodynamics and Kinetics, taught at the Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava (MTF STU).

Project title Development of the Fe based PM components with increased fatigue strength.

Coordinator doc. Ing. Martin Kusý, PhD. Start Date 01/07/2019 End Date 30/06/2022

Program APVV

Annotation The problem of the current serial production of PM-based Fe parts in the case of uniaxial single compression in combination with sintering, calibration and heat treatment for commercially used powder mixtures (in particular FeCu1.8C0.7 and FeMo0.5Ni0.5C0.6) is its density in range 6.9 -7.1 g.cm-3. In the case of the use of such components for the "high-performance" applications in engines and transmissions where resistance to dynamic load, high strength or fatigue properties is required, residual porosity is a limiting factor. The aim of the present project is therefore to develop PM-based Fe parts with a higher density > 7.4 g.cm-3 in series production to reduce porosity (mainly open and bonded pores) and its potential use in "high-performance" applications. With regard to the manufacturing infrastructure of Miba Sinter Slovakia Ltd. (subcontractor of the project), it is necessary to examine in detail the impact of the modification of the powder mixture (with respect to the amount of lubricant) and compression parameters (pressure and velocity) on residual porosity and fatigue strength. However, production technology must be designed with respect to the quality of the die, which is currently designed to working pressure up to 600 MPa.

Project title Study of non-conventional glasses modified by ion exchange or ion implantation

| Coordinator | Mgr. Ondrej Bošák, PhD. |
|---------------|--|
| Start Date | 01/02/2020 |
| End Date | 31/12/2022 |
| Program | APVV |
| Annotation | The proposed project deals with the modification of surface of chalcogenide glasses by Na and K cations doping in order to modify their refractive index and/or their electrical conductivity. Glass samples will be prepared, modified by ion exchange or ion implantation and next they will be tested for their optimal functionality. Electrical and dielectrical properties will be used for characterization of ion content and transport in the investigated glasses. Analyses will be focused on the so-called phenomenon mixed-alkali effect. Surface of glasses prepared by ion implantation will be analyzed by RBS/ERDA and PIXE spectroscopy. |
| Project title | Preparation and chracterisation of disordered materials for aplication in |
| | infrared spectra |
| Coordinator | doc. RNDr. Vladimír Labaš, PhD. |
| Start Date | 01/03/2020 |
| End Data | 21/12/2022 |

End Date 31/12/2022 Program APVV Annotation Project is oriented on support of scientific cooperation of institutes from four contries and education of Ph.D. students in the field of special glasses. By using international cooperation, new glass systems based on chalcogenides and heavy metal oxides will be prepared. The thermal, optical, structural and electrical properties of prepared glass systems will be analysed using instrumentation of all partners. The influence of technological parameters on the chalcogenide glasses with gradient chemical composition influenced by gamma radiation as well as on selected glasses based on heavy metal oxides, will be studied. The possibilities of diagnostics of investigated glasses will be verified by monitoring of selected electrical parameters.

Project Title Reseach on the electron beam weldability of hard to join dissimilar materials

Coordinator Ing. Martin Sahul, PhD.

Start Date01/04/2021End Date31/12/2023

Program APVV

Annotation

The metallurgical joining of dissimilar materials (DM) is difficult, due to the different physical, chemical, and mechanical properties. Therefore, joining DM is a great challenge. One material is usually not able to ensure the complex properties required in demanding operating conditions. Prospective combinations include copper with austenitic stainless steel (ASS) and nickel with titanium. Challenges in terms of weldability of mentioned materials are obvious, high thermal conductivity of copper can cause problems with maintaining the weld temperature necessary to achieve full penetration, the crystal structure of Cu, Ni and ASS are prone to hot cracking. Titanium is characterized by a high affinity to oxygen. The most suitable procedure is to use a vacuum to protect the weld pool from contamination by gases from the environment, and thus to eliminate significant embrittlement. These issues are exacerbated when welding DM. While the formation of hard and brittle intermetallic compounds (IMCs) is not observed in the first combination (Cu + ASS), the second combination of materials (Ti + Ni) forms 3 kinds of IMCs. In order to depress the formation of mentioned IMCs, highly concentrated electron beam welding (EBW) is proposed for research into the weldability of DMs. The equipment with the largest vacuum chamber for EBW in Slovakia will be used for the production of welded joints. The initial stage of experiments will be based on the design of experiment method to determine the influence of welding parameters on the responses. Butt and overlapped welded joints will be produced. Light microscopy and high-resolution scanning electron microscopy (including EDS analysis) will be used for detailed analysis of the microstructure of the welds. A detailed chemical analysis of the local areas of welded joints of dissimilar materials will be performed. The mechanical properties will be determined by automatic microhardness measurements and static tensile testing.

Project Title Novel multi-principal element alloys – design, characterization and properties

Coordinatordoc. Mgr. Marián Palcut, PhD.Start Date01/07/2021End Date30/06/2025

Program APVV

Annotation To expand the alloy design space, recent efforts have shifted toward the development of alloys with several principal elements. These materials are referred to as multi-principle element alloys (MPEAs), complex concentrated alloys (CCAs), or high-entropy alloys (a subset of MPEAs). The aim of this project is to design and characterize a series of novel MPEAs. We shall prepare and study several ternary, quaternary and multiple element alloys with different chemical composition. We shall study the relationship between chemical composition, phase constitution and alloy microstructure. We will investigate the effects of processing conditions (annealing time, cooling rate) on the phase evolution. The materials will be characterized in terms of their thermodynamic stability. The major part of the project will be the electrochemical corrosion study of different alloys in aqueous electrolytes. We aim to investigate the electrochemical stability of the phases and explore the relationship between their corrosion activity and chemical composition. We aim to investigate the effects of various electrolytes. We shall study the corrosion mechanisms and identify the various corrosion products. The project will also include the study of MPEAs mechanical properties and reliability. Furthermore, we shall investigate the alloys mechanical properties at elevated temperatures (stress corrosion cracking) and under simulated atmospheric conditions (salt spray test). In the end, we aim to identify corrosionresistant and mechanically stable materials for practical applications.

Project Title Optimization of round high-temperature supercnoducting cable for pulse magnetic field

Coordinator Dr.-Ing. Marcela Pekarčíková

Start Date 01/07/2021

End Date 30/06/2025

Program APVV

The project is focused on an optimization of a cable made of high temperature Annotation superconducting tapes wound on a core in form of a tube with the possibility of cooling the cable by the coolant flowing through the former. The purpose of the optimization is a significant decrease of AC losses, which can be achieved through three modifications of the cable. The first one is to reduce the width of the 4 mm superconducting tape down to 1 mm with steps smaller than 0.2 mm. The tuning of the tape width should allow to prepare the cables with optimal packing of the cable layers and with greater flexibility. The second modification is an additional narrowing of the superconductor width by striation scribing the superconducting layer along the tape with already optimized width. Both processes require a development of a suitable method for the cutting and scribing process of the superconducting tapes with minimal impact on their mechanical, structural and electrical properties. The third modification is the innovation of the central former, which should fulfill requirement of significantly reduced electrical conductivity. Modified superconducting tapes and cables prepared from them will be characterized in terms of mechanical and electromagnetic properties. Most of the experiments will be supported by computer modeling.

PROJECTS OF THE INSTITUTE OF PRODUCTION TECHNOLOGIES

Project Title Optimization of geometry of cutting tools produced by foundry technology and powder metallurgy to increase durability

Coordinatorprof. Ing. Alexander Čaus, DrSc.Start Date01/01/2019End Date31/12/2022ProgramVEGAAnnotationGeometry of cutting edge has

Geometry of cutting edge has significant effect on wear resistance as well on durability of cutting tools. It is possible to produce near-net-shape cutting tools by both the foundry technology and the powder metallurgy and in the case of high speed steel (HSS) with significantly higher wear resistance compared to similar tools produced by conventional metallurgy using machining of wrought profiles. Optimization of cutting tool geometry will be carried out by numerical simulation of machining conditions and load for the tool in cutting process. Application of additive technologies, namely 3D printing of casting patterns from castable resin for investment casting into ceramic shell moulds, and cemented carbides (CC) from metal powder, provides flexible production of cutting tools with optimal shape without using very expensive and shape-complicated injection moulds for production of castable/burnout casting patterns as well as for forming dies for powder material compaction.

Project titleCoating of powder metallurgical Titanium using electromagnetic radiation
under working atmosphere, study of microstructure and coatings propertiesCoordinatorprof. Ing. Peter Šugár, CSc.

Start Date01/01/2020End Date31/12/2022ProgramVEGA

Annotation The project deals with the possibility of surface treatment of titanium, which was prepared from titanium powder by low temperature methods of powder metallurgy. It is envisaged to use an energy beam of electromagnetic radiation incident on the surface of the PM titanium either in the form of laser beam or in the form of focused solar radiation. When heated under the working atmosphere, the reaction of titanium with oxygen or nitrogen molecules is assumed and coatings based on oxides, nitrides or their mixtures are expected to be formed. Subsequently,the microstructure and selected properties of the prepared coatings will be studied. The aim is to explore the possibilities of surface treatment of PM titanium, depending on future applications, to prevent surface damage during friction, to improve the surface for biocompatibility and to increase corrosion resistance of PM Ti, which are the most important reasons for surface treatment of usual titanium components.

Project title Accurate calculations, modeling and simulation of new surfaces based on physical causes of machined surfaces and additive technology surfaces in machinery and robotical machining conditions

Coordinator prof. Dr. Ing. Jozef Peterka Start Date 01/01/2020

End Date 31/12/2022

Program VEGA

Annotation

The central idea of the project is to use accurate calculations based on analytical equations as a basis for predicting roughness characteristics of machined surfaces. At the center of interest are the physical causes of machined surfaces studied at the level of geometrical-kinematic, mechanical-physical and technological properties of members of the machining system. Our intention is to create mathematical models and simulation algorithms for individual physical causes of the machined surface. As study prototypes, we will consider type-defined and undefined cutting edge technologies and exception-additive technology. Another target group of research is the inclusion of significant dynamic and stiffness characteristics. machines and machining robots. It is in robots that more time and emphasis will be placed on studying the effects of motion, kinematic bonds and trajectories. The inclusion of a robot technology and additive technology system is an important element of our research as a central project note.

Project title Research of joining the metallic and ceramic materials in production of power semiconductor

Coordinatorprof. Ing. Roman Koleňák, PhD.Start Date01/01/2020End Date31/12/2023ProgramVEGAApproximationThe preject is simple to function

Annotation The project is aimed to fundamental research of solderability of metallic, composite, non-metallic and ceramic materials applied in packaging of power semiconductor parts (chips, transistors, diodes etc.). The solution will be oriented to direct joining without application of coating for wettability assurance. Joining of semiconductor materials as Si, SiC and GaN is considered. Furthermore Al2O3, Si3N4, AlN and Cu/SiC composite material, which is applied mainly for the cooling of chips are also taken into account. Cu will be applied as an etalon material. New solder alloys alloyed with a small amount of active elements (Ti, La etc.) will be manufactured and also the solder alloys containing Bi and Zn, applicable for higher service temperatures. The solders will be designed with the aim to be suitable for direct soldering with application of power ultrasound. These new solders will be then tested for technological solderability. The interactions of solder alloys with the surface of substrates will be studied.

Project Title Research into the weldability and brazeability of materials with different melting temperatures joined with highly concentrated energy sources.

| Coordinator | doc. Ing. Erika Hodúlová, PhD. |
|-------------|--------------------------------|
| Start Date | 01/01/2021 |
| End Date | 31/12/2024 |
| Program | VEGA |
| Annotation | The proposed project will be |
| | basic research in the field of |
| | melting points by technologie |
| | |

The proposed project will be solved as a scientific research project focused on basic research in the field of welding and brazing of materials with different melting points by technologies utilizing high concentrated joining methods of materials. The Response surface method as the planning of the experiments will be used to determine the optimal parameters of high-productive joining methods (laser, electron beam, CMT, brazing of the two types of joints (butt and lap joint). Macro- and microstructural analysis of the joints will be used as experimental methods to evaluate the structural integrity of welded and brazed joints. EDX and XRD analysis and extended to high-resolution transmission electron microscopy will be used to determine the creation of different phases and change in chemical composition as well as the identification of excluded phases in joints. The mechanical properties of the joints will be evaluated by tensile strength and shear tests.

Project title Modern educational tools and methods for forming creativity and increasing practical skills and habits for graduates of technical university study programmes

Coordinator Dr. h. c. prof. Ing. Pavol Božek, CSc.

 Start Date
 01/01/2019

 End Date
 31/12/2021

Program KEGA

Annotation

4th Industrial Revolution (Industry 4.0) covers a wide range of large-scale and mass production in Slovakia. At present, the automotive industry is the dominant industry in Slovakia. So far, we have just been a "workshop", with no added value. Unfortunately, technical programme graduates at universities have neither the qualitatively nor quantitatively the required creativity and practical skills and habits to be applied in the companies involved. For manufacturing companies, however, it is necessary to educate a new generation of educators and students who will understand these technologies and know how to use them. This project offers the methodology and tools that are absolutely necessary to be implemented in the educational process in the technical study programmes at Slovak universities. This is mainly about a transfer of newly acquired knowledge from current research and views at contemporary manufacturing businesses in line with industry 4.0 requirements. In this context, it will be very important to include practical lessons in educational process with clearly defined conditions and a defined evaluation methodology. The project considers the use of knowledge based on the literary resources analysis from the creativity forming area of students of technical study programmes using modern educational tools and technologies. At the same time, the approach will be used, followed by synthesis in the formation of creativity and the enhancement of practical skills and abilities of technical study programmes graduates. The practical verification of the selected methods will be realized by applying modern educational tools with a connection to the real requirements of the production practice.

| Project title | Progressive form of interdisciplinary education and support for the development of the study of vocational subjects in the university environment |
|---------------|---|
| Coordinator | Dr. h. c. prof. Ing. Pavol Božek, CSc. |
| Start Date | 01/01/2021 |
| End Date | 31/12/2023 |
| Programme | KEGA |
| Annotation | The main objective of the project is to increase the applicability of students in the |
| | labor market by expanding interdisciplinary cooperation of interested teachers |

and increasing the readiness of graduates to perform in international academic or professional space, which would contribute to the popularization of vocational subjects and their teaching at the Faculty of Materials Science and Technology of the Slovak University of Technology in Trnava and the Faculty of Technology of the Technical University in Zvolen in all three levels of higher education in the following specialized subjects: Design and operation of production systems, Digital Enterprise and Virtual Reality, Basics of Using CAD Systems, Informatics for Technicians, Algorithms and Programming, Programming Robots - Through Progressive Training Methods. The added value of the proposed project will also be the intensification of international cooperation in the field of education with several foreign universities with which cooperation agreements have been signed with the Faculty of Materials Science and Technology of the Slovak Technical University in Trnava and the Faculty Technology. The project will also include the transfer of research results into the pedagogical process and the improvement of the equipment of specialized laboratories, which will serve the needs of the project activities after implementation.

Project title Modernisation of education in the area of joining of engineering materials

Coordinatorprof. Ing. Milan Marônek, CSc.Start Date01/07/2019End Date31/12/2021ProgramKEGAAnnotationThe project focuses on the desi

Innotation The project focuses on the design and implementation of a new concept of study literature creation with regard to the demands and expectations of the current young generation (Generation Z). The proposed concept will support the implementation of multimedia content that greatly helps to facilitate understanding of the issue and reflects the behavioural characteristics of the young generation that is essentially linked to Internet content and social networks. The concept is based on the creation of information database on the progressive joining of materials available online in one place. In each theme, there will be a technology principle, equipment description, explanation of the technological parameters, practical applications of technology and visual demonstrations in the form of animations, videos and pictures.

Project title Improving profesional competences of the university graduates of the branch Manufacturing Technology by applying dual education principles

Coordinatorprof. Ing. Peter Šugár, CSc.Start Date01/07/2019End Date31/12/2021ProgramKEGA

Annotation The projects solves the conceptual, methodological and content issues of the second grade university education in the Production Technologies study programme with the aim of more intensive developing of the graduates professional competences and their ability to fulfill the requirements of modern manufacturing practice. The expected output of this project is to upgrade the existing model of the student education in the Machining and Forming study programme by implementing the elements of dual and online asynchronous e-

learning system. The definition and the verification of the practical training methodology and the content will be implemented in terms of the industrial partners. At the same time, the project output also will be the development of an integrated e-system for an education and the management of praxis-orientated educational activities together with the establishment of the conditions for the face-to-face laboratory trainings focusing on the development of the creative solution for the actual and verifiable-by-praxis tasks. The tasks will be solved in the field of production technologies and the company process management, taking into account the need to quickly adapt the graduate to the bilingual business environment.

Project Title Creation of new study materials including multimedia textbook in field of technical preparation of production in welding and joining

prof. Ing. Roman Koleňák, PhD. Coordinator Start Date 01/01/2020 31/12/2022

End Date KEGA

Program

Annotation The project is focused on the design and creation of a new modern university textbook and didactic tools for teaching the subject: "Technical preparation of production in welding and joining materials". The subject is part of a new study program at the MTF STU entitled "Welding and Joining Materials", to which there are no suitable teaching texts or other didactic tools in historical context. The proposed concept is aimed to creating a textbook and an electronic version of a textbook with multimedia content. The creation of new study materials will directly influence the understanding of the issue under consideration in order to prepare graduates for the profession of welding technician as well as technician in engineering. The textbook will contain the materials needed to understand the technical documentation of welding and bonding. Understanding the preparation and implementation of the documents needed before, during and after the release of the engineering product to production is very important in terms of time and quality. The accompanying product is the creation of multimedia content, which will include a chronological approach to creating technical and welding documentation with explanations of operations using graphical representations and practical examples. The aim of the course is to prepare a student who is able to prepare materials for the construction of connected structures from the breakdown of materials through their security, storage, labeling, distribution to individual workplaces for preparatory operations and their progress to the final workplace for joining parts to individual nodes and units.

Project Title Research into the Unique Method for Treatment of Cutting Edge Microgeometry by Plasma Discharges in Electrolyte to Increase the Tool Life of **Cutting Tools in Machining of Difficult-to-Machine Materials**

Coordinator prof. Ing. Alexander Čaus, DrSc. Start Date 01/07/2017 End Date 30/06/2021 APVV Program

Annotation The cutting edge preparation (CE) is currently the most advanced method of increasing tool life. Cutting edge preparation in the production of cutting tools means treatment of microgeometry of cutting edge (cutting edges) of newly sharpened cutting tools. Suitable microgeometry of the cutting edge (fillet, chamfer) is essential for achieving high productivity machining mainly difficult-to-machine materials (DTM) such as austenitic stainless steels and superalloys. Therefore, the research deals with the machining of X6CrNiTi18-10 stainless steel and NiCr19FeNbMo superalloy. Machining superalloys disseminate knowledge in the energy and aerospace industries since it requires a greater commitment superalloys in future years. Our proposed project is focused on research into a completely new and own unique method of preparation of CE microgeometry of cutting tools by plasma discharge in an electrolyte (PVE). This method is developed originally at Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava (STU MTF).

Project Title Research of direct bonding of the ceramic and metallic materials by use of active soldering alloys

Coordinator prof. Ing. Roman Koleňák, PhD.

Start Date01/07/2018End Date30/06/2022ProgramAPVV

Annotation The project deals with the study of direct bonding of ceramic and metallic materials by application of active soldering alloys. The active alloys will be based on tin or indium and alloyed with active metal, as for example Ti, La, Zr, Y etc. It is supposed that the active element will react with the substrate surface during soldering process and will thus assure the wetting of solder on a ceramic or other hard-to-solder material. The project is based on idea of direct fluxless bonding. Heating will be provided by the high-concentrated heat sources as the laser and electron beam. Power ultrasound will be employed for activation of the new soldering alloys. Material solderability of the new developed solders will be studied. The following solderability criteria will be determined: wettability, spreadability, diffusion etc. Also interactions on the substrate/solder interface will be studied. Individual mechanisms of bond formation from the viewpoint of joint strength, speed of bond formation, life etc. will be compared.

Project Title Research of progressive methods of welding and soldering of corrosionresistant steels and copper

| Coordinator | doc. Ing. Erika Hodúlová, PhD. |
|-------------|--------------------------------|
| Start Date | 01/07/2019 |
| End Date | 30/06/2023 |
| Program | APVV |

Annotation The proposed project will be solved as a scientific research project focused on basic research in the field of welding and brazing/soldering of stainless steel with copper alloy by technologies utilizing progressive joining methods of materials. Several modern scientific methods will be used within the project in order to fill up the objectives set in particular stages of the project. In the early stages of the project, method of scientific analysis and planning of the experiments using Design

Expert software package will be used to determine the optimal parameters of high-productive joining methods (laser beam, electron beam, CMT, brazing/soldering) of the two types of joints (butt joint and lap joint). To achieve the stated objectives working procedures will be developed based on the knowledge and gathered information. Macrostructural and microstructural analysis of the joints will be used as experimental methods to evaluate the structural integrity of welded and brazed joints. EDX analysis and extended to high-resolution transmission electron microscopy will be used to determine creation of different phases and change in chemical composition as well as the dentification of excluded phases in joints. For the determination of internal defects of welded joints the computer tomography will be involved. The mechanical properties of the joints will be evaluated by tensile strength test in case of butt welds, by shear strength in case of lap joints, micro-hardness and bend test.

Project Title Research of progressive methods of welding and soldering of corrosionresistant steels and copper

Coordinatordoc. Ing. Ladislav Morovič, PhD.Start Date01/07/2019End Date30/06/2023

Program APVV

The shape stability of the steel tubes has a major influence on the further Annotation technological process of the tube processing, i. e. on secondary production. It is a very important parameter in terms of functionality, for example, active and passive parts of a car, where the dimensional tolerance fields are one of the toughest in terms of prodution itself. It is important to pay attention to the research of the shape stability of the tubes by means of contact metrology systems (coordinate measuring machine with touch probe) and non-contact measuring systems (optical 3D scanner using active triangulation (structured light)). The resulting properties of the tubes depends on a number of factors, e.g. from the shape instability in the individual phases of the production process in the process of production of tubes in Železiarne Podbrezová. The shape stability and the occurrence of geometric deviations are affected by the eccentricity that occurs primarily in the perforation process due to the off-centered punch, where there is uneven distortion due to the change in the original cross-sectional area of the blank on the radial removing of the material. In the process of producing tubes at the tensile reduction, a polygon is formed which results in uneven deformation caused by the stands in which the rolls are placed. Uneven distortion affects the internal structure of the material and hence the shape stability in the subsequent operation due to the anisotropy of properties. Experimental processes will be numerically simulated in the software DEFORM 3D. The aim is to identify, quantify and subsequently determine the effect of geometrical deviations on the instability of the tube dimensions and their technological inheritance, which is supposed to meet the most stringent technical and supplier conditions for the industry.

Project Title Prototype development of an industrial device for electrolytic-plasma polishing of parts of lung ventilators and other medical devices

Coordinatordoc. Ing. Štefan Podhorský, CSc.Start Date16/09/2020End Date31/12/2021ProgramAPVVAnnotationThe surface of products intende

The surface of products intended for biologically active environments must meet significant quality requirements. This also applies to parts of the lung ventilators. Low surface roughness is required because the ability of microorganisms to be trapped on a smooth surface is significantly worse than on a rough surface. Microscopic defects of the surface layer of the material have a significant negative effect, as well, which represent a significant risk factor not only in terms of possible biological contamination of the surface, but also in terms of microbiological corrosion. Although mechanical polishing methods reduce the surface roughness, they effect on the surface by force and heat, creating a number of microscopic defects that are usually furthermore contaminated with impurities during polishing. Therefore, it is common practice to polish the surface of such products electrochemically, but this necessitates the use of aggressive substances, usually a mixture of concentrated corrosives. Disposal of used solutions, containing a lot of dissolved metals, means a significant environmental and financial burden. An ecologically and technologically advantageous alternative to electrochemical polishing is a unique technology of plasma polishing in electrolyte, which is still relatively unknown worldwide. The team of the research laboratory has been devoting a long time to the development of this progressive technology, but the most significant obstacle to its introduction into industrial practice is the nonexistence of equipment that would be directly usable in the production process. The goal of the presented project is to solve this problem. The aim of the project is the development of technological equipment for plasma polishing in electrolyte and the realization of a prototype.

Project Title Research on properties of stainless alloys components made by additive manufacturing

Coordinatorprof. Ing. Milan Marônek, CSc.Start Date01/07/2021End Dat30/06/2025ProgramAPVV

Program

Annotation The currently used additive manufacturing systems utilize a powder bed and for the remelting of the metal powder, the power laser or electron beam. Despite very high precision and low dimensional tolerances achieved with these techniques, the cost of the devices is high, the rate of component formation is low, resulting in longer production times and increased production costs. Among alternative methods of components fabrication by additive manufacturing, methods using additive material in the form of wire appear to be perspective. In the case of using an electric arc to melt wire, the acronym WAAM (Wire Arc Additive Manufacturing) is employed; using a laser beaminstead of an electric arc, the designation DMD (Direct Metal Deposition) is applied. Unlike specialized powder bed systems, WAAM and DMD can also be implemented on conventional 3-axis welding systems as well as robotic work cells. The originality and novelty of the project lies in its complexity. Its ambition is to bring a new, comprehensive knowledge in the field of component fabrication by progressive arc (CMT, TIG) and laser beam overlay welding of titanium, aluminium and nickel alloys. The project will focus on defining the key process parameters and strategies of torch and laser head movements, analysing the mechanical and structural properties of the produced components, as well as acquiring new, original knowledge in the field of machining of the fabricated components. In this area, the attention of the team will be focused on the design and production of suitable cutting tools for machining the finished components, analysis of the impact of machining strategies on the characteristics of fabricated surfaces, deformations of components after machining as well as assessment of the lifetime of the used cutting tools.

PROJECTS OF THE INSTITUTE OF INDUSTRIAL ENGINEERING AND MANAGEMENT

| Project Title | Work competencies in the context of Industry | 4.0 development. |
|---------------|--|------------------|
|---------------|--|------------------|

| Coordinator | doc. Mgr. Dagmar Cagáňová, PhD. |
|-------------|---------------------------------|
| Start Date | 01/01/2019 |
| End Date | 31/12/2021 |
| Program | VEGA |

Annotation Project is aimed at identifying specific new job requirements in form of key work competences and digital skills according to qualification levels defined by the National Qualification Frame of Slovak republic (NQF) in the context of the development of the technological and working environment Industry 4.0. Project is based on an analysis of developments in the field of industry 4.0 development. The aim of the project is to contribute to the actual flow of information between labor market actors, reflecting the development of key competencies and digital skills in practice. The methodological objective of the project is to specify new job requirements according to the qualification levels of the National Qualification Framework in selected production sectors. The project reflects the key challenges in the Industry 4.0 strategy development in Slovak Republic.

Project Title Identification of priorities for sustainable human resources management with respect to disadvantaged employees in the context of Industry 4.0

| Coordinator | prof. Ing. Miloš Čambál, CSc. |
|-------------|-------------------------------|
| Start Date | 01/01/2020 |
| End Date | 31/12/2023 |
| Program | VEGA |
| Annotation | The essence of the scientific |

Annotation The essence of the scientific project is to analyze the impact of changes in the performance of industrial enterprises on the priorities of sustainable HRM. Management approaches focus mainly on employee and business performance. Changes in the performance of industrial enterprises, related to the digitization increase, the reduction of live work in production, processes improvement, technologies are aimed at organization's efficiency and effectiveness increase. Implementation of new approaches can have an impact on employees of different generations, while the potential negative effect of these risks is not sufficiently analyzed. The aim of the project is to identify risks in the emergence of new practices, critical impact areas on employees, and explore

mechanisms to eliminate these risks. The purpose of the project is to explore the potential of employing disadvantaged groups of employees in the context of changing conditions for enterprises, respecting the uniqueness of different generations of employees.

Project Title Network visualization of common and specific elements and documented information of integrated management systems with respect to relevant ISO standards

| Coordinator Start Date | doc. Ing. Alena Pauliková, PhD. 01/01/2020 |
|---------------------------|---|
| End Date | 31/12/2022 |
| Program | KEGA |
| Annotation | The subject of this project is to elaborate a comprehensive overview used on a global scale and subsequent coordination of individual areas of management systems as part of a comprehensive integration for industrial operations including quality management, environment, OSH, energy, information security, transport, corporate social responsibility, business continuity and more. The set of selected areas will include the organization's connections with industrial operations, key customer requirements, leadership, planning, operational support, operations, performance evaluation, and improvement. Co-ordination will be performed using hierarchical organizational diagrams and final visualized by small world networks - Small World Networks and Scale-Free |

Project Title The implementation of innovative educational methods and MM guide for decisionmaking area and application of analytical methods in the teaching process of selected subjects in the field of Industrial engineering

Coordinator doc. Ing. Henrieta Hrablik Chovanová, PhD.

Start Date 01/01/2021

Networks.

End Date 31/12/2023

Program KEGA

Annotation The project is focused on creating an interactive multimedia educational application (portal) in order to increase the level of the pedagogical (educational) process with the necessary video sequences, images, and other multimedia conditions by innovating educational methods of the selected key subjects in the field of Industrial Engineering (Operational Research, Statistical Methods, Business Logistics). It will serve full-time (combined) and external students of colleges/universities with a technical and economic focus, as well as for the professional public and those interested in the field. The submitted project will be a pilot project for other subjects in the field of Industrial Engineering. The use of multimedia in several forms will support the more intensive, effective, and rational perception of information in the selected subjects (texts, diagrams, photographs, speech, animations, video sequences, e-tests). Nowadays, it is important for students and graduates to be able to orientate themselves in a huge amount of information, to analyze and interpret the available information, and to be able to find an essential idea and focus on the goal. Interactive multimedia and hypertext, which the student (interested in the field) can access at any time and individually, are a suitable tool to support study information, easy search, testing, and easy orientation in them.

PROJECTS OF THE INSTITUTE OF INTEGRATED SAFETY

Project Title Implementation of progressive technologies, methods and forms to education in the study branch Safety and Security Science

Coordinatorprof. Ing. Jozef Martinka, PhD.Start Date01/01/2020End Date31/12/2022ProgramKEGA

The project is aimed at improving the quality of the educational process of Annotation students of the 1st and 2nd degree of university study in the study branch Safety and Security Science (Rescue Services) at the Technical University in Zvolen (Fire Protection and Safety Study Programme) and at the Faculty of Materials Science and Technology in Trnava (Integrated Safety Study Programme) based on application of advanced technologies, methods and forms of education. For selected coursed and core thematic areas of the study branch the innovative electronic learning materials and video tutorials will be created, as well as new modern teaching aids using 3D and large-format printing technology. Teaching materials will be prepared for practical exercises based on direct interaction of teacher – student, using modern ICT devices and with Microsoft Education Tools (part of Microsoft Office 365). The level of knowledge will be verified by on-line tests. In addition to creating new multimedia interactive learning materials and improving the competences of students and graduates, online access and the availability of up-to-date learning materials will also be a benefit for students at other universities and practitioners.

Project Title New forms of education for crisis management (e.g. COVID-19) using artificial intelligence

| Coordinator | prof. Ing. Jozef Martinka, PhD. |
|-------------|---------------------------------|
| Start Date | 01/01/2021 |

| End Date | 31/12/2023 |
|----------|------------|

Program KEGA

Annotation The aim of the project is to create e-learning focused on innovative education (rapid transfer of information) of professionals in the field of crisis management, other professions directly or indirectly involved in crisis management, university students (directly or indirectly involved in crisis management) and the general public. E-learning will consist of three levels. The first level, intended for the general public, will be freely accessible. The second level, intended for teachers, university students, occupational safety and health technicians and occupational health service staff, will be accessible after registration - a university or specified e-mail address will be required for registration. The third level, intended for crisis management specialists, will be accessible after registration(registration will only be allowed to specified persons). For professionals (students, occupational safety and health technicians, occupational health workers and crisis management specialists), elearning will focus mainly on providing the latest information in the field - focused mainly on the application and use of artificial intelligence, neural networks and data mining. Basic information will be provided to the public (the system will be prepared in the event of an unexpected crisis situation for the very fast publication of currently necessary information).

Project Title Building an innovative teaching laboratory for practical and dynamic education of students in the field of occupational safety and health

Coordinator doc. Ing. Richard Kuracina, PhD.

 Start Date
 01/01/2021

 End Date
 31/12/2023

End Date 31/12 Program KEGA

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The project is focused on building an innovative teaching laboratory for practical Annotation education of students of the Faculty of Materials Science and Technology in Trnava in the field of integrated safety. The teaching laboratory will provide students and other interested persons with dynamic education in the form of practical exercises carried out on unique devices enabling the study not only fire - explosion characteristics of dusts, but also measurement and evaluation of workplace parameters closely related to occupational safety and health. These exercises will be dynamic, mainly due to the possibility of transferring information from exercises taking place in real time to other places. The aim of this project is to increase the interest of high school students to study at technical universities and also as a response to the situation resulting from the global pandemic which significantly reduced or completely eliminated the contact method of teaching. The innovative teaching laboratory together with software and hardware support will enable university students of full-time and part-time study to acquire knowledge and skills that are currently required by professional practice. By applying the acquired knowledge in simple examples and practical demonstrations, they will gain an overview of the basics of safety engineering, risk analysis and risk management methods, dangerous substances, theory of fires and explosions, safety of working environment. All teaching materials(texts, presentations, multimedia videos, sample examples) will be published on a website created for this purpose.

Project Title Worldwide unique progressive methods of testing electrical cables for the needs of conformity assessment and verification of the constancy of their parameters as construction products

Coordinator doc. Ing. Jozef Martinka, PhD.

Start Date01/07/2017End Date30/06/2021ProgramAPVV

Annotation For most electrical cables within the meaning of Annex V to the Directive of European Parliament and the Council no. 305/2011 on the assessment and verification of constancy of parameters is used system 1+. On 01/07/2017, ends the transitional period and the assessment and verification of constancy of parameters of most electrical cables in the European Union will be carried out only in accordance with EN 50575: 2014. For manufacturers, this will mean the obligation of performing tests of power, control and communication cables for general use in accredited testing laboratories at yearly intervals. Costs for annual testing for one type of cable are in the order of thousands of euros. At a range of

several hundred kinds of cables - power, control and communication cables of different diameters, different rated voltage and current load will this obligation mean a heavy financial burden on the production of cables. In the Slovak Republic, production and distribution of electrical cables directly and indirectly employs thousands of workers and represents a significant contribution to GDP. Despite this fact exhibit Slovak cable manufacturer in comparison to the other producers in Europe, but also US and China, low volume of production. For that reason, the costs on annual tests will more significantly share in the price of products. These may significantly jeopardize the competitiveness of Slovak producers in the European Union markets. Even producers in the European Union have in comparison with producers from the US and China low volume of production. Consequences of that fact, and their costs significantly reflected in the price of the product will also threatens their competitiveness. The solution is to develop new innovative tests that will maintain current safety requirements and substantially reduce the cost of testing. The project aims to develop tests satisfying the above conditions.

PROJECTS OF THE INSTITUTE OF APPLIED INFORMATICS, AUTOMATION AND MECHATRONICS

Project Title Holistic approach of knowledge discovery from production data in compliance with Industry 4.0 concept

prof. Ing. Pavol Tanuška, PhD. Coordinator

| Start Date | 01/07/2018 |
|------------|------------|
| Start Date | 01/07/2018 |

End Date 31/12/2021

- Program VEGA
- Annotation

The main project goal is creation of a holistic approach of knowledge discovery from production data of heterogeneous control systems in compliance with Industry 4.0 concept. This includes Big Data, Internet of Things, smart sensors, forecasting and decision support methods and tools. The main topic will be proposal of analytic platform to collect, process and analyse big structured and unstructured data sets, utilising Hadoop and NoSQL technologies, for complex process control in production companies. Proposed analytic platform (utilising statistical and inductive learning techniques, e.g. neural networks, fuzzy modeling, decision trees, cluster analysis, etc.) will provide possibilities for gaining new, potentially useful knowledge from data. Subsequently, control strategies will be developed from the gained knowledge using synthesis. Results can be implemented in real-time predictive maintenance and optimization of relevant control paramet.

Project Title Development of advanced models for design and optimization of heat treatment and joining processes of newly developed high-strength steels doc. RNDr. Mária Behúlová, CSc. Coordinator Start Date 01/01/2020 End Date 31/12/2023 VEGA Program

Annotation The project is focused on the design and preparation of the new types of highstrength steels (AHSS) for automotive industry, including the technologies of their heat treatment and thermo-mechanical treatment, to obtain the optimal of combination specific properties of these materials (weight/strength/elongation). The next step is the investigation of the possibilities of metallurgical joining of newly designed AHSS and the analysis of development of dissimilar weld joints of AHSS and light-metal alloys (Al, Mg, Ti). The chemical compositions of steels will be proposed using the ThermoCalc software and JMatPro. The influence of technological parameters of heat treatment and material joining processes on the phase composition, microstructure and the final properties of AHSS will be predicted using advanced materials models and simulation models, using which the numerical simulations of investigated processes will be performed in ANSYS, DEFORM and SYSWELD software.

Project Title Innovation and new learning opportunities in industrial process management with PLC

Coordinator Ing. Andrea Némethová, PhD.

Start Date 01/01/2020

End Date 31/12/2022

Program KEGA

Annotation The presented project, entitled "Innovation and New Learning Opportunities in Industrial Process Control with PLC", aims to innovate an existing laboratory focused on industrial processes control by PLC. The laboratory currently contains 8 workplaces containing physical models enabling the simulation of selected processes. The aim of this project is to innovate the laboratory to simulate Inovácia a nové možnosti vzdelávania v oblasti riadenia priemyselných procesov pomocou PLC 3/21 Identifikátor: 20190425141260810 the realization of full-fledged workplaces with complex distributed control systems. The aim of this project is to innovate the laboratory so that all workplaces can be fully utilized and even more complex distributed systems can be simulated. This modernized laboratory will also allow the extension of the subject "Programmable Logic Controllers". Another benefit is the possibility of solving bachelor, master and dissertation theses. After implementing new workplaces and elements in the laboratory, this can be used to carry out workshops, create teaching materials and sample enclosures from individual workplaces.

Project Title Innovations of teaching process of technical subjects by implementation of augmented and virtual reality

CoordinatorIng. Ladislav Rolník, PhD.Start Date01/01/2021End Date31/12/2023ProgramKEGAAnnotationThe project is focused of

notation The project is focused on the innovation of teaching technical subjects using augmented reality and virtual reality. The project also envisages equipping the laboratory with new types of machine parts and assemblies created by 3D printing, to improve students' technical imagination and skills in the field of construction and creation of technical documentation. In this project will be created a mobile application using augmented reality and virtual reality technologies and a web interface, where students will be able to view in an interactive way models of 3D components created in the CAD / CAM / CAE system CATIA V5. The prepared parametric models can then be printed on a 3D printer and will be used in exercises as study aids that will significantly help students understand the principle of orthographic projection of components. Really made functional models of kinematic systems will allow students to intuitively understand the functionality of mechanisms used in practice. In the following subjects (Finite element method, Parts and mechanisms of machines) it will be possible to analyze the created parts using the finite element method in terms of thermal and mechanical stress in the CATIA V5 and ANSYS systems. The aim of the project is to increase the attractiveness of technical directions through an innovative approach to teaching subjects related to the construction of machinery. Another goal is to create macros in the Visual Basic for Automation VBA environment to support the automated process of constructing machine parts in CATIA V5.

PROJECTS OF THE ADVANCED TECHNOLOGIES RESEARCH INSTITUTE

| Project title Coordinator Start Date End Date Program Annotation | Computational design of novel functional materials doc. Mgr. Mariana Derzsi, PhD. 01/01/2019 31/12/2022 VEGA The project focuses on broadening the vistas of the technologically important systems with transition metals and lanthanides by predicting and targeted design of new as-yet unknown phases using theoretical approaches based on atomic- scale quantum-mechanical modelling, evolutionary algorithms and direct phonon method. The studied systems will encompass new electronic materials for spintronics, multiferroics and superconductors. This study will allow for designing of the most effective and technologically attractive structural forms of the newly predicted phases with metallic elements particularly tuned for the functionality in question in accessible pressure and temperature ranges. |
|--|--|
| Project title Coordinator Start Date End Date Program Annotation | Searching for multicomponent character of the flickering in accreting systems Mgr. Andrej Dobrotka, PhD. 01/01/2020 31/12/2022 VEGA The aim of the project is to study fast stochastic variability generated by mass accretion in cosmic objects, where the main drive mechanism is disc driven accretion, i.e. (for our current focus) cataclysmic interacting binary stars with a white dwarf, X-ray binaries with black holes, or active galactic nuclei with a supermassive black hole in the center. This stochastic flickering do not originate only from one source and has a complicated morphology. The proposed project aims to study the frequency spectrum of variability in order to identify the source. |

Since all mentioned objects have the same physical process as the main engine,

the flickering morphology must also have common features. Our goal is to look for these common features and to create a complex concept of flickering for all objects. For this purpose, we will use high-quality, extensive and multi-frequency data from space missions such as Kepler and XMM-Newton.

Project title Quest for novel inorganic compounds with nickel, palladium, copper and silver by DFT modelling and ion beam synthesis

Coordinator Ing. Pavol Noga, PhD. Start Date 01/07/2019

| Start Date | 01/0//2019 |
|------------|------------|
| End Date | 30/06/2023 |
| Program | APVV |

Annotation The current project aims at a thorough theoretical and experimental study of all important stoichiometries, which are currently missing from the structure map of binary oxides and halides of Group 10 (Ni, Pd) and 11 (Cu, Ag) metals. Absence of these simple chemical stoichiometries is disturbing and calls for an explanation. What are the reasons for these white spots on the huge seas of chemical stability? Are these compounds truly unstable? Or, maybe, they could be stable but not enough attention was paid to them? Answers to these and related questions will be given within the project using state-of-the-art approaches for search of new materials that will rely on combination of computational modelling at the atomic level and experimental physicochemical techniques, reactive magnetron sputtering deposition and ion implantation. Our strategy meets the urgent need of the modern world for highly effective screening of the unknown potential of available natural resources and the most economic use of available research infrastructures.

Project title Quantum Monte Carlo for strongly correlated electronic systems

Dubecký, PhD.

| Coordinator | Ing. Matúš D |
|-------------|--------------|
| Start Date | 01/07/2019 |
| End Date | 30/06/2023 |
| Program | APVV |
| Annotation | In recent ve |

In recent years, single-determinant fixed-node diffusion Monte Carlo (FNDMC) Annotation reached high-standard accuracy in a number of diverse systems (where mean-field methods like DFT do not suffice) ranging from weakly bound noncovalent complexes to strongly correlated systems like solid transition-metal oxides at high pressures. Thanks to its favourable CPU cost scaling, parallelism, and direct access to periodicity, FNDMC gains popularity as an unprecedented benchmark tool for large realistic complex many-electron systems. Recent results however suggest, that the expected accuracy is not always accessible, sometimes the results are overvalued, or they depend on the parameters that have been ignored to date. The reason being incomplete understanding of FN approximation (FNA) and its interplay with other possible biases. Our goal is identification and development of deep conceptual understanding of the key FNDMC error sources in strong interaction limit. We plan to uncover the currently unknown links between generic nodal (position-space) properties (e.g., topology) of fermionic wave functions, and, their connection to the structure of many-determinant expansions and 1-particle reduced density matrix occupation numbers, as well as separation of electron

correlation energy to dynamic and nondynamic (strong, multireference) component, which will enable fundamental understanding of FNA limits and decoupling of FN-bias from other bias sources of FNDMC. We also plan screening of FNDMC accuracy in strongly interacting model systems and unprecedented method developments that go beyond FN approximation. In addition to deep physical insights to the strong correlation effects in complex many-electron systems and limits of FNDMC methodology, the results of the project will enable rational usage and fine bias control of this method valuable for large systems.

Project Title Modern electronic devices based on ultrawide bandgap semiconducting Ga2O3 for future high-voltage applications

CoordinatorIng. Pavol Noga, PhD.Start Date01/07/2021End Date30/06/2025ProgramAPVV

Annotation Wide bandgap (WBG) semiconductor devices represent one of the key technologies in development of high power and high frequency systems for electric power conversion and telecommunications owing to their fundamental benefit of higher breakdown electric fields, in some cases increased electron mobility, and possibility to form heterostructures and 2D electron gas. GaN and SiC, two typical WBG examples also benefit from moderate values of thermal conductivity allowing for more efficient sinking of generated waste heat, lower channel temperatures, and enhanced device reliability. New emerging semiconductor materials with even higher bandgap energies Eg>3.4eV) referred to as ultrawide bandgap materials allow for further improvements in high power voltage handling solid-state electronic devices. Currently, and high semiconducting gallium oxide (Ga2O3) is under extensive study and expected to provide base material for rectifying Schottky-gate diodes and field-effect transistors for applications operating in kV range thanks to its good scalability, relatively simple synthesis, availability of native melt-grown substrates, and wide range of achievable n-type doping levels. The main aim of the proposed project constitutes material research and development of technology for epitaxial growth of epitaxial α -, β -, and ϵ -Ga2O3 layers and for processing of basic unipolar and bipolar electronic devices based on prepared Ga2O3 layers for future high voltage/power applications. Ga2O3 layers will be grown using liquid injection metalorganic chemical vapour deposition on sapphire, and higher thermal conductivity SiC substrates. We also aim to prepare Schottky diodes, FETs, and alloxide Ga2O3 PN diodes using naturally p-type oxides (e.g. NiO, In2O3, CuO2). Comprehensive structural, electrical, optical, and thermal study of prepared epitaxial layers and devices will be conducted and numerous original, high-impact results are expected to be obtained.

PROJECTS OF THE CENTRE FOR NANODIAGNOSTICS OF MATERIALS

Project Title Towards lithium based batteries with improved lifetime Coordinator Ing. Viliam Vretenár, PhD. Start Date01/07/2021End Date30/06/2025ProgramAPVVAnnotationWith the st

With the steadily increasing energy requirements of portable electronics and electromobility, conventional lithiumion batteries are facing new challenges. In the proposed project, we aim to stabilize the capacity and lifetime of lithium-ion batteries employing ultra-thin interfacial layers prepared by means of atomic layer deposition (ALD). The primary functions of interfacial layers are: i) preventing the dissolution of the cathode materials into electrolyte and ii) stabilizing the cathode morphology during lithiation and de-lithiation. Although the positive effect of ALD fabricated interfacial layers has already been demonstrated, systematic studies are still missing. The main bottleneck of such studies is the identification of appropriate feedback analytical techniques that enable real-time and in-operando insights into the charging/discharging mechanisms on the nanoscale. The conventional electrochemical characterization methods can only provide hints on the ongoing mechanism during degradation processes. Here we propose to utilize in-operando small-angle and wide-angle X-ray scattering (SAXS, WAXS) to track the morphology and phase changes that occur during the charging/discharging of lithium-ion batteries in realtime. The main focus of this project is on the application of real-time SAXS/WAXS studies under laboratory conditions. In these circumstances, extensive, systematic studies of various ALD interfacial layers can be performed.