

DMSRE 2024
33rd Joint Seminar

**DEVELOPMENT
OF MATERIALS SCIENCE
IN RESEARCH AND
EDUCATION**



BOOK OF ABSTRACTS OF THE 33rd JOINT SEMINAR

9 – 13 September 2024
Tatranská Štrba

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Tatranská Štrba

Editors

Mária Behúlová and Zdeněk Kožíšek

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**DEVELOPMENT OF MATERIALS SCIENCE
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*Hotel RYSY***, Tatranská Štrba, 9 – 13 September 2024*



Organized by

Slovak Expert Group of Solid State Chemistry and Physics
Czechoslovak Association for Crystal Growth

Under the auspices of

Crystallographic Society

*Faculty of Chemical and Food Technology STU in Bratislava
Faculty of Materials Science and Technology STU in Bratislava
Institute of Physics of the Czech Academy of Sciences, Prague
Regional Committee of Czech and Slovak Crystallographers*

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FOREWORD

The seminar “Development of Materials Science in Research and Education – DMSRE” is the 33rd in a series that began in Gabčíkovo in 1991, initiated by the Czech and Slovak Association for Crystal Growth and the Slovak Expert Group of Solid State Chemistry and Physics.

The seminar provides an excellent opportunity for the presentation and discussion of results in the fields of materials engineering, chemistry, solid-state physics, production technologies, materials processing, and related areas.

Additionally, the seminar aims to facilitate the exchange of experiences in teaching technical subjects, chemistry, and physics at universities, and to explore the connections between university research and practical applications.

The scientific session will cover the following main topics:

- Trends in development of materials research
- Education of materials science at the universities
- Information about the research programmes of individual institutions
- Information about equipment for preparation and characterization of materials
- Results of materials research

The program will include two invited keynote lectures (40 minutes each), given by Shelley Lorimer from MacEwan University, Edmonton, Alberta, Canada, and Jan Džugan from COMTES FHT a. s., Dobřany, Czech Republic; 52 contributions presented as short lectures (20 minutes each); and two company presentations.

Dear Colleagues, we warmly welcome you to the 33 rd DMSRE Joint Seminar and hope you enjoy your stay in the High Tatras.

Organizers

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PROGRAM

Monday, 9 September 2024

- 12:00 – 15:00 Registration (Hotel Lounge)
15:00 – 15:10 Opening (Lecture Hall)
-
- 15:10 – 16:30 **Monday Session 1**
Location: Lecture Hall
(chairperson: Mária Behúlová, Milan Nad’)
- 15:10 – 15:50 Jan Džugan
AM deposited metallic materials mechanical properties assessment with the use miniaturized samples
- 15:50 – 16:10 Monika Losertová
Influence of specimen dimensions on tensile behavior of NiTi alloy
- 16:10 – 16:30 Maroš Martinkovič
Measuring the toughness of weld joints on a tensile test machine.
- 16:30 – 17:00 Coffee break
-
- 17:00 – 18:30 **Monday Session 2**
Location: Lecture Hall
(chairperson: Zdeněk Kožíšek, Roman Yatskiv)
- 17:00 – 17:20 Zdeněk Remeš
Nanosecond photoluminescence decay in Mo-doped ZnO nanorods observed by TCSPC and phase shift methods
- 17:20 – 17:40 David John
Influence of annealing on Raman and photoluminescence spectra of single crystal ZnO
- 17:40 – 18:00 Radim Novák
Theoretical modelling of the frequency-dependent phase shift between-emission and excitation in ZnO nanorod photoluminescence spectra
- 18:00 – 18:20 Zdeněk Potůček
Effect of sample illumination on the content of luminescence active defects in Sn₂P₂S₆ crystals
- 18:30 – 19:30 Dinner
20:15 – 22:00 Welcome party (Hotel Restaurant)

Tuesday, 10 September 2024

08:40 – 10:00 **Tuesday Session 1**

Location: Lecture Hall

(chairperson: Zdeněk Remeš, David John)

- 08:40 – 09:00 Roman Yatskiv
New insight into the gas-sensing properties of β -Ga₂O₂ nanowires by near-ambient pressure XPS
- 09:00 – 09:20 Tomáš Hostinský
Silver borophosphate glasses modified with tungsten and molybdenum oxide
- 09:20 – 09:40 Jan Zich
Transport properties deviation of polycrystalline Bi₂O₂Se: Causes and solutions
- 09:40 – 10:00 Antonín Sojka
Thermoelectric properties of doped Bi₂O₂Se
- 10:00 – 10:30 Coffee break

10:30 – 12:30 **Tuesday Session 2**

Location: Lecture Hall

(chairperson: Maroš Martinkovič, Tomáš Vopát)

- 10:30 – 10:50 Jana Knedlová
The effect of moisture on laser beam wood machining
- 10:50 – 11:10 Hana Vrbová
Evaluating surface quality of heterogeneous surfaces produced by non-conventional machining technologies: methodological advances and challenges
- 11:10 – 11:30 Ondřej Bílek
The impact of surface roughness of replaceable cutting inserts treated with MRF technology on the turning process
- 11:30 – 11:50 Milena Kubišová
Analysis of measurement uncertainties in mechanical production and subsequent use for process stability control
- 11:50 – 12:10 Miroslava Puchoňová
Polymorphism of methylsalicylatocopper(II) complexes
- 12:10 – 12:20 Martin Cyprich
Hermes LabSystems - provider of solutions for laboratories
- 12:20 – 12:30 Miroslav Kamenský
TESTOVACÍ TECHNIKA s.r.o. - company presentation

- 12:30 – 13:30 Lunch
-
- 14:00 – 15:00 **Tuesday Session 3**
-
- Location: Lecture Hall*
(chairperson: *Monika Losertová, Miroslava Puchoňová*)
- 14:00 – 14:20 Ivona Černíčková
Comparison of experimental and thermodynamic approaches in the study of Ga-enriched SAC305 lead-free solders
- 14:20 – 14:40 Libor Ďuriška
Structural and thermodynamic studies of SAC108 lead-free solders enriched with Ga
- 14:40 – 15:00 Tereza Machajdíkova
Impact of nickel addition on the phase composition and properties of Sn-Ag-Cu solder alloys
- 15:00 – 15:30 Coffee break
-
- 15:30 – 18:10 **Tuesday Session 4**
-
- Location: Lecture Hall*
(chairperson: *Peter Šugár, Libor Ďuriška*)
- 15:30 – 16:10 Shelley Anne Lorimer
Using a Compositional Thermal Reservoir Simulator (STARS) to Examine Mechanisms and Scaling of Enhanced Oil Recovery Processes
- 16:10 – 16:30 Martin Podhorský
Site-controlled growth of InGaAs quantum dots with buried stressor for the development of microlasers and quantum light sources
- 16:30 – 16:50 Boris Pätoprstý
Surface modification of additively manufactured parts by drag finishing
- 16:50 – 17:10 Vladimír Šimna
The impact of generator parameters on cutting width in machining nickel alloys using WEDM technology
- 17:10 – 17:30 Marek Vozár
Comparison of optical measurement methods utilization for complex high feed tool geometry
- 17:30 – 17:50 Tomáš Vopát
Statistical evaluation of the influence of plasma polishing parameters on the material removal rate and the cutting edge radius sizes
- 17:50 – 18:10 František Jurina
Monitoring of selected aspects during the plasma polishing of cemented carbide end mills
- 18:30 – 19:30 Dinner

Wednesday, 11 September 2024

09:00 – 11:30 Current Trends in Teaching Technical Subjects: A Panel Discussion
Location: Lecture Hall

12:30 – 13:30 Lunch

14:00 – 15:30 Membership meeting of the Slovak Expert Group of Solid State
Chemistry and Physics
Location: Lecture Hall

16:00 – 17:00 Joint meeting of the Slovak Expert Group of Solid State Chemistry
and Physics and CSACG
Location: Lecture Hall

18:00 – 19:30 Dinner

Thursday, 12 September 2024

08:30	–	10:10	Thursday Session 1
<i>Location: Lecture Hall</i> <i>(chairperson: Jana Šugárová, Milena Kubišová)</i>			
08:30	–	08:50	Milan Uhríček <i>Effect of heat treatment on the internal damping of magnesium alloys</i>
08:50	–	09:10	Milan Uhríček <i>Effect of structure on the fatigue properties of aluminum casting alloys</i>
09:10	–	09:30	Viera Zatkalíková <i>Electrochemical characteristics of austenitic stainless steel after different times of sensitization</i>
09:30	–	09:50	Lenka Markovičová <i>Assessment of the suitability and durability of a recycled polymer product as a building component</i>
09:50	–	10:10	Daniel Ďugel <i>Modern composites in transportation constructions</i>
10:10	–	10:40	Coffee break
10:40	–	12:20	Thursday Session 2
<i>Location: Lecture Hall</i> <i>(chairperson: Robert Král, Tomáš Hostinský)</i>			
10:40	–	11:00	Vladimír Kuchtanin <i>The journey of nickel</i>
11:00	–	11:20	Alexandra Kucmanová <i>Let's reveal the secrets of chemistry in the environment to children</i>
11:20	–	11:40	Marek Kudláč <i>Influence of final turning on SCC susceptibility and corrosion properties of austenitic stainless steel 08Ch18N10T</i>
11:40	–	12:00	Jaroslava Maroszová <i>Efficiency of selected sorbents for eliminating PCBs from soil</i>
12:00	–	12:20	Margita Ščasná <i>Biochars from Cardboard as an Alternative adsorbent for the Removal of Pesticides from the Water Environment</i>
12:30	–	13:30	Lunch

14:00	–	15:20	Thursday Session 3
<i>Location: Lecture Hall</i>			
<i>(chairperson: Zdeněk Potůček, Vladimír Kuchtanin)</i>			
14:00	–	14:20	Zdeněk Kožíšek <i>Homogeneous versus heterogeneous nucleation in aluminum droplet at low supercooling: nucleation rates and the total number of nuclei</i>
14:20	–	14:40	Robert Král <i>Study of thermochromic materials and their properties for visual indicators</i>
14:40	–	15:00	Kateřina Křehlíková <i>Ternary lithium manganese (II) chloride as a new red-emitting neutron scintillator</i>
15:00	–	15:20	Juraj Kajan <i>Improving the efficiency of crystal growth process control by HDC method</i>
15:20	–	15:50	Coffee break
15:50	–	17:50	Thursday Session 4
<i>Location: Lecture Hall</i>			
<i>(chairperson: Ondřej Bílek, Viera Zatkalíková)</i>			
15:50	–	16:10	Jana Šugárová <i>Surface roughness evaluation of the formed parts produced by the multi-pass cold metal spinning applying laser textured tool</i>
16:10	–	16:30	Richard Antala <i>Roughness and wettability of the Ti Grade 2 surfaces modified by nanosecond laser</i>
16:30	–	16:50	Filip Ferenčík <i>Impact of sputtering power on trace impurities in binary oxides: A ToF-ERDA characterization study</i>
16:50	–	17:10	Matej Kubiš <i>Effects of high fluence helium ion irradiation on the micromechanical properties of Eurofer97 and ODS Eurofer steels</i>
17:10	–	17:30	Diana Fabušová <i>Theoretical investigation and DFT modelling of novel Pd₂O polymorphs using educated guess and evolutionary algorithms</i>
17:30	–	17:50	Radovan Bujdák <i>Exploring novel phases in the nickel-oxygen binary system with evolutionary algorithms and density functional theory modeling</i>
19:30	–	24:00	Conference banquet (Hotel Restaurant)

Friday, 13 September 2024

09:00 – 10:00 **Friday Session 1**

Location: Lecture Hall

(chairperson: Ivona Černíčková, Lenka Markovičová)

- 09:00 – 09:20 Milan Naď
Analysis of the influence of geometric and material parameters of fixing edge layers on the modal properties of plate structures.
- 09:20 – 09:40 Rastislav Ďuriš
The determination of basic material properties using DIC
- 09:40 – 10:00 Eva Labašová
Methods for determining reliability of complex systems
- 10:00 – 10:30 Coffee break

10:30 – 12:00 **Friday Session 2**

Location: Lecture Hall

(chairperson: Rastislav Ďuriš, Jaroslava Maroszová)

- 10:30 – 10:40 Ivo Říha
CEDEG - a partner for your business, research and innovations
- 10:40 – 11:00 Jana Jakubčínová
Interdisciplinary education of chosen parts of natural sciences for pre-service teachers
- 11:00 – 11:20 Thaer Syam
CFD analysis of damping characteristics of a hydraulic damper through geometrical modification and velocity variation
- 11:20 – 11:40 Eva Babalová
Numerical simulation of dissimilar laser welding of titanium and AISI304 steel parts
- 11:40 – 12:00 Mária Behúlová
Modelling and numerical simulation of temperature fields during WAAM production of an aluminium part
- 12:00 – 12:10 Closing

ABSTRACTS

Roughness and wettability of the Ti Grade 2 surfaces modified by nanosecond laser

Richard Antala, Peter Šugár, Jana Šugárová, and Michal Moško

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Surface characteristics of the materials dedicated to application in a biological environment play an important role. Chemical and phase composition, surface morphology and roughness determine the processes on the interface implant-surrounding bone, therefore many researchers are looking for optimal implant's surface integrity with an emphasis on micro and nano roughness alternation, in combination with the improved thickness of passivation layer and enhanced surface energy [1 - 4]. One of many ways how to improve the surface properties of materials for biomedical applications is laser structuring [5]. In this study, the impact of laser structuring parameters on the surface roughness and wettability of flat Ti Grade 2 surfaces was examined. Five experimental surfaces were prepared applying different levels of laser pulse energy maintaining the constant value of the scanning speed and five surfaces were prepared using various values of scanning speed while keeping the pulse energy constant. The surface morphology was documented employing high-resolution digital microscopy followed by the surface roughness parameters measurement using the contact profilometer. Finally, the surface wettability was measured using the sessile drop technique [6]. Experimental results confirmed a tendency of the surface contact angle to increase with the increase of the scanning speed, which corresponds with the trend of surface roughness parameters R_{sk} and R_{ku} to be higher when the scanning speed is increased. An opposite tendency of the contact angle decrease was observed with the rise of the laser pulse energy. It is consistent with the trend of a slight decrease in the surface profile kurtosis R_{ku} when the pulse energy grows.

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Numerical simulation of dissimilar laser welding of titanium and AISI304 steel parts

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Laser welding of titanium Grade 2 and AISI304 steel parts is commonly used in industries such as aerospace, automotive. These two metals have unique characteristics that make them ideal for various applications, but their differences in thermal conductivity, melting points, and chemical composition make achieving a strong and durable joint challenging [1]. Numerical simulation plays a crucial role in understanding and optimizing the laser welding process. By using numerical simulation it is possible to predict the behavior of the weld pool, heat distribution, and residual stresses in the welded material. This allows for the optimization of process parameters such as laser power, welding speed, and focal spot size to achieve better weld quality and efficiency [2]. This article focuses on analysing the temperature fields during the laser welding of 2 mm thick plates of AISI 304 steel and Ti Grade 2 through numerical simulations using ANSYS software. A simulation model for producing butt joints was developed to evaluate the impact of laser welding parameters, including laser power, welding speed, and laser beam offset towards the AISI 304 side, on temperature distribution and weld-pool characteristics. The laser heat source was modeled using a conical model with a Gaussian distribution of laser beam power. Material properties of AISI 304 steel and Ti Grade 2 were calculated as a function of temperature using JMatPro software. Cooling of the welding plates via convection and radiation with the argon shielding gas and surrounding air was applied using a third-kind boundary condition. Subsequently, the simulation model was employed to design appropriate technological parameters for laser welding these dissimilar metals. Using the DoE (Design of Experiment), the influence of technological parameters such as welding speed and laser power on the size of the melted zone on the top and bottom of the weld was analysed. An optimization was carried out, on the basis of which the area of optimal parameters for creating a weld with good quality was designed [3].

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Modelling and numerical simulation of temperature fields during WAAM production of an aluminium part

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Wire arc additive manufacturing (WAAM) is a notably promising direct energy deposition (DED) technology for the production of large-scale metallic components of various shapes without the need for complex tooling, molds, or dies. The main advantages of this technology include high material efficiency, lead time reductions, a high deposition rate, and low production costs [1-2]. WAAM offers numerous benefits for a wide range of metallic materials, including metals with high reflectivity like aluminum, copper, and magnesium, and their alloys [2-4]. The paper investigates the thermal cycles and temperature fields that develop during the additive manufacturing of an AA5087 aluminum alloy part using conventional Cold Metal Transfer (CMT) with varying deposition parameters. Thermal cycles were experimentally measured using an Ahlborn Almemo 5690-2 measuring station equipped with K-type thermocouples, while temperature fields were captured with a FLIR E95 infrared camera. A simulation model of the deposition process was developed to study the effect of deposition parameters on temperature distribution and the geometrical characteristics of weld beads. Results from numerical simulations using ANSYS software were compared with the macrostructural features and weld bead dimensions in single layers.

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The impact of surface roughness of replaceable cutting inserts treated with MRF technology on the turning process

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This work investigates the effect of the surface roughness of uncoated replaceable cutting inserts (RCIs) on the turning process. The surface of the RCIs was modified using sandblasting and magnetorheological finishing (MRF) technology, and the results were compared with the original untreated surface. The experimental research was conducted on DMG Mori's NTX 1000 turn-mill center, where cutting forces were measured using a Kistler 9129AA dynamometer and analyzed using Dynoware software. The results showed that the roughness of RCI significantly affected the final workpiece quality, cutting forces and chip compression coefficient. The MRF-treated RCI showed lower cutting forces and better workpiece surface quality. In addition, MRF technology allows for more precise control of surface roughness and quality. Therefore, optimizing RCI roughness is critical for efficient and energy-saving turning operations.

This work and the project were realized with the financial support of the internal grant of TBU in Zlín No. IGA/FT/2024/002, financed from the resources of specific university research.

Exploring novel phases in the nickel-oxygen binary system with evolutionary algorithms and density functional theory modeling

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Transition metal oxides present a vast array of materials with innumerable technical and chemical applications. Recently, binary oxides of nickel have attracted significant attention due to their emergence as a family of new superconducting materials, as well as their relevance in various industrial processes, such as metallurgy, catalysis, and semiconductor fabrication. Known binary nickel oxides have a wide application area, and the prediction and description of new phases in Ni-O binary system might uncover new attractive and functional materials. In our work, we explore and characterize either completely unknown or poorly characterized phases in binary transition metal oxide system Ni-O. We utilize a methodology that integrates state-of-the-art approaches such as Density Functional Theory (DFT) calculations in combination with Evolutionary Algorithms (EA) for the theoretical prediction of structures of new phases. We focus on analyzing crystal chemistry across various stoichiometries within the Ni-O binary system, examining large datasets generated by EA+DFT to uncover statistical patterns, relationships, and preferences in the data. Our findings contribute to a deeper fundamental understanding of the nickel-oxygen binary system.

This work was supported by Project No. SK-SRB-23-0035 - A synergy of ion beam methods and 2D materials with bulk and nano systems for energy and sensing applications. Presented research results were largely obtained using the computational resources procured in the national project National competence centre for high performance computing (project code: 311070AKF2) funded by European Regional Development Fund, EU Structural Funds Informatization of society, Operational Program Integrated Infrastructure.

Comparison of experimental and thermodynamic approaches in the study of Ga-enriched SAC305 lead-free solders

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The aim of the work was the study of lead-free solders SAC305 alloyed with gallium and comparison of experimental and thermodynamic approaches. In the experimental investigation, scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction and differential scanning calorimetry were used. It has been observed that with the addition of gallium in the solders, the thermal properties of the solders are improved. Also at low gallium content, a refinement of the microstructure was observed. However, at high gallium content, the exclusion of the inappropriate gallium-rich phase was found. The experimental results are compared to thermodynamic calculations of the Sn-Ag-Cu-Ga system obtained using the Thermo-Calc software.

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Modern composites in transportation constructions

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The large variety of existing modern composite materials and products on the construction market provides a number of possibilities for their use. However, at the same time the world is facing many challenges due to the daily deterioration of the environment and the depletion of non-renewable resources. New technologies and materials are being sought to combat these issues. As one of possible solutions is the innovative use of polymers in transport construction. This paper focuses on the investigation of the material properties of two different materials (hybrid composite and foam concrete). The main idea of the research is the development of new composite materials with higher strength and durability compared to traditional types of materials used on construction site.

The determination of basic material properties using DIC

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In determining the basic material properties, in recent years contact the strain gauge techniques of deformation measurements are often replaced by non-contact deformation measurement techniques. Digital image correlation (DIC) is currently one of the most popular non-contact optical method. The robust computational correlation algorithms developed so far allow a sufficiently accurate description of the movement of material points during the deformation of the tested sample. They effectively provide an estimate of the distribution of deformation field. For this reason, the relatively simple optical DIC method is widely used to estimate displacements and deformations in various applications: material characteristic investigation, structural condition monitoring, fatigue crack growth tracking, high temperature testing, etc. The adaptability of the DIC technique lies in the technology of image capture by standard cameras, applicability to a wide range of dimensions and materials of the tested samples and constructions. The contribution is focused on the use of the open source MATLAB 2D DIC software Ncorr [1] to evaluate the deformations of the test sample during the static tensile test. Tensile tests were carried out on flat samples made in different dimensions and with different materials. The influence of selected parameters of the correlation algorithm in the settings of the Ncorr program on the estimation of deformations was evaluated. The results of uniaxial strains obtained by the DIC method were verified by experimental measurements using an installed strain gauge and a reference extensometer. Subsequently, the basic parameters of the material of the samples were determined: Young's modulus of elasticity and Poisson's ratio.

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Structural and thermodynamic studies of SAC108 lead-free solders enriched with Ga

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In recent years, lead-free solders based on Sn-Ag-Cu (SAC) have been considered as the most promising alternative to Sn-Pb solders [1,2]. The most preferred candidates used in industry are SAC387 (95.5 wt.% Sn, 3.8 wt.% Ag, and 0.7 wt.% Cu) and SAC 305 (96.5 wt.% Sn, 3.0 wt.% Ag, and 0.5 wt.% Cu) [1]. However, there is a tendency to reduce the overall cost of the solder by reducing the Ag content. Despite the fact that a lot of work has been done in recent years, properties of lead-free solders have not been fully optimized compared to lead-based solders [3]. However, it was found that additional alloying elements (e.g., Ga, In, Bi, Ni) can lower the melting temperature and optimize the thickness and morphology of the intermetallic compound (IMC) layer [4-6]. Considering the above facts, this work is focused on the study of SAC108 (98.2 wt.% Sn, 1.0 wt.% Ag, and 0.8 wt.% Cu) enriched with Ga. The main aim is to study the influence of Ga on structural, thermal, and mechanical properties of SAC using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), differential scanning calorimetry (DSC), and Vickers hardness testing (HV1). The phase composition and morphology is discussed. The hardness and melting point of studies solders are evaluated. The effect of the Ga addition is also discussed in terms of thermodynamic calculations performed by the Thermo-Calc software.

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AM deposited metallic materials mechanical properties assessment with the use miniaturized samples

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Additive manufacturing (AM) has seen a dramatic surge in interest, necessitating precise characterization of mechanical properties for its successful integration into engineering structures. It is well-established that the mechanical behavior of AM-produced components is highly sensitive to deposition parameters such as location, orientation, and wall thickness, resulting in substantial property variations. Moreover, the size dependency and surface quality of AM parts significantly impact their mechanical performance, rendering standard test samples often unsuitable. While miniaturized samples are undergoing standardization for tensile testing, there remains a critical gap in methodologies for fatigue, fracture toughness, and creep evaluations. This paper provides a comprehensive overview of mini-sample utilization for these tests and outlines ongoing standardization efforts in this field.

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Theoretical investigation and DFT modelling of novel Pd₂O polymorphs using educated guess and evolutionary algorithms

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Transition metal oxides represent a significant category of materials with wide-ranging applications in technical and chemical fields. Among these, binary oxides of palladium have recently attracted significant interest due to their exceptional catalytic properties [1], particularly in industries such as automotive, pharmaceutical, and agriculture. Despite their importance, palladium oxides remain poorly characterized, with only PdO [2] and PdO₂[3] being well-recognized. In this study, we focus on the challenging task of identifying and characterizing new phases within binary palladium oxides, specifically Pd₂O. Utilizing a strategy that combines Density Functional Theory (DFT) calculations with educated guesses and evolutionary algorithms, we aim to predict and explore the structure of Pd₂O. Palladium oxide, Pd₂O has been only identified in ultrathin palladium films and cuprite structure with space group *Pn-3m* was proposed [4]. However, it was not further characterized and its properties remain unknown. Therefore, in order to gain deeper insights into the properties of Pd₂O we have calculated crystal, electronic and phonon structure of the reported cubic Pd₂O phase and evaluated its thermodynamic stability using Density Functional Theory. Additionally, in combination with evolutionary algorithms for crystal structure prediction we have proposed other potential new polymorphs of Pd₂O. Our results show that Pd₂O can form various polymorphs with more favorable formation enthalpy than previous reported cuprite structure. This study not only advances the understanding of Pd₂O but also demonstrates the effectiveness of integrating theoretical methods in the exploration of poorly characterized transition metal oxides.

Research results was obtained using the computational resources procured in the national project National competence centre for high performance computing (project code: 311070AKF2) funded by European Regional Development Fund, EU Structural Funds Informatization of society, Operational Program Integrated Infrastructure.

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Impact of sputtering power on trace impurities in binary oxides: A ToF-ERDA characterization study

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Performance of Binary oxides, used especially in the semiconductor industry, are significantly affected by impurity concentrations. Power density is one of the sputtering parameters that significantly affects these impurities. Increasing the power density reduces the amount of contaminants in the thin film metals. This study examines how power density in magnetron sputtering impacts hydrogen, carbon, and other impurities in silicon, titanium, copper, silver, and palladium binary oxides, which are common in the semiconductor industry and needed further investigation for comparison with metals. We focused on a narrow power density range of 200-300W using DC reactive magnetron sputtering on a 3-inch target. Six samples of each material were prepared under fixed conditions of $5 \times 10E-3$ mbar pressure in an Argon and Oxygen atmosphere with a flow rate of 40/10 sccm. Data analysis was performed on films of the same thickness, ignoring the surfaces of both the substrate and the film. Using Time-of-Flight Elastic Recoil Detection Analysis (ToF-ERDA), we detected very low but important changes in impurity concentrations and understood how they relate to the sputtering power density. The results offer new insights into optimizing deposition parameters to improve film purity and performance.

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Interdisciplinary education of chosen parts of natural sciences for pre-service teachers

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The preparation of pre-service teachers and the training of professionals, technicians and engineers are the main focus of new fields of study, curricula and educational approaches. The multidisciplinary elements of chemistry are emphasised in university chemistry teacher preparation programs. The aim is to educate pre-service teachers by integrating the chemical and physical disciplines through specific laboratory assignments. The above disciplines enhance the effectiveness of pre-service student-teacher preparation in acquiring pedagogical skills related to developing flexible structural aspects of teaching practices to meet a specific learning objective. The aim is to foster creativity and provide positive motivation for the science disciplines (chemistry and physics) using interdisciplinary approaches. The examples given in the paper focus on physics for chemists. Laboratory exercises are also included as an educational optimising factor based on the relationships between science disciplines. The students apply the acquired theoretical knowledge to experimental activities on a physical basis. They perform basic measurements on available laboratory instruments and evaluate the data. Laboratory exercises are an essential tool to improve the quality of education for the following reasons: the essence is practical learning and experimentation, developing as well as promoting technical and practical skills that help in the development of critical thinking and problem-solving, consequently promoting interaction and cooperation, and above all validating theoretical knowledge. Laboratory exercises in the education of pre-service teachers will help students understand chemistry and physics concepts through hands-on learning and interactive activities. Expectations, outcomes, and benefits of the laboratory exercise among the pre-service chemistry and physics teachers were orientated in the teaching: improving memorisation and understanding of physicochemical concepts and relationships through laboratory exercises and interactive activities; increasing the engagement of student pre-service teachers in the teaching process and encouraging their active participation in solving physicochemical problems; strengthening the practical skills and competencies of pre-service teachers, which can contribute to better use of modern technologies in teaching; creating a stimulating and innovative learning environment through interdisciplinary learning. The results highlighted the importance of improving chemistry teaching, increasing student motivation, developing skills and promoting interactive learning. These implemented applications and activities can contribute to more effective and interesting teaching of chemistry and physics and support the development of students' comprehensive chemical knowledge in interdisciplinary education.

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Silver borophosphate glasses modified with tungsten and molybdenum oxide

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This contribution deals with study of mixed glass former effect (MGFE) and its effects in two series of borophosphate glasses of $40\text{Ag}_2\text{O}-20\text{MO}_3-(40-x)\text{P}_2\text{O}_5-x\text{B}_2\text{O}_3$ (where $M = \text{W}, \text{Mo}$) in a composition range of $x = 0-30$ mol% B_2O_3 . Basic physico-chemical properties were determined, and thermal properties studied by differential thermal analysis and thermomechanical analysis. The glass structure was investigated using Raman spectroscopy and both 1D and 2D ^{11}B and ^{31}P MAS NMR spectroscopy. Behavior and oxidation states of tungsten and molybdenum throughout the series was investigated using EPR spectroscopy. The electrical properties of the glasses were obtained by using impedance spectroscopy. In both series, glass transition temperature, T_g , increases in range of 0-10 mol% B_2O_3 , further additions results in slight decline of T_g values. Results from impedance spectroscopy reveal non-linear increase in DC conductivity which can be attributed to MGFE and therefore changes in the structure of the glass network. The second possible explanation of the development in DC conductivity can be attributed to the presence of reduced forms of W and Mo which can affect the resulting conductivity by the polaron hopping phenomenon. This phenomenon has already been studied and confirmed on glasses of similar systems [1]. Structure of the glasses was probed with multiple MAS NMR experiments. To get first information about the glass network, standard 1D experiments of ^{11}B and ^{31}P nuclei were performed. From obtained ^{31}P MAS NMR spectra is visible the transformation of the dominant phosphate structural units in the direction of $\text{Q}^2 \rightarrow \text{Q}^0$ with B_2O_3 additions, and thus the shortening of the phosphate chains. Development in ^{11}B MAS NMR spectra reveals presence of both BO_4 and BO_3 structural units through the series. Interconnections between phosphate and borate species was further studied by multiple 2D correlation techniques. Namely 2D ^{31}P INADEQUATE sequence was used to probe direct through bond connections between phosphate structure units, which confirmed shortening of phosphate chains. As next was done investigation of the P-O-B linkages using the $^{11}\text{B}(^{31}\text{P})$ D-HMQC sequence. This experiment confirmed presence of both P-O-B^[4] and P-O-B^[3] structure units connection inside the glass network. And lastly 2D ^{11}B DQ-SQ sequence was used to investigation of presence and nature of B-O-B bonds. This experiment reveals presence and evolution of all three $\text{BO}_3\text{-BO}_3$, $\text{BO}_3\text{-BO}_4$ and $\text{BO}_4\text{-BO}_4$ pairs inside the glass network. By combining all these methods, we were able to prepare an approximate structural model of these glasses, which could be used to explain the macroscopic properties of the studied glasses.

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Effect of structure on the fatigue properties of aluminum casting alloys

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Casting alloys are materials used for producing shape castings, specifically aluminum alloy products with intricate geometries. These alloys are increasingly prevalent and find numerous applications in modern industry [1]. Aluminum alloys are critical engineering materials extensively utilized in various fields such as automotive parts, aircraft components, wire ropes, and overhead electrical cables due to their high strength-to-density ratio. However, in these applications, aluminum alloys are also susceptible to fatigue damage [2]. Aluminum alloys used in the automotive industry must exhibit a suitable balance of strength and ductility. Sheets or profiles are typically formed into final shapes, such as body panels or bumper beams, through cold deformation. Therefore, bendability is crucial for both fabrication and application, where ductility ensures optimal energy absorption. While uniaxial tensile testing is commonly employed to determine the mechanical properties of metals, it may not accurately reflect the deformation modes experienced by a component. In such cases, the three-point bending test is a more appropriate method for assessing mechanical properties. Several factors influence bendability, including hardening behavior, constituent particles, shear band formation, microstructure, and texture/anisotropy [3]. The aim of this work is to study and analyze the properties of aluminum alloys for casting. The experimental measurement is aimed at material evaluation and fractographic analysis of fracture surfaces after three-point bending loading.

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Influence of annealing on Raman and photoluminescence spectra of single crystal ZnO

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Zinc oxide exhibits high electron mobility, wide 3.3eV band gap, ability to sustain large electric fields, relative low electronic noise, and strong luminescence at room temperature. These properties make ZnO invaluable for a broad range of applications. It is therefore important to study to influence of treatment on its properties under various conditions. In this work we compare Fourier transform infrared Raman (FTIR Raman, 1064 nm laser excitation, 70-3500/cm spectral range, 1/cm spectral resolution) and photoluminescence (PL, 360 nm UV LED excitation, 375-700 nm spectral range, 1 ns time resolution) optical spectra of as the received and annealed ZnO single crystals. The annealing has been done in oxidizing and reducing atmosphere at 350, 500 and 700C. The Raman spectra show two characteristic peaks at 100/cm and 440/cm associated with the sublattice oscillations of Zn and O, respective, and a broad PL band in the visible spectrum with mean time decay about 10 microseconds. The optical measurements are correlated with the topographical information obtained by atomic force microscopy (AFM). We analyze trends in the optical spectra related to vacancy rearrangements in the lattice, and showed a possible next course of action for further research.

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Monitoring of selected aspects during the plasma polishing of cemented carbide end mills

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The article deals with the monitoring of selected characteristics of the plasma discharge process during the polishing of cemented carbide milling cutters. The aim of the experiment is to evaluate the change in current, voltage, temperature of the electrolyte and the cutting edge radius sizes with respect to the polishing time. These results bring new knowledge in the specific field of cutting edge preparation of cemented carbide milling cutters by plasma discharge in electrolyte

Improving the efficiency of crystal growth process control by HDC method

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In order to determine the stability of crystallization conditions, four experimental processes of sapphire crystal growth by the horizontal directional crystallization (HDC) method were carried out. The heater power was regulated based on real-time crystal-melt boundary position data obtained using video monitoring, which provided a stable crystal growth rate. The obtained curves of the dependence of the heater power on the length of the growing crystal indicate the similarity of physical phenomena regardless of the degree of melting of the seed crystal, the length of the container, and the effectiveness of thermal shielding. The analysis of the heat flow balance revealed that heat transfer from the heater is dependent on the melt surface area.

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The effect of moisture on laser beam wood machining

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Wood moisture can affect various parameters of the engraving process, such as the depth of engraving, the structure and surface of the wood, and thus the overall quality of the created image. The investigation of the influence of moisture contained in different types of wood on their machining was carried out on samples of oak, beech, pine, spruce, alder, ash and cherry produced using the laser device ILS 3NM, CO₂, with a wavelength of 10.6 μm and a maximum power 100 W, with a maximum feed speed of 1524 mms⁻¹. The depth of ablation and the surface of the machined surface were studied for selected samples with the moisture of the wood plants in the laboratory room, the outdoor and with the moisture created by immersion in the water bath.

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Homogeneous versus heterogeneous nucleation in aluminum droplet at low supercooling: nucleation rates and the total number of nuclei

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Crystallization processes determine the quality of the product obtained and understanding the molecular mechanisms that occur during crystallization remains a scientific challenge. As a model system, we have chosen aluminum (Al), whose crystallization temperature $T_C \approx 642$ °C (corresponding to an undercooling $\Delta T_C \approx 18.3$ °C) and can be well detected by differential scanning calorimetry (DSC) under non-isothermal conditions [1]. On the contrary, the crystallization event was repeatedly detected by the isothermal DSC after several tens of minutes at the undercooling $\Delta T \approx 6.8$ °C. The standard kinetic model of homogeneous and heterogeneous nucleation was solved numerically to determine the size distribution of the nuclei, the nucleation rate, and the total number of nuclei. In our previous analysis of Al crystallization via homogeneous nucleation, we have determined [1] the most probable values of the interfacial energy and the kinetic barrier of nucleation. Heterogeneous nucleation of Al on the concave droplet surface is modeled for the wetting angle $\vartheta = 90$ °C when the nucleation barrier of heterogeneous nucleation $W^{het} \approx 1/2$ of the homogeneous nucleation barrier W^{hom} and thus the probability of heterogeneous nucleation would be much higher than homogeneous one. On the other hand, the number of nucleation centers, where cluster formation starts, is much higher for homogeneous nucleation. As a result, the two nucleation processes are comparable in the Al sample of the mass 9.91 mg. Homogeneous nucleation starts at shorter times, but heterogeneous nucleation prevails in longer times.

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Study of thermochromic materials and their properties for visual indicators

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Recently, chromogenic materials brought attention due to their wide application potential [1]. They belong into a broad family of functional materials containing discoloration substances and other auxiliary components, which change color when exposed to varying external conditions such as temperature, pressure, gas, etc. Specific group are the thermochromic materials, also called as temperature sensitive material(s), with unique color change occurring (reversibly or irreversibly) under thermal treatment [2]. Thus, these materials can be applied in scientific, industrial, and technological applications due to their ability to provide visual indication of thermal changes at specific environmental conditions or external influences. This may be used in aerospace, military, smart windows (to block solar radiation), printing technology, textile, architectural coatings, etc. [2,3]. However, the most significant application may be ascribed to food packaging and food safety, to monitor whether the food was properly stored while transported. Our main goal is to study selected thermochromic compounds based on Co- and Ni-phosphites to understand the mechanism behind their color properties and changes. However, due to their complex composition, which results in multiple transitions and decompositions at higher temperatures, we decided to firstly study thermochromic transitions on model compounds such as cobalt chloride hexahydrate ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$) and nickel chloride hexahydrate ($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$). In this work we explored and analyzed properties of above mentioned model compounds using various thermoanalytical methods e.g. thermomicroscopy, simultaneous differential thermal analysis and thermogravimetry coupled with mass spectrometry, and thermomechanical analysis. Further, their structural and physical properties were investigated as well.

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Ternary lithium manganese (II) chloride as a new red-emitting neutron scintillator

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Neutron detectors play an important role in many application fields, such as nuclear power generation, nuclear decommissioning and decontamination, border and homeland security control, nuclear non-proliferation and medicine [1,2]. The current world source of ³He comes mostly from the decay of tritium originating in nuclear weapons programs in the U.S. and Russia. Since 2008, ³He has become extremely expensive as the supply became limited and the world has been facing the shortage [1,3]. As ³He proportional counters still represent the industry standard for neutron detection [4,5], there is still high demand for an alternative scintillation material, which would have potential to be mass-produced at low-cost from promptly available materials and technology [3]. Good neutron detection efficiency, gamma-neutron separation and robustness for deployment are the most important properties sought after [1]. From the group of inorganic scintillators, red-emitting ternary lithium manganese (II) chloride (Li₂MnCl₄) could represent a promising new material for neutron detection. In this study, undoped and Ce³⁺ and Eu²⁺ doped Li₂MnCl₄ single crystals were grown by vertical Bridgman method and basic structural, compositional, physical, thermal, optical, luminescence, and scintillation characterizations were performed.

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Effects of high fluence helium ion irradiation on the micromechanical properties of Eurofer97 and ODS Eurofer steels

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This study aimed to address the challenge posed by elevated levels of transmutation helium in materials for advanced nuclear reactors, both fusion and fission, which leads to the formation of helium bubbles, causing embrittlement and swelling [1]. While current research primarily examines fundamental aspects such as defect evolution and void swelling at the nanoscale, our study specifically investigates the bulk properties of these materials and their practical engineering applications. To study the effects of transmutation helium, we subjected Eurofer97 and its ODS variant, as well as five other structural steels—SIMP, PM2000, OSD Eurofer, SS 310S, and 800H—designed for use in demanding radiation environments, to high fluence helium ion irradiation. Using multiple ion energies ranging from 17 MeV to 1 MeV, we conducted the irradiation experiment with the 6 MV tandem accelerator at the ion beam laboratory at ATRI MTF STU. We systematically decreased the energy levels to create a uniform "box-profile" with a helium concentration of 1000 appm [2]. This method resulted in a consistently irradiated layer approximately 65 μm thick, allowing us to focus on assessing changes in the micromechanical properties, particularly hardness, of the irradiated Eurofer97 and its ODS variant using the nanoindentation method. In this contribution, we present the initial findings of our work, focusing on the nanoindentation analysis of the irradiated steel samples.

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Analysis of measurement uncertainties in mechanical production and subsequent use for process stability control

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In the current industrial environment, where quality is a key factor of competitiveness, the measurement and control of the stability of production processes plays a vital role. This work focuses on the analysis of measurement uncertainties in mechanical production and their subsequent use for process stability control. Measurement uncertainties are an inherent part of any measurement system, and their understanding and proper management is necessary to ensure the accuracy and reliability of production processes. The MSA (Measurement Systems Analysis) method enables the assessment of the capability of measurement systems and the identification of sources of variability. Emphasis is placed on the standard uncertainties of type A and B and the ways in which they affect the measurement process. The work also includes a description of the implementation of statistical process control (SPC) and its importance for maintaining a stable production process. SPC makes it possible to continuously monitor production processes and quickly identify deviations, which leads to timely correction and minimization of defects. To achieve these goals, quality tools such as the Ishikawa diagram, histogram and Pareto diagram are used. This work provides a comprehensive view of the importance of measurement and data analysis to ensure stability and quality in manufacturing processes.

The journey of nickel

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Nickel has been found in metallic artefacts dating back more than 2,000 years. It was first identified and isolated as an element by the Swedish chemist, Axel Cronstedt, in 1751. In the 19th century, it came to prominence in plating and in alloys such as “nickel silver” (German silver) in which it is alloyed with copper and zinc. This alloy was named for its colour and does not contain any silver! 15th century miners in Germany found a brown-red ore which they believed to contain copper. They called it Kupfernickel or Devils’ Copper because they couldn’t recover copper from it. Coins in the USA first used nickel alloyed with copper in 1857. The “nickel” was not made from pure nickel but in 1881, pure nickel was used for coins in Switzerland. Stainless steels were discovered early in the 20th century and nickel was found to have a very beneficial role in many of the common grades, which continues to this day. Alloys based on nickel were found to have excellent corrosion resistance and could withstand high temperatures, which made them suitable for chemical plants and also allowed the practical realisation of the jet engine. As a result of these developments, nickel has enjoyed a very strong growth of demand over the past century. This continues today because of the essential role nickel plays in many technologies. While the concentration of nickel in the earth’s crust is 80 parts per million, the earth’s core consists mainly of a nickel-iron alloy.

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Let's reveal the secrets of chemistry in the environment to children

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This article aimed to determine the effectiveness of an innovative approach to teaching chemistry through experiential learning in a chemical laboratory followed by theoretical instruction by teachers and subsequent theoretical teaching by teachers. Experiential learning and an excursion were completed by twelve-year-old elementary school pupils together with their chemistry teacher in the chemical laboratory at the Institute of Integrated Security, where they were shown simple chemical experiments. During the theoretical classes, the processes that they had previously seen in the laboratory, were explained. During the excursion, the pupils carried out practical experiments under the guidance of university teachers, which enabled them not only to visualize theoretical knowledge but also to gain practical experience with chemical techniques. Subsequent teaching was designed to link practical experience with theory, improving overall understanding and retention of the subject matter. Preliminary observations indicate that combining the theoretical curriculum with practical examples increases students' motivation and interest even in such a subject as chemistry. This can lead to a better understanding and long-term retention of acquired knowledge. In addition, the article focuses on investigating the impact of an innovative approach on the environmental awareness of pupils, as the experiments were focused on chemical processes related to environmental protection. The preliminary results of the processing of the results from the interviews with pupils during the excursion and the structured interview with the teacher indicate a positive impact of this innovative method on the educational process of the pupils. The article provides valuable insights for educators and education experts aiming to implement experiential learning into the pedagogical process to improve the understanding of the basic principles of chemistry and promote environmental awareness among younger generations.

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Influence of final turning on SCC susceptibility and corrosion properties of austenitic stainless steel 08Ch18N10T

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Final machining, such as final turning or final milling, aims to smooth the given machined surface of the material and obtain dimensional tolerance. However, with tough materials like austenitic stainless steels, where deformation hardening also occurs, the machining of these materials is complicated, and consequently the character and properties of the machined surface of these steels can have a negative impact on corrosion resistance. The affected parameters may include surface microhardness, roughness or residual stresses. In this work, the influence of final turning on stress corrosion cracking susceptibility and corrosion resistance of austenitic stainless steel 08Ch18N10T was monitored where as a toll a replaceable double-sided sintered carbide cutting plate with a negative rake angle was used. A combination of two machining parameters was set up: feed (0.12, 0.2 and 0.3 mm) and cutting speed (100 and 250 m min⁻¹). The roughness, microhardness and the surface deformation zone depth were analysed on the machined surface. It was found that hardness but also roughness increased with increasing tool feed. Using the exposure of samples in a boiling MgCl₂ solution, susceptibility to stress corrosion cracking was observed. Density of cracks as well as the depth or length of cracks into the material were studied and evaluated using SEM and ImageJ software. With increasing feed, the density of cracks decreased, on the contrary, the length and depth of cracks increased. Electrochemical potentiokinetic reactivation analysis, a double loop method, was used to determine sensitization to intergranular corrosion. The samples were determined to be non-sensitized. This method also showed the effect of roughness on the resulting polarization scans.

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Methods for determining reliability of complex systems

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The contribution deals with the determination of the final reliability function, the mean time to failure and the hazard rate of complex systems. These systems cannot be simplified to a combination of series and parallel connected blocks [1]. The systems were set by using a reliability block diagrams [2]. Each block represents an element of the system, the connections between these elements are set by lines. Ties connections might be one-way or double-way, what is shown by the arrows. The aim of the contribution is to determine the reliability function of the complex system on the model example. Three methods were used to determine the reliability function: the method of minimum paths, the method of critical sections and the decomposition method. The Matlab program was used for calculations. The article presents the basic principles of individual methods and the functional relationships used to determine reliability function of the systems [3]. Virtual block diagrams of the respective system are also shown for all three methods. In terms of calculation efficiency, the decomposition method seems to be the most suitable. It is not necessary to apply the idempotence transformation because neither of elements of the system is repeated in virtual models more than once. In the methods of minimal paths and critical sections, it is necessary to apply the idempotence transformation, because some elements of the system can be found more than once in virtual models.

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Using a Compositional Thermal Reservoir Simulator (STARS) to Examine Mechanisms and Scaling of Enhanced Oil Recovery Processes

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Understanding scaling of enhanced oil/bitumen recovery processes is essential in moving laboratory scale experimental results to field scale. Scaling theory for thermal processes, was developed by Pujol and Boberg [1], but for many processes such as Steam-Assisted Gravity Drainage (SAGD), solvent enhanced oil recovery and in-situ combustion [2], scaling from lab scale to field scale is not well understood. This talk summarizes research done at MacEwan University that uses a commercial thermal compositional reservoir simulator to study the mechanistic behavior and scaling of SAGD, solvent and combustion processes in Athabasca bitumen. This work stems from Shook et al. [2] who used reservoir simulation to confirm scaling groups for waterflooding. A similar strategy to Shook et al. was used in this work whereby the scaling of the enhanced oil recovery processes was examined using reservoir simulation at three different reservoir scales: lab scale, semi-field scale and field scale. Parameters were chosen to investigate the capability of the reservoir simulator for capturing scalability with a focus examining the results considering scaling groups that define the mechanisms for each of the processes. Compositional reservoir simulation is extremely flexible as it permits the numerical modeling of many physical mechanisms for enhanced oil recovery in a porous media. A wide variety of mechanisms such as chemical kinetics, diffusion, dispersion, gravity and/or drive forces, viscous forces, and capillary effects can be readily examined and analyzed. In addition, multiple components can be used in a 3D examination of complex reservoir properties such as permeability and porosity. Temperature, oil saturation and water saturation profiles and process recovery variables were examined at the three different scales. Results confirmed scalability of the processes when the simulation results were non-dimensionalized. Other parameters included effects of capillary pressure, and other injection parameters on scalability. Scaling approaches are summarized for each process as well as a discussion about the suitability of reservoir simulation as a tool in examining the mechanisms that drive each process and whether or not reservoir simulation supports the scaling groups for the processes.

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Influence of specimen dimensions on tensile behavior of NiTi alloy

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Nitinol is a shape-memory alloy composed of nickel and titanium that can exist in three different states, each with unique properties and behaviors. The three states are martensite, superelastic austenite capable of transforming into stress-induced martensite, and stable austenite. The main variable that affects the presence of these states for given chemical composition of the alloy is the temperature. The Young's modulus of the NiTi alloy is reported to range from 28 to 83 GPa, with higher values corresponding to superelastic austenite. Nevertheless, his Young's modulus is more closely aligned with the elastic properties of human bone than any other metallic material utilized in the field of biomedicine. It is therefore of great importance to identify an appropriate phase composition in order to ensure the convenient superelastic properties and mechanical strength of plates or nails that can be used in traumatology or orthopedics. The mechanical properties of NiTi specimens are studied by the tensile testing that is usually conducted either up to specimens breaking or only to superelasticity region manifestation with subsequent unloading. This work investigates the specimen dimension effect on the tensile behavior for NiTi alloy with the composition of 56.31 wt.% Ni and 43.69 wt.% Ti. The development of the curves at tensile testing of two different dimensions of NiTi was evaluated. The phase composition of the NiTi testing material was determined by XRD and DSC analysis.

This work has been realized in the framework of the following projects: FV40306 "Development of new implants for correction of angular pediatric deformities in sterile design", NU23-08-00043 "Additive manufacturing of NiTi alloys for applications in orthopedics and traumatology" and SGS SP2024/062 - Influence of production, processing parameters and degradation mechanisms on the resulting material properties and lifetime of structural materials.

Impact of nickel addition on the phase composition and properties of Sn-Ag-Cu solder alloys

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Lead-free solders have been adopted widely due to the environmental and health concerns associated with lead. However, these alloys face several challenges that impact their performance and reliability in electronic applications, e.g. high melting temperature, decrease in mechanical properties, and formation of brittle intermetallic compounds. [1] The addition of nickel has the potential to improve the properties of lead-free solder alloys. [2-4] This study focuses on the addition of Ni into the solder alloy with varying nickel content (0.1-4 mass% Ni) using computational thermodynamics and experimental techniques. For the computational part, the phase equilibria of the system was predicted to analyse the effect of nickel on the solder properties. The experimental part employed various techniques (scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction, and differential scanning calorimetry). From the experimental results, it was found that the primary phases identified were Ag₃Sn, β -Sn, and Cu₆Sn₅. At a nickel content of 1 wt.% or higher, the Ni₃Sn₄ phase also appeared. As the nickel content increased, the alloy's melting temperature rose sharply, and changes in the solubility of other elements, as well as the stabilization of the Ni₃Sn₄ and Cu₆Sn₅ phases, were observed. The analysis revealed that Nickel content significantly influences the phase composition of the alloy.

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Assessment of the suitability and durability of a recycled polymer product as a building component

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The aim of this work is to assess the influence of natural environmental conditions (temperature, time, humidity, microorganisms, UV radiation) on the modification of the properties of rubber composites. The study evaluates the suitability and durability of recycled polymer products by investigating changes in tensile strength, hardness and fire performance under natural ageing conditions. Recycled polymers offer environmental benefits, but their long-term properties require careful assessment for practical applications. Samples were exposed to natural weathering for a specified period and mechanical properties were measured periodically. Tensile strength was evaluated to determine structural integrity, hardness to assess surface durability and fire properties to ensure compliance with safety regulations. The results showed an initial slight increase in tensile strength and hardness. With increasing length of exposure, the composite started to degrade gradually which was reflected by a decrease in the monitored parameters. The fire resistance proved to be insufficient as the composite exhibited poor fire safety in both horizontal and vertical directions, but this can be improved by the addition of fire retardants. The study concluded that although recycled polymers show promising durability, specific formulations may require improvements to maintain mechanical properties over time.

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Efficiency of selected sorbents for eliminating PCBs from soil

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Polychlorinated biphenyls (PCBs) are physically and chemically very stable substances with a serious negative impact on the health of the human organism as well as on the surrounding environment. In addition to acute symptoms in the form of dermatoses or nausea, chronic toxicity is especially serious, in the form of hepato-, nephro-, neuro-, immuno- and other toxicities, including hormonal disorders and disorders of the excretory system. Due to their optimal physico-chemical properties, they were massively produced all over the world. Chemko Strážske - a factory in eastern Slovakia, was also an important producer of these substances. Gradually, after the identification of serious toxic effects on health and the environment, the production of PCBs was suspended worldwide (in Czechoslovakia as one of the last countries in 1984). However, due to the prohibition of production and distribution, a large amount of these substances remained in the premises of the former plant and its surroundings, together with the by-products of their production, as a significant toxicological risk. After the partial elimination of solid waste from the premises of the former factory, the question of cleaning up the environment in the wider area also comes up. These are mainly water and soil from the surrounding area. The present paper will present possible technological procedures that can be helpful in removing this environmental burden from surrounding.

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Measuring the toughness of weld joints on a tensile test machine.

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In the tensile strength of weld joints, the sample breaks at the point of least strength or at the point of the defect. If there is a fracture of the basic material, we do not get an overview of the strength of the individual parts of the weld joint [1]. For that reason a shear test have been developed. This process implies that it would be possible to measure shear strength and toughness in butt welds of base materials, in different places of the heat affected zone, in weld metal. Mechanical properties of the welded joint can be characterized by determination of strength and from the force-displacement dependence by the toughness. Shearing in predetermined part of the welded requires fixation of the sample in the required position using a holder. This causes that it is not possible to determine the specific shear energy for samples with different shear areas. Fracture energy consists of two components - shear energy and rupture (final failure) energy. Shear energy is related to the deformation properties of the joint - the energy of deformation until the joint deforms and a crack does not appear, that is, it is related to the resistance to crack formation, the fracture energy to the resistance to crack propagation [2]. The fracture in the shape of the S curve subsequently causes a decrease in the gradient of the decrease in force by mutual friction with the created surface, which increases the value of the measured fracture energy. Therefore, it is possible to exactly determine the energy only up to the maximum value of the force. In the shear test a special device with universal testing machine was used. For accurate force measurement, the strain gauge force sensor of the universal testing machine was calibrated using an externally calibrated strain gauge pressure sensor.

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Analysis of the influence of geometric and material parameters of fixing edge layers on the modal properties of plate structures.

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The appropriate vibroacoustic properties, such as natural frequencies and mode shapes, are very important conditions for the required behaviour of mechanical structures. It is clear that these properties are dependent on the so-called spatial properties, which consist of mass, stiffness and damping properties of the given mechanical structure. In many cases, when the dynamic properties of these structures are unsatisfactory, it is necessary to vary the structural behaviour to solve noise and vibration problems. The technique by which it is possible to achieve the required dynamic properties consists mainly in changing the mass, stiffness and damping properties of the structure, is called structural dynamic modification. The plate structures can be considered as important building components of many technical equipment. These plate structures are very often exposed to periodically repeating dynamic loads and in the case of inappropriately designed parameters of plate structures, these loads lead to the resonant states. This state is inappropriate and the structural modifications of plate structures are necessary. One of the very effective methods of plate structural modification is the method edge fixing of plate and also change of fixation parameters at the edges of the plate structure. The modification of dynamical properties of plate structures using fixing edge layers is presented in this paper. Structural modification of the selected geometrical shapes of plate structures is based on the shapes and geometrical parameters of the layers. By changing the width, thickness and slope of the fixing edge layers is possible to achieve modification of modal properties (especially natural frequencies and mode shapes) of the given plate structures. The results obtained by computer simulations using the ANSYS program confirm that this method of structural modification provides a suitable tool for the so-called "dynamic tuning" of plate structures.

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Theoretical modelling of the frequency-dependent phase shift between emission and excitation in ZnO nanorod photoluminescence spectra

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Hydrothermally growth, zinc oxide (ZnO) nanocrystals are known for their interesting scintillation and photocatalytic properties. In our previous paper we presented an optical setup for measuring spectrally resolved photoluminescence (PL) mean decay time using conventional UV LED with sinusoidal excitation and a phase shift method with about 10 ns time resolution [1], recently upgraded to 1 ns. Photoluminescence decay is the process by which the excited state of a material, induced by the absorption of photons, returns to the ground state, emitting light in the process. This process can be measured in time domain, with the decay rate indicating how quickly the material returns to its ground state after excitation, or equivalently in frequency domain, with the difference between the phase of the light wave at the moment of excitation and the phase of the light wave at the moment of emission. Here we report on the theoretical modelling of the frequency-dependent phase shift between emission and excitation in photoluminescence spectra of ZnO nanorods.

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Surface modification of additively manufactured parts by drag finishing

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The production of parts by additive manufacturing is a quickly progressing area. The issue with additively manufactured parts is surface treatment with conventional methods. One of the possibilities is the treatment of the surface by drag finishing, when it is possible to modify even the complicated shapes of the parts. The article deals with the modification of additively produced parts by drag finishing. The goal was to find out to what extent is it possible to modify the integrity of the surface of parts produced by additive manufacturing. Simple cylindrical parts were produced by Fused Deposition Modelling technology. The parts were made of ABS plastic with different layer thickness. Surface roughness changes over time were monitored. As a drag finishing machine, a device developed at Faculty of Material Science and Technology was used. Two drag finishing media were used for part processing - Al_2O_3 and SiC + walnut shells. It was determined that the roughness of the surface of additively manufactured parts can be significantly improved.

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Site-controlled growth of InGaAs quantum dots with buried stressor for the development of microlasers and quantum light sources

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Quantum dots (QD) have proven to have many applications in optoelectronics [1.], photonics [2.], quantum photonics [3.,4.] and telecommunications [5.]. This work focuses on the systematic optimisation of the growth and fabrication parameters of site-controlled InGaAs quantum dots (SCQDs), grown with buried stressor method [6.], to enhance the precision, uniformity and reproducibility of the quantum dot placement and local density for their advanced optoelectronic applications, such as low-threshold microlasers and quantum light sources. The impact of the growth and the fabrication on the structural and optical properties of SCQDs is thoroughly investigated via atomic force microscopy (AFM), scanning electron microscopy (SEM), confocal laser scanning microscopy (CLSM), X-Ray diffraction (XRD) and photoluminescence (PL) spectroscopy.

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Effect of sample illumination on the content of luminescence active defects in Sn₂P₂S₆ crystals

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Tin hypthiodiphosphate Sn₂P₂S₆ is promising uniaxial semiconductor ferroelectrics with favorable photorefractive properties in the red and near-infrared spectral regions, a pronounced photoconductivity, and large values of pyroelectric, piezoelectric, and electrooptic coefficients. Moreover, Sn₂P₂S₆ crystals exhibit photoluminescence (PL) in the red and near-infrared spectral regions at low temperatures that is related to intrinsic crystal defects [1]. In comparison to conventional orange tinted crystals the photorefractive properties of brown tinted Sn₂P₂S₆ crystals were improved by modification of crystal growth conditions and they are not noticeably sensitive to crystal pre-illumination as well. However, the nature of defects involved in photorefractive processes was not satisfactorily explained up to now. Since PL intensity is sensitive to the photoinduced changes in the content of luminescence active defects and energy levels of the same defects may influence photorefractive properties and photoconductivity of Sn₂P₂S₆ crystals, the dependence of PL intensity on exposure time was studied on four Sn₂P₂S₆ crystals as a function of temperature (12 - 360 K) and illumination wavelength (300 - 800 nm). All the Sn₂P₂S₆ crystals studied showed PL in the red and near-infrared spectral regions. Both PL spectral distribution and integral intensity were markedly sample-dependent under the same conditions. The variations with time of PL intensity were observed for all the crystals at temperatures lower than 170 K as a result of sample illumination with light with wavelength shorter than 710 nm at the same temperatures. The integral PL intensity of all the crystals cooled in the dark decreased at 12 K with time of steady-state excitation with monochromatic light with wavelength shorter than 510 nm. With respect to position of the absorption edge of the Sn₂P₂S₆ crystals near 496 nm at 10 K this finding indicates that PL excitation via the fundamental crystal lattice absorption decreases integral PL intensity of the crystals cooled in the dark. Likewise, the integral PL intensity of the orange tinted crystals cooled in the dark decreased at 12 K with time of steady-state excitation with monochromatic light with wavelength longer than 510 nm. On the contrary an increase of integral PL intensity was observed in the brown tinted crystal demonstrating opposite effect of illumination in the spectral region where PL of Sn₂P₂S₆ crystals is excited through absorption of crystal defects on the integral PL intensity of brown and orange tinted crystals. Heating of the crystal to suitable higher temperature partially or fully restored the initial PL intensity observed in the crystal cooled in the dark pointing to partial or full restoration of the initial content of corresponding luminescence active defects. The possible photoinduced changes of the charge state of supposable luminescence active defects in Sn₂P₂S₆ crystals resulting in the variations with time of PL intensity observed in the crystals illuminated in a suitable way at temperatures lower than 170 K are discussed.

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Polymorphism of methylsalicylatocopper(II) complexes

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Copper complexes containing N-donor ligands are traditionally studied from different points of view, the phenomenon of polymorphism and isomerism of transition metal complexes being one of them. In recent decades, various polymorphs and isomers of carboxylatocopper(II) complexes have been investigated [1,2]. Building upon previous research, we have focused on Cu(II) complexes with various position isomers of methylsalicylate anions (MeSal) in presence of 2-hydroxymethylbenzimidazole (2HMBzim). The synthesis in the presence of 3-methylsalicylate anion led to formation of two complexes with the same composition [Cu(3-MeSal)₂(2-HMBzim)₂] (**1a** and **1b**). The structures of the newly prepared complexes were determined by single-crystal X-ray analysis. The complexes were characterized by spectroscopic methods (IR, UV-vis and EPR spectroscopy). Based on the crystal structures and in accordance with experimental and computational studies it was concluded, that the systems **1a** and **1b** were conformational isomers/polymorphs. With the help of the state-of-the-art computer simulation, it was predicted, that the presence of methanol or acetonitrile as solvents played a pivotal role in folding the molecular components into a specific polymorphic form.

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Nanosecond photoluminescence decay in Mo-doped ZnO nanorods observed by TCSPC and phase shift methods

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Hydrothermally grown, pellet-pressed Mo-doped zinc oxide (ZnO) nanocrystals were investigated for time-resolved photoluminescence at room temperature under UV excitation. Two optical setups were compared. The TCSPC setup was based on ns-short-pulse excitation followed by time resolved histogram-like counting of emitted photons. The phase-shift method was based on the frequency-resolved phase delay between sinusoidal excitation and emission [1]. Whereas the TCSPC method is nowadays a commercially available and widely used, the second method was built as a low-cost student's setup with a conventional UV LED as the excitation source, sine-wave voltage generator, an old dispersive monochromator, optical band-pass and long-pass filters, a red-enhanced photomultiplier and a lock-in amplifier [2]. Recently, the setup was upgraded by a new HF2LI Zurich Instruments 50 MHz lock-in amplifier, which also includes pulse generator and a current amplifier to measure the PMT photocurrent. Both methods gave a similar time resolution slightly below 1 ns. While the time resolution of the TCSPC was limited by the excitation pulse width, the time resolution of the phase shift method was limited by the maximum operating frequency of the UV LED (several MHz). To be able to measure the PL decay in ps range, we need to replace UV LED by a new, faster UV excitation source to increase the excitation frequency up to the 50 MHz limit of our lock-in amplifier.

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CEDEG - a partner for your business, research and innovations

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Biochars from Cardboard as an Alternative adsorbent for the Removal of Pesticides from the Water Environment

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Hydrothermal carbonization (HTC) is a promising method for converting biomass into carbonaceous materials with high adsorption capacity. In this study, we investigated the effect of different HTC conditions on the production of hydrochars from egg cardboard waste and their subsequent efficiency in removing metribuzin from the water environment. Biochars are presented as a sustainable alternative to commonly used sorbents, which often have limitations such as high cost and environmental impact. All hydrochar samples were produced using the same amount of dry biomass and distilled water, varying only the time (2, 3, 4, and 5 h) and temperature (200 °C, 220 °C, 240 °C) of the HTC process. The organic carbon content of each sorbent was measured using the *Ťurin* method modified by Nikitin. Metribuzin removal efficiency was evaluated using comparison measurements after 3 and 6 hours of adsorption. The morphological properties of the hydrochars were analysed by scanning electron microscopy (SEM). The results showed that temperature and HTC time significantly affect the structure, organic carbon content, and adsorption capacity of the hydrochars. The highest metribuzin removal efficiency was observed for samples produced at 240 °C after 6 h, which correlated with a better-developed porous structure and higher organic carbon content confirmed by SEM analysis. Conversely, lower temperatures and shorter HTC times produced hydrochar with a less developed porous structure, lower organic carbon content, and lower adsorption capacity. The study's findings suggest that optimising HTC conditions are crucial for maximizing the efficiency of hydrochars in removing organic contaminants from water environment. These results contribute to a better understanding of the relationship between hydrochar production conditions, organic carbon content, and adsorption properties, which is important for its future applications in water treatment and environmental engineering.

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The impact of generator parameters on cutting width in machining nickel alloys using WEDM technology

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The objective of this study is to analyze the influence of generator parameters on the kerf width in Wire Electrical Discharge Machining (WEDM) technology for the nickel alloy Inconel 718. An experiment was designed using selected parameters that could affect the kerf width based on the acquired knowledge. The introduction covers the general principles of EDM and WEDM technology, discusses the method of spark generation using a generator, and focuses on how electrical discharge machining impacts Inconel 718. The experimental part was conducted on a WEDM machine from Charmilles Technologies. During the experiment, two responses were recorded: the groove width, measured using Dino-Lite and Alicona optical devices, and the cutting speed. The final part of the thesis presents a statistical evaluation of the influence of individual parameters on the cut.

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Thermoelectric properties of doped Bi₂O₂Se

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Over the past decade, Bi₂O₂Se has emerged as an interesting 2D material. It has excellent carrier mobility and mechanical properties in its single crystal form. Thanks to its remarkable transport properties, Bi₂O₂Se has also been explored in polycrystalline form for thermoelectric applications. Bi₂O₂Se is an n-type thermoelectric material characterized by a quasi-2D layered structure. Numerous studies have shown that this material can achieve low thermal conductivity, and its carrier concentration and mobility can be adjusted through doping. In this study, we have examined the substitution of Bi with transition metals, focusing on manganese as a case study. Our analysis of transition metal-doped Bi₂O₂Se polycrystalline samples included X-ray diffraction, scanning electron microscopy, and measurements of electrical conductivity, Seebeck coefficient and thermal conductivity. We compared the solubility limits, transport properties, and other parameters of our samples with existing literature data, offering explanations for the significant discrepancies observed.

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Surface roughness evaluation of the formed parts produced by the multi-pass cold metal spinning applying laser textured tool

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Metal spinning is an incremental forming process based on the forming a flat metal disc on a lathe into many different shapes. It is used in wide spectrum of production areas including those requiring parts with high precision and improved surface integrity. There are a lot of metal spinning parameters which defines and affects the quality of the produced components. Some of them are parameters related to the tool-workpiece interface. These parameters have essential influence on the final surface integrity of processed parts [1-5]. According to this, the paper brings the results of an experimental study of the multi-pass cold metal spinning process employing a laser-textured tool of 90MnCrV8 (1.2842) steel. The tool with a nose radius surface modified by pulse laser machined hexagonally arranged texture made up of dimple-like depressions with a diameter of 100 μm , depth of 20 μm and density of 6 % was applied for testing of surface hardening of DC01 low carbon steel sheet of the thickness 1 mm by applying various spinning tool pass profiles (convex, linear, and concave), mandrel speeds of 400, 800, and 1200 min^{-1} and tool feeds of 0.4, 0.8, and 1.2 mm. On the cylindrical-shaped spun samples the surface roughness of the spun cup wall was evaluated. The measurements in 0°, 45° and 90° directions related to the blank material rolling direction were realised and these responses were compared with those, which have been observed on the parts produced by the conventional, non-textured, tool. The analysis showed that applying a laser-textured roller reduces the arithmetic mean height of the spun part roughness profile R_a by about 30 % compared to this, achieved using the non-textured roller. The R_a reduction of about 15.2 % compared to the initial roughness of the blank material was documented while the influence of the planar anisotropy of the material on the surface roughness was not proven.

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CFD analysis of damping characteristics of a hydraulic damper through geometrical modification and velocity variation

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Shock absorbers or hydraulic dampers are a power dissipating device. Fluid flow passages are responsible for variation in the damping or hydraulic characteristics in terms of damping force with respect to velocity. The piston inside the damper has a various orifice or piston valves that cause different flow losses. They play a crucial role in the performance and stability of systems, especially those involving fluid dynamics and mechanical vibrations. In this work, a Computational Fluid Dynamics (CFD) method is used to study the flow behaviour inside a rear side two-wheeler automobile mono tube damper for different number of orifices in the piston which are two, six and ten orifices opening with changing the throttling velocities based on previous experimental work in the literature. ANSYS 17R software is used to carry out CFD analysis, the continuity, and the Reynolds averaged Navier-Stokes (RANS) equations are used to describe the throttling behaviour inside the rebound and compression chambers. A new proposed model comprises a modification of the throttle valve by changing one of the original models with 6 orifices with geometrical design freedom, aiming to achieve better damping characteristics and design freedom. The damping action has been studied and verified by throttling viscous oil through orifices for different cases. The damping action is not affected by changing the location of the orifice for the same number. It is concluded that the damping force increases with increasing the velocity of the piston. However, the damping coefficient decreases. The damping force decreases as the number of orifices increases in the piston valve. Creating designs that are safe both for the operator, the machine itself and the surrounding environment is par for the course with shock absorbing and vibration technologies.

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Effect of heat treatment on the internal damping of magnesium alloys

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The gradual accumulation of mechanical energy within a material leads to alterations in its mechanical and physical properties. These changes can degrade material performance, resulting in decreased accuracy of machine tools, the initiation of fatigue cracks, increased noise and vibration in the working environment, modifications to material properties, reduced corrosion resistance, and the deterioration of regulatory devices and sensors. Ultimately, this can cause damage to the entire device. Measuring internal damping provides a means to monitor these structural changes and the various mechanisms involved [1, 2]. Today, there is a significant demand for the efficient use of magnesium-based materials. Magnesium alloys are particularly attractive for various industrial applications due to their specific weight, corrosion resistance, density, and strength. The damping capacity of these alloys is closely related to microstructural defects, including solute atoms, secondary phases, and voids. The interaction between moving dislocations and point defects is a primary mechanism of internal friction in magnesium alloys, meaning precipitates affect the damping capacity and contribute to damping properties. Pure magnesium exhibits very high damping capacity at room temperature due to the easy movement of dislocations. However, an increased concentration of solute atoms such as Al, Ca, and Zn, as well as impurities and precipitates, can restrict dislocation mobility, potentially reducing the friction capacity of magnesium alloys [2, 3]. Internal damping is a highly sensitive method effectively used to investigate structural defects and their mobility. It facilitates the examination of transport processes in materials and phase transformations in the solid state, which are otherwise difficult to detect. The experimental setup includes measurement and control components, along with heating and ultrasonic elements. An ultrasound generator produces a sine wave, which is then amplified and converted into a mechanical wave using a piezoceramic transducer.

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Statistical evaluation of the influence of plasma polishing parameters on the material removal rate and the cutting edge radius sizes

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The paper introduces an innovative method for preparing the edges of cemented carbide cutting tools using plasma discharges in an electrolyte. This environmentally friendly technique rounded the cutting edges by immersing the cutting inserts into the electrolyte. The aim of the article is to statistically evaluate the influence of the process parameters on the material removal rate and the cutting edge radius sizes. The measured data were analysed in the software Minitab. Measured responses were normally distributed, thus the assumption for performing ANOVA (Analysis of Variance) analysis was fulfilled. The associated p-value of less than 0.05 for the model (95% confidence level) indicates that the input process parameters in model are statistically significant. From the results of the ANOVA analysis for material removal rate and cutting edge radius sizes, it is obvious, that all observed input process parameters had a significant influence on measured responses. Moreover, the influence of values of individual process parameters (electrolyte concentration, voltage, electrolyte temperature and polishing time) on the cutting edge radius sizes and material removal rate was evaluated.

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0071. This work was supported by the Science Grant Agency - project VEGA 1/0266/23.

Comparison of optical measurement methods utilization for complex high feed tool geometry

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High Feed Machining (HFM) is an advanced machining technique that offers the potential for up to three times faster machining speeds compared to conventional methods. The geometric characteristics of HFM cutting tools differ significantly from those used in traditional machining, posing challenges when it comes to their precise measurement. Cemented carbide solid high feed mills feature specialized end profiles that enable the utilization of chip thinning mechanisms to achieve substantially increased feed rates. Grinding is a widely adopted manufacturing process for production of carbide tools. The tool's geometry is attained through the coordinated movement of the grinding wheel and the workpiece while employing a cooling medium. The precision of the resulting cutting tool geometry directly impacts the machining process. In the context of the experiment, five HFM tools were manufactured. The primary focus was to assess the geometry of these tools using two distinct measurement methods: a dedicated optical measuring machine designed for cutting tools and a 3D optical scanner. The results from each measurement method were subsequently compared and evaluated using the GOM Inspect software. Based on the analysis of measured data, it's possible to confidently determine that optical scanning represents a reliable and effective method for quality control of the macrogeometry of cutting tools.

This work was supported by the Slovak Research and Development Agency of the Slovak Republic under Contract no. APVV-21-0071 and VEGA grant agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences, no. 1/0266/23.

Evaluating surface quality of heterogeneous surfaces produced by non-conventional machining technologies: methodological advances and challenges

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This paper is focused on the evaluation of heterogeneous surface quality. In the realm of scientific practice, there exists a significant inconsistency in the methodologies employed to investigate heterogeneous surfaces produced by non-conventional machining technologies. Traditional approaches are inadequate for these types of surfaces due to the presumption of surface roughness homogeneity, which does not account for the complexities and variations inherent in heterogeneous surfaces. The utilization of unsuitable assessment methods can significantly hinder the research and development efforts related to these advanced technologies, potentially stalling innovation and the optimization of machining processes. However, through an initial investigation of roughness data obtained from heterogeneous surfaces, discernible patterns have emerged. These patterns suggest a promising opportunity for the development of a coherent and standardized approach to surface quality assessment. Such an approach would enhance the accuracy and reliability of evaluations, thereby supporting the continued advancement and refinement of non-conventional machining technologies. The findings underscore the necessity for a shift towards more sophisticated and tailored assessment methods that can accommodate the unique characteristics of heterogeneous surfaces.

This work and the project were realized with financial support from the internal grant of TBU in Zlín No. IGA/FT/2024/002, funded by the resources of specific university research.

New insight into the gas-sensing properties of β -Ga₂O₃ nanowires by near-ambient pressure XPS

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Gas sensors play an essential role in environmental monitoring, medical diagnosis, chemical processing control, energy efficiency, and emission control in combustion processes. Traditionally, various metal oxides have been used as active sensing materials. The key advantages of metal-oxide sensors are their high sensitivity, rapid recovery and response times, low cost, compact size, easy production, and simple measuring electronics. Among the various metal oxides, Ga₂O₃, which is an ultrawide-bandgap n-type semiconductor [1-3], is an excellent material for the detection of both oxidizing (O₂, NO_x, CO₂) and reducing (H₂, CO, NH₃, ethanol, acetone, and CH₄) gases over a wide temperature range [4]. It has been demonstrated that at high temperatures (T>800°C), the formation of oxygen vacancies and complex lattice defects are responsible for their sensitivity. In contrast, at lower temperatures, the sensing mechanism remains unclear, and it is assumed that surface reduction-oxidation reactions play an essential role in sensing. The objective of this study [5] was to evaluate the potential of β -Ga₂O₃ nanorods as gas sensors and to elucidate their sensing mechanism at low temperatures. Using near-ambient pressure X-ray photoelectron spectroscopy, we demonstrated that adsorbed oxygen species play a crucial role in the gas-sensing properties of β -Ga₂O₃ nanorods. Our results confirmed that the interaction of oxidizing/reducing analytes with adsorbed oxygen species changes the resistivity of the β -Ga₂O₃ nanorods and that redox reactions govern the sensing mechanism at low temperatures. Furthermore, we provided new insights into the ethanol-sensing mechanisms at different temperatures. Our findings revealed that at 400°C ethanol reacts with chemisorbed oxygen on the surface of β -Ga₂O₃ via the acetaldehyde pathway, whereas at 100°C, the gas-sensing mechanism includes the adsorption of ethanol molecules, which are partially oxidized to ethoxy due to the dissociative chemisorption of ethanol.

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Electrochemical characteristics of austenitic stainless steel after different times of sensitization

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Austenitic stainless steels are highly resistant to general corrosion in a wide range of corrosive environments. They have good balance of strength and ductility and appropriate toughness at both low and high temperatures. An advantage is also their weldability by most standard welding techniques. Common limitations to the use of austenitic steels are their susceptibility to the pitting in chloride-containing environments and also to the intergranular corrosion after their sensitization. This phenomenon is related to an exposure in the temperature range of 500-800 °C with consequent slow cooling which can lead to chromium content drop under the passivity limit near the grain boundaries due to chromium carbides precipitation. Sensitized, locally chromium depleted austenitic grains become susceptible to intergranular attack typically combined with pitting if aggressive environment contains chlorides. Sensitization of austenitic stainless steel can occur during various industrial and operational processes where the material is exposed to the critical temperatures in the sensitization range for a certain period. It is typical for heat exchangers, especially used in chemical, petrochemical, and oil/gas industries; chemical processing equipment; food processing equipment; intermediate temperature components for nuclear power plants, and also for exhaust systems. The conditions for the significant extensive sensitization of austenitic stainless steels can be determined according to the diagram of carbon solubility in austenite. The minimum sensitization time is affected by various factors as alloy chemical composition, temperature, carbon content and heating rate. Under specific conditions local sensitization can be caused by a short-term heating. This study deals with the corrosion behavior of AISI 304 stainless steel after 10, 6, 2, 1-hour sensitization time at the 650 °C temperature. Sensitization of the specimens is verified by ASTM A262 test. Corrosion resistance is evaluated by electrochemical characteristics of the potentiodynamic polarization performed in 1 M NaCl solution at the temperature 20 ± 3 °C on the specimens with high temperature surface oxides and after their removal by pickling. The electrochemical etching test in oxalic acid confirmed the ditch structure and the complete sensitization after 10 and 6 hours sensitization time. After 1 hour, the material showed only slight local signs of sensitization. The electrochemical characteristics of the potentiodynamic polarization were significantly affected by the surface state of the sensitized specimens. Regardless of the sensitization time, the specimens with high-temperature surface oxides behaved like an actively corroding metal. After pickling, they retained the passivity region, but with a higher passive current density than the as received material.

The research was funded by Scientific Grant Agency of Ministry of Education, Science and Sport of Slovak Republic and Slovak Academy of Sciences, grant KEGA 016ŽU-4/2023.

Transport properties deviation of polycrystalline Bi₂O₂Se: Causes and solutions

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Bismuth oxyselenide (Bi₂O₂Se) is a promising thermoelectric (TE) material known for its high carrier mobility, non-toxic composition, and cost-effectiveness. However, its low intrinsic electrical conductivity necessitates doping to enhance performance. A major challenge is the significant variation in transport properties of bulk polycrystalline samples, even when synthesized using similar methods. This study examines the causes of these deviations and suggests solutions. Through analysis of literature and synthesis of samples using different compounds and methods, we identified that impurities and foreign phases significantly impact the transport properties of undoped Bi₂O₂Se. Techniques such as powder X-ray diffraction (PXRD), scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDS), Raman spectroscopy, and ATR IR spectroscopy were used to detect these impurities. To combat this issues, we propose a reproducible low-temperature solid-state synthesis process to produce high-purity Bi₂O₂Se. This method minimizes presence of high temperature associated secondary phases and ensures a consistent crystal structure, leading to improved and reliable transport properties. By refining synthesis techniques and controlling impurity levels, we aim to establish a standard for achieving consistent performance in Bi₂O₂Se.

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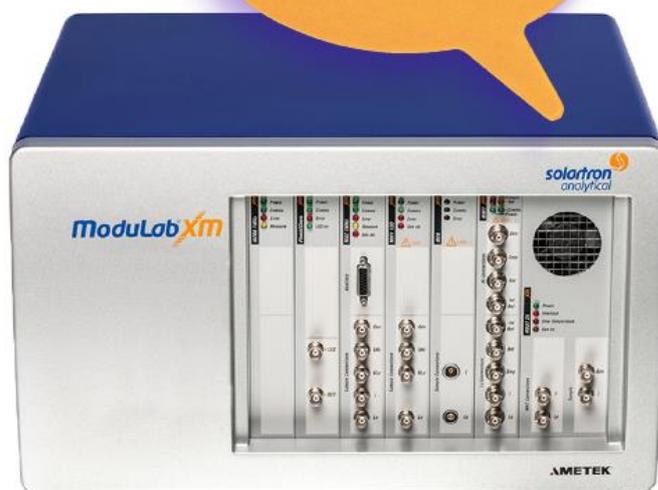


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