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2022

**The 4th International Conference on Materials:
Advanced and Emerging Materials**

19–21 October 2022 | Barcelona, Spain

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4th International Conference on Materials: Advanced and Emerging Materials

MGS Auditorium
Barcelona, Spain
19 – 21 October 2022

Conference Chairs

Prof. Dr. Maryam Tabrizian
Prof. Dr. Filippo Berto

Organised by



Conference Secretariat

Elena González	Delia Dragusin
Selina Yang	Divena Dai
Yulia Zhao	

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**4th International Conference on Materials:
Advanced and Emerging Materials**
19 – 21 October 2022, Barcelona, Spain

	Wednesday 19 Oct 2022	Thursday 20 Oct 2022	Friday 21 Oct 2022
Morning	Registration Welcome <i>S1. Materials Characterization - Part I</i>	<i>S4. Soft and Bio-materials - Part I</i>	<i>S4. Soft and Biomaterials - Part II</i>
	Coffee Break	Coffee Break	Coffee Break
	<i>S2. Nanotechnology in Material Sciences and Engineering - Part I</i>	<i>S3. Materials Processing and Manufacturing</i>	<i>S2. Nanotechnology in Material Sciences and Engineering - Part II</i>
	Lunch	Lunch	Closing Remarks & Awards Ceremony
Afternoon	<i>S6. Optical, Electrical and Magnetic Materials</i>	<i>S1. Materials Characterization - Part II</i>	
	Coffee Break & Poster Session A	Coffee Break & Poster Session B	

Wednesday 19 October 2022: 08:15 - 13:05 / 14:35 - 17:40

Thursday 20 October 2022: 09:00 - 13:05 / 14:35 - 17:50 / **Conference Dinner: 20:00**

Friday 21 October 2022: 09:00 - 13:15

Conference Programme

Wednesday 19 Oct 2022

- 08:15 Registration Desk Open (Check-in)
08:45 – 09:00 Welcome from the Chairs
09:00 – 09:45 **Plenary Talk** : **Kazunori Kataoka** - Engineered nanosystems and nanoconjugates with smart functionalities for targeted therapy of intractable diseases
Chair: **Maryam Tabrizian**

Session 1. Part I

Materials Characterization

Session Chairs: **Tomasz Garbowski** and **Emil Babić**

- 09:45 – 10:00 **Emil Babić** - Are compositionally complex alloys intrinsically better than conventional ones?
10:00 – 10:15 **Damian Mrówczyński** - The role of imperfections in numerical homogenization of multi-layered panels with a corrugated core
10:15 – 10:30 **Natalia Staszak** - Numerical homogenization of three-layer plates with a soft core
10:30 – 10:45 **Lukmanul Hakim Zaini** - Nanofibrils from oil palm trunk: Effect of delignification and fibrillation technique
10:45 – 11:00 **Ewa Olewnik-Kruszkowska** - The role of surfactants in the formation of homogenous polymeric films based on polylactide and cellulose acetate propionate

11:00 – 11:30 **Coffee Break**

Session 2. Part I

Nanotechnology in Material Sciences and Engineering

Session Chairs: **Tohid Didar** and **Danatbek Murzalinov**

- 11:30 – 11:50 **Keynote Talk** : **Tohid Didar** - Micro and nano engineered bio-interfaces for diagnostics, therapeutics and public health
11:50 – 12:05 **Ateeque Siddique** - Chemotherapy-Eluting Nanoparticle Acrylic Bone Cement for Local Adjuvant Treatment of Spinal Metastases

- 12:05 – 12:20 **Shadmad Khan** - Patterning Pathogen-responsive DNAzymes onto Food Packaging for Real-time Food Monitoring in situ
- 12:20 – 12:35 **Chongchong Tang** - Phase formation and thermal stability of quaternary MAX phase thin films in the Cr-V-C-Al system: an experimental combinatorial study
- 12:35 – 12:50 **Danatbek Murzalinov** - Formation of light-emitting particles with different parameters by coating ZnO on a silicon surface with several porosity levels
- 12:50 – 13:05 **Alessandro Corozzi** - Bioinspired Hydrophobic Coatings for Antifouling Application

13:05 – 14:35 Lunch

Session 6

Optical, Electrical and Magnetic Materials

Session Chairs: **Federico Bella** and **Kristen Dellinger**

- 14:35 – 15:05 **Invited Talk** : **Federico Bella** - Advanced Materials Supporting the Lithium and post-Lithium Energy Technologies
- 15:05 – 15:20 **Agnieszka Pawłowska** - A new type of an Organic Memristive Device based on interactions between polymer thin-films
- 15:20 – 15:40 **Keynote Talk** : **Kristen Dellinger** - Next-generation substrates for surface-enhanced Raman spectroscopy
- 15:40 – 15:55 **Anamika Kumari** - A scheme to determine the carrier density distribution, potential profile, and subband quantization of a conducting interface LaVO₃/SrTiO₃

15:55 – 17:25 Coffee Break and Poster Session A

Thursday 20 Oct 2022

09:00 – 09:45 **Plenary Talk** : **Molly Shoichet** - Emulating the Environment : Soft Materials Enable 3D Cell Culture

Chair: **Maryam Tabrizian**

Session 4. Part I

Soft and Bio-materials

Session Chairs: **Derek Rosenzweig** and **Frej Mighri**

09:45 – 10:05 **Keynote Talk** : **Derek Rosenzweig** - Leveraging 3D biofabrication, bioengineering and biophysical approaches for musculoskeletal tissue regeneration and local therapeutic delivery

10:05 – 10:20 **Leandro S. Oliveira** - Preparation of hybrid films of locust bean galactomannans and starch from cassava peels

10:20 – 10:35 **Florina Daniela Cojocar** - Polysaccharides-calcium phosphates beads for the treatment of osteoporotic fractures

10:35 – 10:50 **Frej Mighri** - Development and characterization of biocompatible porous PLA-Chitosan scaffolds without solvent treatment

10:50 – 11:05 **Piotr Rychter** - Hydrolytic degradation of methylene carbonate/lactide copolymers with functional, active carboxylic side groups as a carrier of biologically active agent, including drugs for use in dermatology and cosmetology

11:05 – 11:35 **Coffee Break**

Session 3.

Materials Processing and Manufacturing

Session Chairs: **Antanas Ciuplus** and **Regita Bendikiene**

11:35 – 11:50 **Rafał Zybala** - Residual stress measurement and properties investigation of cold sprayed titanium and titanium alloy coatings after laser surface treatment

11:50 – 12:05 **Katherine Pérez** - Formation of PEO coatings on binary material Mg-33wt%Ti processed by high energy ball milling (HEBM)

- 12:05 – 12:20 **In Gyeong Kim** - Manufacture of Invar Sheets Using a Continuous Electrodeposition Technique for the OLED FMM
- 12:20 – 12:35 **Sharon Koppka** - Influence of microstructure and porosity on bending strength of nanoporous, selective laser-sintered glasses
- 12:35 – 12:50 **Jorge Santos** - Effect of a physical vapor deposition film applied on decorative electroplated coatings of plastic substrates
- 12:50 – 13:05 **Anne-Marie Layher** - Additive Manufacturing of Preforms for Special Glass Fibres made of Al-doped Fused Silica

13:05 – 14:35 Lunch

Session 1. Part II Materials Characterization

Session Chairs: **Joseph Poon** and **Lilia Sabantina**

- 14:35 – 15:05 **Invited Talk : Joseph Poon** - High-Entropy Alloys: Opportunities, Challenges, and Progress
- 15:05 – 15:20 **Huseyin Zengin** - Evolution of microstructure, mechanical properties and corrosion resistance of Mg–2.2Gd–2.2Zn–0.2Ca (wt%) alloy by extrusion at various temperatures
- 15:20 – 15:35 **Adriana S Franca** - Development of antioxidant films based on oil/water emulsions with sunflower proteins and cellulose nanoparticles
- 15:35 – 15:50 **Jakub Mokrzycki** - Assessment of ammonium ions removal from aqueous solutions using zeolite-composite materials derived from fly ash
- 15:50 – 16:05 **Constantin Mulaja Tshakatumba** - Tailings recycling into fired building bricks and anti-acid bricks
- 16:05 – 16:20 **Nadia Muhammad Hussain** - Characterization and Minimization of the Four-Point Probe for Direct Blood Impedance Measurements in Vacutainer Tube

16:20 – 17:50 Coffee Break and Poster Session B

20:00 Conference Dinner at Abrassame

Friday 21 Oct 2022

Session 4. Part II
Soft and Bio-materials

Session Chairs: **Roman Perez** and **Pierre Bagnaninchi**

- 09:00 – 09:30 **Invited Talk : Roman Perez** - Therapeutic biomaterials for the stimulation of tissue regeneration
- 09:30 – 09:50 **Keynote Talk : Pierre Bagnaninchi** - Imaging cell and tissue physical properties
- 09:50 – 10:05 **Martin Humenik** - Microstructured arrays based on self-assembled fibrillar networks for specific cell immobilization
- 10:05 – 10:20 **Raquel Giménez** - Soft functional materials by bottom-up 1D assembly of pyrazole dendrons
- 10:20 – 10:40 **Keynote Talk : Arnab Chanda** - Investigation of Mechanical Properties in Novel Auxetic Skin Grafts
- 10:40 – 10:55 **Faisal Abdelrahim** - Influence of Anodization Parameters on The Surface and Corrosion Resistant Characteristics of Titanium Nanotubes Formed on Ti Substrate in Simulated Body Fluids

10:55 – 11:30 **Coffee Break**

Session 2. Part II
Nanotechnology in Material Sciences and Engineering

Session Chair: **Zeinab Hosseinidoust**

- 11:30 – 12:00 **Invited Talk : Konstantin Neyman** - In-silico designing bimetallic nanoparticles
- 12:00 – 12:15 **Zeinab Hosseinidoust** - Self-Assembling Nanofibrous Viral Microgels as Sprayable Antimicrobials Targeting Multidrug-Resistant Bacteria
- 12:15 – 12:30 **Mansi Pahuja** - Ni-Foam-Graphene-CNTs-SnSeP: An efficient electrocatalyst covering universal pH range and tap water splitting for hydrogen evolution reaction
- 12:30 – 12:45 **Karolina Ogródowska** - Nanosilica Modification of Epoxy Matrix in Hybrid Basalt-Carbon FRP Bars - Impact on Microstructure and Mechanical Properties
- 12:45 – 13:00 **Gema Tabares** - Fabrication of MoTe₂(1-x)Se_{2x} alloy-based hydrogen gas sensor

13:00 **Awards Ceremony and Closing Remarks**

Welcome from the Chairs

Dear colleagues, friends, and the wider material science community:

On behalf of the organizing committee, it is our great pleasure to invite you to the 4th International Conference of Materials, organized by MDPI's Open Access journal *Materials*. This conference will be held in the beautiful city of Barcelona from October 19 to October 21, 2022. The first three editions of the conference were in electronic format, and each was a great success. This has encouraged the organizing committee to take this tradition to the next level by organizing the 4th edition of this conference in Barcelona, where all stakeholders working on various aspects of materials science and material engineering can come together. The aim is to make this event a forum for discussion, knowledge exchange and fruitful interactions among participants in this exponentially growing field.

Stakeholders from academia and industry as well as from governments and research institutes are welcome to join this event and share their findings on various topics related to materials, such as:

- Materials Characterization
- Nanotechnology in Material Sciences and Engineering
- Materials Processing and Manufacturing
- Soft and Bio-materials
- Fibers and Membranes
- Optical, Electrical and Magnetic Materials

We are very enthusiastic about this 4th Materials Conference and are relying on you to make it a successful event.

We look forward to meeting you in Barcelona!

Prof. Dr. Maryam Tabrizian
Conference Chair



Editor-in-Chief of *Materials*.
McGill University, Canada

Prof. Dr. Filippo Berto
Conference Chair



Associate Editor-in-Chief of
Materials. Norwegian University of
Science and Technology, Norway



materials

an Open Access Journal by MDPI

Materials (ISSN 1996-1944) is a peer-reviewed, open access journal of materials science and engineering published semimonthly online by MDPI. *Materials* provides a forum for publishing papers which advance the in-depth understanding of the relationship between structure, properties, and functions of all kinds of materials. It covers all aspects of materials science and engineering including synthesis, structure, mechanical, chemical, electronic, magnetic, and optical properties, as well as their various applications.

Among other databases, *Materials* is indexed by the Science Citation Index Expanded (Web of Science), MEDLINE (PubMed), and Scopus.

Journal Webpage: <https://www.mdpi.com/journal/materials>

Impact factor: **3.748** (2021); 5-Year Impact Factor: 4.042 (2021)

MDPI, the Multidisciplinary Digital Publishing Institute, is a publisher of fully peer-reviewed, Open Access journals with a focus on robust and rapid editorial processes. Our aim is to ensure that high-quality research is verified and made available to the research community as quickly as possible. MDPI stands at the forefront of the Open Access movement, having launched its first online journal *Molecules* in 1996. Today, MDPI is a leader in Open Access, publishing more than 400 journals across all research disciplines and offering publishing-related initiatives to scholars:

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- Preprints - A multidisciplinary not-for-profit platform for rapid communication of research results before peer-review.
- JAMS - A complete manuscript submission system that incorporates all steps from initial submission to publication, including peer-review.
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If you would like more information about open access or any of our services listed above, be sure to talk to us at the MDPI booth. See you there!



4th International Conference on Materials: Advanced and Emerging Materials will be held at the MGS Auditorium, Barcelona, on 19 – 21 October 2022.

This conference seeks to gather experts in the field of Advanced and Emerging Materials, and aims to provide a forum for discussion, knowledge exchange and fruitful interactions among participants in this exponentially growing field.

Conference Venue

MGS Auditorium
Carrer d'Entença, 335, 08029 Barcelona

Registration Desk

The desk for registration, information and distribution of documents will be open from 08:15h on 19 October 2022.

Certificate of Attendance

Participants of the event will be able to download an electronic Certificate of Attendance by accessing their dashboards on Sciforum.net once the event is concluded. The certificates will be found under "My Certificates" category.

Disclaimer

Delegates will receive a name-badge at the Information Desk, upon registration. The badge must be worn prominently in order to gain access to the congress area during all scientific and social events. Admission will be refused to anyone not in possession of an appropriate badge.

Insurance

The organizers do not accept liability for personal accident, loss, or damage to private property incurred as a result of participation in *ICM 2022 –The 4th International Conference on Materials: Advanced and Emerging Materials*. Delegates are advised to arrange appropriate insurance to cover travel, cancellation costs, medical, and theft or damage of belongings.

Barcelona and Catalonia

Barcelona is the capital and largest city of Catalonia and is Spain's second largest city, with a population of over one and half million people.

Located on the northeastern Mediterranean coast of Spain, this city has a rich and diverse history, with its roots dating back to Roman times. The fruitful medieval period established Barcelona's position as the economic and political centre of the Western Mediterranean. The city's Gothic Quarter bears witness to the splendour enjoyed by the city from the 13th to the 15th centuries.



The 20th century ushered in widespread urban renewal throughout Barcelona city, culminating in its landmark Eixample district, which showcases some of Barcelona's most distinctive Catalan art-nouveau, or modernista, buildings. The Catalan Antoni Gaudí, one of the most eminent architects, designed buildings such as La Pedrera, the Casa Batlló and the Sagrada Família church, which have become world-famous landmarks.

In 1992, Barcelona gained international recognition by hosting the Olympic games which brought about a massive upturn in its tourism industry. For visitors, this has translated into the very modern, yet incredibly old city you see now in the 21st century, where new elements work to both preserve and celebrate both the city's heritage and origins.

Barcelona is plenty of outdoor markets, restaurants, shops, museums, and churches. The city is also very walkable, with an extensive and reliable Metro system for more far-flung destinations.

For a complete overview, see [wikitravel.org](https://www.wikitravel.org/en/Barcelona) or visit [barcelonaturisme.com](https://www.barcelonaturisme.com).

The MGS Auditorium

Address: Carrer d'Entença, 335, 08029 Barcelona

The conference will be held at MGS Auditorium, Barcelona, Spain. The MGS Auditorium is located next to Avenida Diagonal, one of the most modern areas of Barcelona and also the main financial area of the city.

The MGS auditorium can be accessed through the lifts located at the reception of the MGS building. **Take any of the four lifts to the -1 floor.** It can also be accessed through the interior stairs.



Conference Dinner

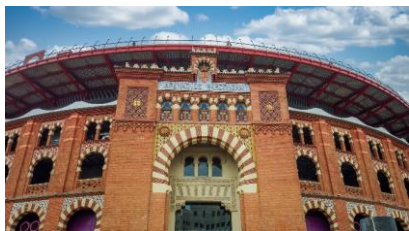
Thursday 20 October, 20:00

Price: 40€ Tickets must be purchased in advance, but you can ask for availability at the Information Desk.



We invite you to join us at the Conference Dinner at **Abrassame**, a cutting-edge restaurant specialised in Mediterranean cuisine which, in addition to its location at the picturesque terrace of Arenas de Barcelona, will make of your evening at the restaurant an experience to remember.

Abrassame is located at the top of **Arenas de Barcelona** (Address: Gran Via de les Corts Catalanes 373 – 385), only a few minutes away from one of Barcelona's most emblematic must-sees, Montjuïc. You can easily reach the restaurant from the conference venue either by foot, taxi, or public transport (buses number D40 or V7). To reach the terrace, you could either use the exterior elevator (adults 1€; children, seniors over 65 years old, and people with reduced mobility are free) or climb through the stairs/elevators inside the shopping centre (free).



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Emergency Information

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Ambulance (Ambulancia) and health emergencies: 061 or 112
Fire brigade (Cuerpo de bomberos): 080 or 112
Spanish National Police (Policía nacional): 091

Abstracts

Talks

Engineered nanosystems and nanoconjugates with smart functionalities for targeted therapy of intractable diseases

Kazunori Kataoka

Innovation Center of NanoMedicine, Kawasaki Institute of Industrial Promotion, Kawasaki, Japan

Nanotechnology-based medicine (nanomedicine) has received progressive interest in treating and diagnosing intractable diseases, such as cancer. Engineered polymeric nanosystems play a pivotal role in nanomedicine as drug carriers, gene vectors, and imaging probes. This presentation focuses on the present status and future trends of polymeric nanosystems and nanoconjugates with smart functionalities for the therapy of intractable diseases. Polymeric nanosystems of 10 to 100 nm in size can be prepared by programmed self-assembly of block copolymers in an aqueous entity. A typical example is polymeric micelle (PM) with distinctive core-shell architecture. Smart functionalities, such as pH- and/or redox potential responding properties and endosomal escaping capabilities, can be integrated into the PM structure. Specific ligands may be installed on the PM surface to exert functionalities of crossing histological barriers, such as the blood-brain barrier. These smart PMs loaded with various chemotherapy reagents were proven to have a significant utility in treating intractable cancers. Five different formulations of the PMs developed in our group have already proceeded into clinical trials worldwide. Versatility in drug incorporation is another relevant feature of polymeric nanosystems for drug delivery. Nucleic-acid-based medicine, such as pDNA, mRNA, and oligonucleotides, can be self-assembled with oppositely charged polycationic block copolymers into nanosystems through the ionic interaction (polyplex micelle). A phase I clinical trial using the polyplex micelle loaded with siRNA has started in Japan to treat recurrent breast cancer.

Furthermore, smart nanoconjugates of checkpoint blockade antibody (anti-PDL1 antibody) have been developed in our group to treat intractable glioblastoma multiforme (GBM). Anti-PDL1 antibody was decorated with glucosylated PEG to cross the blood-brain tumor barrier of GBM by recognizing glucose-transporter overexpression on GBM capillaries. By sensing the reductive microenvironment of GBM, PEG palisades are removed from the antibody to recover its checkpoint-inhibiting ability, exerting effective immune-checkpoint blockade (ICB) therapy to achieve the complete remission of GBM.

Are compositionally complex alloys intrinsically better than conventional ones?

Emil Babić¹, Đuro Drobac², Ignacio A Figueroa³, Mathilde Laurent-Brocq⁴, Željko Marohnić⁵, Stefan Michalik⁶, Vesna Mikšić-Trontli⁷, Loic Perriere⁴, Petar Pervan⁵, Ramir Ristić⁸, Amra Salčinović-Fetić⁹, Krešo Zadro¹

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Despite a huge expansion of research on compositionally complex alloys, CCA (such as the approximately equimolar, multi-component high-entropy alloys, HEA and the corresponding high-entropy glassy alloys), their basic understanding is still limited, which is detrimental both for the design of CCAs and for their application. In particular, the prediction of compositions capable of forming random solid solutions (RSSs) and the prediction of their properties is still a problem. Nevertheless, some properties of a few CCAs exceed those of conventional alloys (CA) [1].

The broad compositional range of CCAs enables simple tuning of their properties by varying the contents of their constituent elements. Accordingly, the study of the transition from CCA to CA composed from the same constituents is very important, both for understanding the formation of RSSs in CCAs and for proper evaluation of their potential with respect to that of CAs. However, this transition has so far been studied systematically in only two types of alloys: five isopleths of the CrMnFeCoNi (Cantor) alloy [2] and glassy TiZrNbCuNi/Co alloys with variable Co, Ni or Cu content [3]. Here, we review the effects of the transition from HEA to CA compositions on several properties of these alloys.

In both alloy systems, the variation of a given property with composition depends heavily on the selected principal component (thus, on the evolution of interatomic correlations and related electronic structure) and can be either monotonic (like that in the ideal solid solutions) or non-monotonic. When the variation is non-monotonic, the maximum value of the selected property rarely occurs around the equimolar (HEA) composition.

References

[1] E. P. George, D. Raabe and R. O. Ritchie, *Nat. Rev. Mater.* 4 (2019) 515

[2] G. Bracq et al, *Acta Mat.* 177 (2019) 266 and ref. therein

[3] R. Ristić et al, *J. Appl. Phys.* 130 (2021) 195102; E. Babić et al, *Materials* 14 (2021) 5824 and ref. therein

The role of imperfections in numerical homogenization of multi-layered panels with a corrugated core

Damian Mrówczyński¹, Tomasz Garbowski²

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2 Department of Biosystems Engineering, Poznan University of Life Sciences, ul. Wojska Polskiego 50, 60-627 Poznań, Poland

Multi-layered panels with a corrugated core are usually thin plates composed of very thin layers. One of the most popular examples of such plates is corrugated cardboard, which is an ecological material that is widely used in the packaging industry. To determine the behavior of cardboard, it is necessary to know its strength parameters from several basic laboratory tests, e.g., edge crush resistance, bending, shear, torsional stiffness and many others. Correctly calculating these parameters is crucial as they are often used to analytically determine the load capacity of corrugated board packaging. An additional factor that must be taken into account for the numerical simulation of the behavior of laboratory samples is the initial imperfections, which are of great importance in the compression of the cardboard layers. In the present communication through the use of the finite element method (FEM), the initial global stiffness matrix of the detailed model was determined, which, after condensation, was utilized in the homogenization process. The homogenization method based on elastic strain energy equivalence transformed the 3D model of the corrugated board into an equivalent plate with effective parameters. The method was verified using experimental data and data from the literature. Satisfactory compliance with the experimental data was obtained.

Numerical homogenization of three-layer plates with a soft core

Natalia Staszak¹, Tomasz Garbowski²

1 Doctoral School, Department of Biosystems Engineering, Poznan University of Life Sciences, Poland

2 Department of Biosystems Engineering, Poznan University of Life Sciences, ul. Wojska Polskiego 50, 60-627 Poznań, Poland

Sandwich structures are widely used in many sectors of engineering. They are used in construction but also in the electronics and aviation industries. Their great popularity results, among others, from the fact that the layers of the structure can be freely selected in such a way as to meet specific requirements. In the case of multi-layer panels used in construction, they must meet the appropriate acoustic, thermal insulation, and load-bearing requirements but must also be resistant to various biological or chemical factors. The standard selection of multilayer panels is usually based on the manufacturer's available catalogs. However, in the case of the appearance of holes or non-standard dimensions of plates, this approach is useless. Then, in the calculations, full 3D models must be used, which is very time-consuming and requires specialist knowledge; therefore, the solution to this problem may be the use of a simplified model obtained thanks to one of the homogenization methods. Numerical homogenization allows us to simplify the model computationally and replace the complex structure with a homogeneous plate with equivalent parameters, which ensures very similar behavior to the three-dimensional reference model. The paper presents the procedure of numerical homogenization based on the equivalence of the strain energy. The proposed method was used to analyze a three-layer board with a soft core and with an opening. The complex 3D model of the plate with all details was reduced to a plate element of effective stiffness. The obtained results from the simplified model were compared with the results of the full 3D model. This method allows for the proper homogenization of complex multi-layer structures with a soft core, without the need to create full 3D models.

Nanofibrils from oil palm trunk: Effect of delignification and fibrillation technique

Lukmanul Hakim Zaini^{1, 2}, Stefan Veigel¹, Claudia Gausenbauer¹, Istie Sekartining Rahayu², Muhammad Adly Rahandi Lubis³, Andreas Mautner⁴, Wolfgang Gindl-Altmutter¹

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4 University of Vienna, Austria

Oil palm trunks represent a potential raw material for the preparation of cellulose nanofibers (CNF). The manufacturing of CNF has typically involved the pretreatment and the mechanical fibrillation stage. However, the different methods used will be affecting the resulting CNF from OPT. In order to understand the effect, this study was done to apply less severe delignification and fibrillation techniques to OPT and then further investigate their influence on fibril properties. Morphology analyses showed less severe delignification and fibrillation techniques resulting in rougher surface, low interfacial adhesion, and higher fiber diameter. However, particle size distribution was found comparable between B-H-OPT and A-MH-OPT. FTIR analysis showed minor changes in the chemical compositions following the alkaline treatment and the bleaching process, whereas the samples subjected to mechanical treatment only remained similar. Rheology analysis exhibited the less viscous characteristics of less severe delignification and fibrillation techniques. Less negative zeta-potential after alkali treatment and more negative zeta after oxidation were detected lower electrophoretic mobility while only a slight decrease in zeta potential value after mechanical treatment. TGA analyses showed OPT began to decompose at 253 °C, while less severe delignification exhibited lower thermal stability.

The role of surfactants in the formation of homogenous polymeric films based on polylactide and cellulose acetate propionate

Ewa Olewnik-Kruszkowska, Magdalena Gierszewska

Nicolaus Copernicus University in Toruń, Faculty of Chemistry, Gagarina St. 7, Toruń, Poland

Currently, most products need packaging, especially food. It is an indisputable fact that biodegradable polymers have begun to play a significant role in the packaging process. Consumers are interested in safe and high-quality food while being increasingly conscious of the environmental implications related to disposing of packaging. For this reason, it should be noted that the packaging market is developing towards biodegradable active packaging that is safe for the environment and simultaneously prevents unfavourable changes in the freshness of products. This group of biodegradable polymers includes polylactide (PLA) and cellulose acetate propionate (CAP)—the polymers that are the object of the presented project. The formation of blends consisting of the PLA and CAP seems to be an avenue of research resulting in obtaining a promising material characterised by reduced manufacturing costs of products and desired properties. However, it should be stressed that PLA and CAP form incompatible blend systems. For this reason, a compatibilizer has to be applied. In the ongoing work, six non-ionic surfactants that differ in hydrophilic–lipophilic balance were used as compatibilizers. They have all been approved for contact with food by the Food and Drug Administration. It should be stressed that only a few papers have described the effect of surfactants on the properties of polymeric blends [1,2], which clearly outlines the novelty of the performed study.

Analysis of the obtained films allowed us to establish the most suitable type of surfactant to improve the compatibility of PLA and CAP. Moreover, the compositions of materials containing PLA, CAP, and the selected surfactant, which were characterised by the most favourable mechanical properties and water vapour resistance, have been determined.

References

- [1] Journal of Membrane Science (2022) 120426
- [2] Carbohydrate Polymers 90 (2012) 1452–1460

Micro- and nano-engineered bio-interfaces for diagnostics, therapeutics and public health

Tohid F. Didar

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The biological/non-biological interface system is an important cornerstone for the fabrication of a wide range of biomedical devices. Platforms as diverse as lab-on-chip and point-of-care diagnostics, 3D tissue culture scaffolds, organs-on-chips, implants and antimicrobial surfaces all rely on the effective interaction of cells and/or bio-recognition elements (proteins/peptides, enzymes, oligonucleotides, etc.) with non-biological surfaces. The design and engineering of micro-/nano-patterned interfaces provide powerful tools to study biological phenomena at a micro- and nano-scale and to develop novel technologies for diagnostics and therapeutics. I will present an overview of our research on micro-/nano-scale design of novel biomedical coatings and their integration into in vitro systems such as lab-on-chip, flexible sensing interfaces and antimicrobial coatings as well as in vivo applications to develop efficient medical devices such as catheters and vascular grafts. These will include using lubricant-infused coatings as well as hierarchical micro-/nano-structures for preventing biofouling, pathogen adhesion and blood coagulation.

Chemotherapy-Eluting Nanoparticle Acrylic Bone Cement for Local Adjuvant Treatment of Spinal Metastases

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Polymethylmethacrylate acrylic bone cement is used to fill critical-sized defects created by the surgical resection of spinal metastases. Tumor cells remain hidden and drive cancer recurrence. Doxorubicin (DOX) is a common chemotherapeutic drug; however, it is cardiotoxic when administered systemically. Mesoporous silica nanoparticles are gaining attention for targeted drug delivery to bypass the negative side effects associated with systemic drug administration. Our objectives were to develop a nanoparticle cement for the local release of DOX and test its ability to suppress cancer cells. Various amounts of DOX were loaded onto nanoparticles, and they were then mixed into the cement at 2% and 8% w/w formulations. The drug release from the cement constructs was measured over a period of 4 weeks. The cement constructs were incubated with both 2D and 3D cultures of breast and prostate cancer cell lines, and cell metabolic activity and viability were evaluated. Additionally, cell migration and spheroid growth were assessed in 3D collagen-coated spheroid cultures. A sustained DOX release profile was achieved with the addition of nanoparticles to the bone cement. The release profile of DOX from nanoparticle cement can be modified by changing the amount of the drug loaded onto the nanoparticles and the proportion of nanoparticles in the cement. Cancer cells treated with the cement constructs showed dose- and time-dependent inhibition. Furthermore, cell migration and spheroid growth were impaired in 3D culture. We determined that nanoparticles are essential for a sustained DOX release profile from acrylic bone cement. The release can be modified for an optimal local drug-delivery system. Our findings demonstrate that chemotherapeutic cements can inhibit cancer cells and impair their migration.

Patterning Pathogen-responsive DNazymes onto Food Packaging for Real-time Food Monitoring in situ

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Foodborne illnesses continue to devastate human health globally, with over 600 million cases annually, millions of hospitalizations, and a death toll estimated to be over 420,000. The economic ramifications are similarly severe, with billions of dollars being spent each year on the treatment of such illnesses. Current measures aimed at identifying bacterial pathogens within food products involve lab-based processing and culturing of collected samples, which is an expensive and laborious process. More importantly, its time-consuming nature means that products are distributed before culturing results are obtained. If a pathogen is detected, retroactive food recalls cost manufacturers tens of millions of dollars. While several platforms aimed at real-time pathogen detection have been developed in recent years, they are still expensive and laborious and often exhibit poor detection sensitivity. They also cannot be embedded within packaging but rather require packages to be opened and sampled. This makes individual product monitoring unfeasible. To address this need, we have developed an in situ detection platform using pathogen-responsive RNA-cleaving fluorescent deoxyribozymes (RFDs), which exhibit a significant increase in fluorescence when exposed to their target bacterium. Amine-modified RFDs can be covalently immobilized onto oxygen or carbon dioxide plasma-activated food packaging materials using various chemical crosslinkers. Patterned deposition of the RFDs via contact or non-contact printing approaches yields well-defined microarrays. A handheld fluorescence reader can then be used to monitor these arrays in real-time without the need to open packaging. We have substantiated this technology using *Escherichia coli*-responsive RFD microarrays immobilized onto packaging materials, which demonstrate high stability, sensitivity, and specificity when incubated with contaminated food samples. By using a range of different pathogen-responsive RFDs, we aim to develop a fluorescence barcode that can detect several foodborne pathogens in parallel. The simplicity of the system ensures accessibility to all users along the food production and distribution pipeline.

Phase formation and thermal stability of quaternary MAX phase thin films in the Cr-V-C-Al system: an experimental combinatorial study

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$M_{n+1}AX_n$ phases are atomically layered ternary carbide and nitride compounds that possess remarkable and unusual combination of properties. Tailoring of individual atomic layers via alloying to synthesize quaternary MAX phases is attracting unprecedented interest with discovery of new solid solution and ordered phases.

Nowadays, there is tremendous interest in MAX phase thin films for applications in surface engineering. Intensive efforts are ongoing to explore new approaches for high-quality (i.e., single-phase and textured) ternary thin films, while synthesis of quaternary thin-film materials has been rarely explored yet. In this study, we focus on the growth of $(Cr_xV_{1-x})_2AlC$ quaternary films and study their formation, microstructure, and thermal stability. CrV/C/Al multilayers with pre-defined nanostructured architectures (i.e., periodical stacking of nanolayers and variation of the Cr:V ratio) were deposited by combinatorial experiments in magnetron sputtering using a specific segmented Cr-V, pure graphite, and Al targets. These multilayer precursors were synthesized without substrate heating, and post-annealed from 300°C to 1000°C in vacuum to investigate their temperature-dependent phase formation. For this purpose, and to identify the underlying reaction mechanisms for potential MAX phase formation, in-situ HTXRD analyses were carried out. The composition and microstructure of the films before and after annealing were systematically studied, including methods with both global and local resolution (EPMA, TEM, APT, etc). Crystallization of solid solution $(CrV)_2AlC$ MAX phases above 600°C was confirmed for all multilayer precursors, i.e., for all different compositions and Cr:V ratios. The quaternary MAX phase thin film structures tend to decompose when vacuum annealed at 1200°C for more than one hour. We will discuss how the preferential diffusion behavior triggers the complex quaternary MAX phase structure formation and explore the correlation of their synthesis, microstructure, and properties from the nanostructured multilayer precursors.

Formation of light-emitting particles with different parameters by coating ZnO on a silicon surface with several porosity levels

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Composites of nanomaterials embedded in various matrices are considered promising materials for new generation devices. Porous silicon is of interest due to the use of its inner volume for nano-reactors for the synthesis of various particles. The spatial separation of channels decreases nanoparticle aggregation. By controlling the form and the size of the channels, it is possible to investigate nanosized materials with certain geometrical size and form.

Por-Si was synthesized by electrochemical anode etching. The presence of several porosity levels of silicon affected on growth mechanism and phase formation of synthesizing ZnO film on its surface. During the process of deposition of a film-forming system to a heated substrate, the air in the pores expanded, and crests and troughs formed on the surface of the sample. This explains the formation of clusters during the deposition of 20 layers. An increase in the number of layers up to 25 had led to the enlargement of clusters and the formation of troughs between them. The clusters were the growth center of the layers.

The systems with modified surface morphology contain light-emitting particles. The photoluminescence band at 380 nm is explained by exciton recombination at the boundary of the near band in ZnO films, and the peak at 520 nm is associated with defects—oxygen vacancies. It is noticeable that with an increase in the number of layers deposited, the signal intensity increases by 380 nm. In turn, the signal at 520 nm decreases, since the growth of films implies a decrease in the number of dangling bonds.

The study of defects by the ESR method showed that the samples with deposited layers indicate the signal in the form of a singlet with anisotropy: $\Delta H=1.37$ G, g -factor=1.987. The increase in the number of deposited layers affects to increase of the signal.

Bioinspired Hydrophobic Coatings for Antifouling Application

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Marine bio-fouling consists of undesirable settlement and accumulation of marine microorganisms, plants, and animals on the surface of submerged materials and it has huge adverse influence on infrastructure. Marine bio-fouling increases the weight and roughness of a ships hull, which raises the frictional resistance and causes additional fuel consumption [1]. The microorganisms contained in the sea water in contact with the surface of the hull adhere, causing the growth of biofilm. The aim of this work was to develop coatings capable of improving hydrodynamic performances of marine vehicles, with antifouling (AF) properties acting through a non-toxic mechanism. Hybrid nanocoatings based on a ceramic layer (Al₂O₃ or SiO₂) functionalized with (fluoroalkylsilanes) and “infused” with perfluoropolyether oils with different viscosity (the so-called SLIPS biomimetic approach [2]) have been developed and tested in laboratory for their AF efficacy and bio-safety. These coatings were deposited on materials such as steel, aluminum, and fiberglass. The reduction of the accretion of fouling was investigated by larval settlement test (A. Amphrite, a hard fouler [3]). In addition, release tests were carried out to evaluate the toxicity of the coating for the marine environment in accordance with the ASTM 6442 standard [4].

References

- [1] Li, Y. & Ning, C. Latest research progress of marine microbiological corrosion and bio-fouling, and new approaches of marine anti-corrosion and anti-fouling. *Bioact. Mater.* 4, 189–195 (2019).
- [2] G. Boveri, A. Corozzi, F. Veronesi, M. Raimondo, *Coatings*, 2021;11,77
- [3] Reddy G.K.K. Rajitha K. Nacharaiyah Y.V 2020 Antibiofouling potential of 1-alkyl-3-methylimidazolium ionic liquid: Studies against biofouling barnacle larvae. *Journal of Molecular Liquids*, 302, 112487.
- [4] ASTM D6442-06 (2012)- Standard test method for determination of copper release fate from antifouling coatings in substrate ocean water. ASTM International

Advanced Materials Supporting the Lithium and post-Lithium Energy Technologies

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Europe needs to emerge as a global leader in the field of batteries by accelerating the development of underlying strategic technologies and, in parallel, building a European battery-cell manufacturing industry based on clean energy and the circular economy. Europe has the potential to take the lead if we combine our strengths to create a more coordinated and truly collaborative approach that unites industry, researchers, policymakers, and the public.¹

With the aim of inventing ultra-high-performance batteries that are safe, affordable, sustainable, and have a long lifetime, organic chemistry emerges as a key field to design new materials aiming at targeting battery gigafactory requirements.

In this contribution, the main activities carried out at the Electrochemistry Group of the Politecnico di Torino in collaboration with international organic chemistry groups will be presented, with a special focus on:

- Polymer electrolytes able to ensure the safety and self-repairing ability of lithium batteries;²
- Recovery of cardanol- and lignin-based biomasses to produce post-lithium batteries, e.g. potassium-based batteries.³

This contribution also aims to start new collaborations within the ICM 2022 community dealing with the development of sustainable materials for energy devices.

This project has received funding from the European Union's Horizon 2020 Research and Innovation programme (grant agreement No. 952169, project title: SYNERGY).

References

[1] Battery 2030+, link: battery2030.eu.

[2] F. Elizalde, J. Amici, S. Trano, G. Vozzolo, R. Aguirresarobe, D. Versaci, S. Bodoardo, D. Mecerreyes, H. Sardon, F. Bella, J. Mater. Chem. A 2022, 10, 12588 – 12596.

[3] S. Trano, F. Corsini, G. Pascuzzi, E. Giove, L. Fagiolari, J. Amici, C. Francia, S. Turri, S. Bodoardo, G. Griffini, F. Bella, ChemSusChem 2022, 15, e202200294.

A new type of an Organic Memristive Device based on interactions between polymer thin-films

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Constant technological progress demands new solutions in terms of device architecture, but above all in the field of materials science. In recent years, significant progress in the field of organic semiconductors has been made, enabling the application of them in various types of devices as organic field-effect transistors (OFETs), organic photovoltaics (OPVs), or sensors. This would not have been possible without the synthesis of new compounds and a better understanding of the influence of the interactions at the internal and external interfaces of the devices. A study of the interactions between poly(4-vinylpyridine) (P4VP) and cobalt (II) bromide (CoBr_2), which act as a virtual gate by inducing an electric field, and its effect on the operation of OFET [1], revealed a new effect. An OFET consisting of poly(3-hexylthiophene) (semiconductor) and PEDOT:PSS (gate) with P4VP- CoBr_2 layer in between, showed time evolution of transistor characteristics. More interestingly, the time evolution of current-voltage characteristics is observed even when the PEDOT:PSS gate is left unbiased. Such behavior may be related to the presence of mobile ions in the gate material. The ion displacement induced by an electric field manifests itself as a pinched hysteresis loop in the current-voltage characteristics, which is a characteristic trait of memristive devices. To gain a better understanding of the effect, a device with a gate replaced by a polymer matrix admixed with potassium ions has been investigated. The devices were characterized by in-situ Secondary Ion Mass Spectrometry and various current-voltage measurements. Our studies reveal a unique principle of operation of the device based on interactions between each polymer layer. The results show that the electric field induced by the P4VP- CoBr_2 layer can be modulated by the displacement in polymer matrix which results in an altered conductivity of a semiconductor.

References

[1] Applied Materials Today 21 (2020) 100880, DOI: 10.1016/j.apmt.2020.100880

Next-generation substrates for surface-enhanced Raman spectroscopy

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Surface-enhanced Raman scattering (SERS) is a phenomenon resulting in the amplification of Raman signals via interactions with nanostructured substrates. SERS is understood to be a product of two mechanisms: electromagnetic and chemical. The electromagnetic mechanism is attributed to plasmon excitation in metal nanostructures functioning as a substrate, while the chemical mechanism is broadly attributed to a group of processes associated with the transfer of electrons between a molecule and substrate. While plasmonic materials have formed the bulk of research in SERS, semiconductors have more recently been proposed as materials that may benefit from the chemical mechanism. Indeed, they exhibit several properties that could be advantageous in SERS work, particularly in biosensing applications, given their excellent physical properties, unique chemistries, and tunable interactions with light. To explore this area, we are developing innovative ways to improve Raman signal enhancement in metal oxides, which include tuning the band gap by substitutional doping and exploring coating with plasmonic materials to create hybrid SERS substrates. In this work, we examine the application of zinc oxide (ZnO) doped with magnesium (Mg) to tailor the band gap. We found that the absorption edge of the Mg-doped ZnO nanoparticles was red-shifted compared to pure ZnO nanoparticles, and the band gap estimated using Tauc's plot also showed a decrease with increasing Mg doping. When the 5,5'-dithiobis(2-nitrobenzoic acid) (DTNB) molecule was observed with the various nanoparticle substrates, an enhanced signal was observed for the doped substrates, concurrent with changes in the band gap. Overall, we anticipate this work will serve as a platform for improving the use of SERS substrates in molecular sensing and bio-detection applications.

A scheme to determine the carrier density distribution, potential profile, and sub-band quantization of a conducting interface LaVO₃/SrTiO₃

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The carrier-density distribution near a conducting interface and related band structure is an essential topic in condensed matter physics. We propose a scheme combining photoluminescence (PL) spectroscopy and time-correlated photon counting (TCSPC) with electrical measurements to reveal the distribution of the carriers, the shape of the quantum well, and energy sub-bands, and Fermi surfaces of the conducting interface of LaVO₃ and SrTiO₃ (LVO/STO). LaVO₃ is a Mott insulator and SrTiO₃ is a band insulator, but the interface is conducting. Electronic properties, such as carrier density and mobility estimated from the electrical measurements are in excellent agreement with that estimated from optical spectroscopy-based methods through theoretical modeling. The carrier density is $2.21 \times 10^{14} \text{ cm}^{-2}$, which is very close to the carrier density predicted by the polar catastrophe model ($3 \times 10^{14} \text{ cm}^{-2}$). The proper knowledge of band structure can help us understand the fascinating physics of “Rashba band splitting” due to high spin-orbit coupling which gives rise to the planar hall effect, non-trivial berry phase, etc.

Emulating the Environment: Soft Materials Enable 3D Cell Culture

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We designed hydrogels for 3D cell culture with the goal of screening cells in an environment that mimics that of native tissue. With 3D cell culture, we gain an understanding of both cell invasion and cell viability, thereby providing insights that are inherently limited with traditional 2D cell culture. To achieve a suitable environment, we synthesized hyaluronan-based hydrogels because hyaluronan is often over-expressed in invasive tumours including those in the breast, brain, and lung [1]. To facilitate cell invasion and remodelling of the matrix, the hydrogels are crosslinked with peptides that can be degraded by matrix metalloproteinases (MMPs) secreted by the cells. We use either Diels–Alder or oxime click chemistry to crosslink our hydrogels while also including polymers that provide viscoelasticity, thereby enabling cells to remodel the 3D hydrogel environment. To enhance cell adhesion, the hydrogels are modified with proteins and/or peptides; to facilitate cell invasion, the hydrogels are modified with growth factor concentration gradients [2]. Using well-defined hyaluronan-based hydrogels, we investigate breast cancer [3,4], brain cancer, and lung cancer cell [5] invasion and their response to different therapeutic treatments.

Acknowledgements: We are grateful to NSERC and CIHR for funding.

References

- [1] Fisher, S.; Anandakumaran P.; Owen, S.C.; Shoichet, M.S. 2015 “Tuning the microenvironment: click-crosslinked hyaluronic acid based hydrogels provide a platform for studying breast cancer cell invasion”, *Advanced Functional Materials*, 25: 7163-72; doi: 10.1002/adfm.201502778
- [2] Fisher, S.A.; Tam, R.Y.; Fokina, A.; Mahmoodi, M.M.; Distefano, M.D.; Shoichet, M.S. 2018 “Photo-immobilized EGF chemical gradients differentially impact breast cancer cell invasion and drug response in defined 3D hydrogels” *Biomaterials*, 178: 751-66; doi: 10.1016/j.biomaterials.2018.01.032
- [3] Baker, A.E.G.; Bahlmann, L.C.; Tam, R.Y.; Liu, J.C.; Ganesh, A.N.; Mitrousis, N.; Marcellus, R.; Spears, M.; Bartlett, M.S.; Cescon, D.W.; Bader, G.D.; Shoichet, M.S. 2019 “Benchmarking to the gold standard: hyaluronan-oxime hydrogels recapitulate xenograft models with in vitro breast cancer spheroid culture”, *Advanced Materials*, 31: e1901166; doi: 10.1002/adma.201901166
- [4] Baker, A.E.G.; Bahlmann, L.C.; Xue, C.; Lu, Y.H.; Chin, A.A.; Cruickshank, J.; Cescon, D.W.; Shoichet, M.S. 2022 “Chemically and mechanically defined hyaluronan hydrogels emulate the extracellular matrix for unbiased in vivo and in vitro organoid formation and drug testing in cancer”, *Materials Today*, 56: 96-113; doi: 10.1016/j.mattod.2022.01.023
- [5] Tam, R.Y.; Yockell-Lelièvre, J.; Smith, L.J.; Julian, L.M.; Choey, C.; Baker, A.E.G.; Hasim, M.S.; Dimitroulakos, J.; Stanford, W.L.; Shoichet, M.S. 2018 “Rationally designed 3D hydrogels model invasive lung diseases enabling high-content drug screening”, *Advanced Materials*, 30: 1806214; doi: 10.1002/adma.201806214

Leveraging 3D biofabrication, bioengineering and biophysical approaches for musculoskeletal tissue regeneration and local therapeutic delivery

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Over the past 5–10 years, additive manufacturing, or 3D printing, has become extremely inexpensive and highly accessible. Therefore, the use of 3D printing in biomedical applications has become more mainstream. Fused deposition modeling in particular, using polymers such as polylactic acid, polycaprolactone, or other composites including polyurethanes, are widely used for medical applications including pre-surgical planning, resident surgical training, and patient education. Moreover, these polymeric devices or scaffolds are now combined with bioprinting to open new avenues to cutting-edge research toward musculoskeletal repair and regeneration such as pre-vascularized bone or soft-tissue constructs. Most importantly, these tools are being widely used to generate composite scaffolds representing matrices on which to culture cells of various tissue types such as bone, cartilage, cardiac tissue, and nervous tissue. Various 3D-printed composite matrix scaffolds are being tested in highly sophisticated in vitro and in vivo preclinical models, paving the way for future clinical translation in which the ultimate goal is to generate functional replacement tissues. Other avenues include devices for personalized medicine and drug delivery that are highly applicable to the pharmaceutical industry and beyond. Here, we present our findings from the past few years, whereby low-cost 3D printing is leveraged toward bone and tendon tissue repair strategies as well as generating devices for local drug delivery.

Preparation of hybrid films of locust bean galactomannans and starch from cassava peels

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Agri-food by-products are currently being generated in rather large quantities and being dealt with in a non-profitable manner. Agri-food by-products are a rich source of polysaccharides that can be extracted and used to produce biopolymeric films, which in turn can be employed in a variety of applications, thus adding value to the by-product. In view of the aforementioned, the aim of this work was to develop hybrid biopolymeric films with galactomannans from locust beans and starch from cassava peels by a casting process, as an alternative to promote the application of polysaccharide sources of low cost and add value to cassava processing by-products. Five distinct film formulations were developed: A1 (100% galactomannans), A2 (75% galactomannans and 25% starch), A3 (50% galactomannans and 50% starch), A4 (25 % galactomannans and 75% starch), and A5 (100% starch). The thermal degradation of the films was investigated by TGA analysis, demonstrating the high thermal stability of all film formulations. All films presented a three-stage degradation behavior, with peak mass losses occurring above 300oC and the percent mass losses decreasing with increasing starch content in the film formulation (12.33% mass loss for the film with 100% of galactomannan and 8.24% mass loss for the film with 100% of starch). The mechanical properties of the films were also determined, and it was observed that tensile strength and elongation at break increased with increased contents of galactomannans, indicating that galactomannans promoted increased intermolecular interactions and, consequently, increased the cohesion forces of the films. The preparation of hybrid films by the inclusion of galactomannans into starch film formulations allowed for the improvement of mechanical properties of starch films without significant changes in the thermal stability of the films.

Polysaccharides-calcium phosphates beads for the treatment of osteoporotic fractures

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The adult skeleton is normally stable and permanently active, with balanced resorption and bone formation, coordinated as part of the modeling and remodeling process [1]. Unfortunately, these aspects change a lot as we age, the physiology and structure of the bone being substantially modified[2]. Osteoporosis, a frequent consequence of these changes, is expected to double in the next 20 years due to increased longevity, leading to a huge human and socio-economic impact. Because statistics indicate that every 3 seconds a bone is fractured due to osteoporosis [3], an affordable solution must be found to effectively treat osteoporotic fractures so that the patient can return to their daily life. Given all these aspects, the aim of this study was to prepare and characterize polysaccharides–calcium phosphate beads loaded with drugs as a guide and support for bone regeneration in osteoporotic fractures. After the basic physico-chemical characterization of the beads (morphology, structure, and mechanical properties), the study continued with in vitro characterization. The first step in the complex in vitro characterization process was the immersion of the beads in different acellular aqueous solutions, which have the role of mimicking the physiological environment enough to provide preliminary data about the suitability of the beads as bone implant materials [4]. Furthermore, the MG-63 cell line was used to analyse the in vitro cytotoxicity of the beads and to evaluate their osteogenic behaviour. As promising results were obtained, in the future, the beads will be tested in vivo on an osteoporotic rat model.

Acknowledgment: This work was supported by a grant from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2019-0937, within PNCDI III.

References

[1] Acad Forensic Pathol. 2018;8(3):611-640. [2] Am J Kidney Dis. 2021; 78(4):582-589. [3] <https://www.iofbonehealth.org/facts-statistics>. [4] Int J Appl Glass Sci. 2020; 11:537–551.

Development and characterization of biocompatible porous PLA-Chitosan scaffolds without solvent treatment

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In this work, we will present an original technique to develop open-cell poly(lactic acid) (PLA)/chitosan (Ch)-based scaffolds. First, graft copolymerization of chitosan with PLA was performed to obtain a Ch-g-PLA copolymer. This modification aims to ensure good interaction between Ch and the pore surface of PLA scaffold and effectively promotes Ch/PLA adhesion. Second, we used the internal mixing method to prepare a chemical foaming composite (CFCO) composed of Ch-g-PLA adequately mixed with a chemical foaming agent (azodicarbonamide, ADC) under a mixing temperature below ADC decomposition temperature. Finally, this CFCO was used to develop, by compression molding, PLA open-cell porous scaffolds. Because the CFCO contains Ch-g-PLA, the latter is directly projected on the surface of the developed pores during the decomposition of the foaming agent, leading to strong adhesion between Ch-g-PLA and the PLA matrix. This was confirmed by FTIR analyses. Additionally, improved osteoblast adhesion and proliferation with the developed scaffold were, respectively, confirmed by Hoechst staining and MTT cell proliferation assay.

Hydrolytic degradation of methylene carbonate/lactide copolymers with functional, active carboxylic side groups as a carrier of biologically active agent, including drugs for use in dermatology and cosmetology

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Biodegradable and biocompatible polymers with embedded functional group currently, due to their potential functionality and ability to chemical modification, represent currently attractive materials for biomedical applications. Polymers containing functional carboxylic groups are one of the representatives among this family and due to their chemical activity and ability to form covalent bonds with reactive groups of active agents, including drugs, are particularly important for the synthesis and use of covalently bounded bioconjugates. Such functional polymers represent very promising materials for use as carriers of active agents in the drug and protein delivery systems that are currently being successfully used in pharmacy and cosmetology. The presence of carboxylic groups in proposed polymers allows for the modification of their physicochemical properties, including hydrophilicity, solubility, and the same influence on their (bio)degradation rate, giving them advantages over the conventional aliphatic polyesters and polycarbonates. Thanks to these properties, such a polymers may be used in tissue engineering for the formation of 3D scaffolds towards cell cultures applications. In this study, degradation of MTC-COOH/lactide copolymers with few various ratio of LA/MTC-COOH (70:30, 50:50, and 30:70, respectively) were undertaken at temperature of 37°C in phosphate buffer. ¹H NMR analysis of copolymers composition after one, two, and four weeks of copolymers immersed in buffer was determined. Solubility in PBS were dependent on MTC-COOH/lactide copolymer composition ratio. After four weeks of degradation, all samples were totally disintegrated. Due to fast disintegration of samples, proposed copolymers can be an interesting carrier with active functional groups for many biologically active substances and drugs (especially for use in dermatology and cosmetology).

This research was funded by the NATIONAL SCIENCE CENTER POLAND, grant number UMO-2019/33/B/ST5/00743: "Bioresorbable polymers and polymer blends with bactericidal properties for use in cosmetics and dermatology".

Residual stress measurement and properties investigation of cold sprayed titanium and titanium alloy coatings after laser surface treatment

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Titanium and its alloys are ones of the most commonly used materials. Due to very low specific weight combined with great mechanical properties and corrosion resistance, they are applied in a wide range of applications, e.g., biomedical and aerospace industries. Another reason for their popularity is the possibility of fabricating parts using additive manufacturing (AM) techniques. The remarkable development of AM in recent years is due to the relatively high efficiency of the process. The AM technique, in which Ti and Ti alloys powders are of particular use, is Cold Spraying (CS). CS is a very competitive technology enabling deposition of coatings, repairing machine parts, and manufacturing new components. Unfortunately, for specific applications the surface of cold-sprayed materials may require further processing. This paper reports on our latest attempt at employing laser surface treatment (LST) of cold sprayed titanium and titanium alloy coatings on an aluminium substrate. The influence of 200W laser beam interaction time on the coatings' properties was investigated. Microstructure examinations were performed via optical microscopy and scanning electron microscopy (SEM). Energy-dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD) were utilized for assessing changes in chemical and phase composition, respectively. To evaluate residual stress after CS and LST the $\sin^2\psi$ technique was used. Investigations on Vickers hardness, contact angle, and surface roughness were also performed.

Research was funded by Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme.

Formation of PEO coatings on binary material Mg-33wt%Ti processed by high energy ball milling (HEBM)

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The manufacture of light alloys has caused a significant impact in the world of additive manufacturing. Among the highly attractive light metals in the aeronautical, automotive, and biomaterials industries are titanium and magnesium, which, due to their low density and high strength-to-weight ratio, have been seen as having great potential for application in these areas. Magnesium alloys are of growing interest in many industrial fields, and their properties are being improved and their performance increased; however, their use is still restricted due to their moderate mechanical strength and high reactivity, the latter of which reduces their corrosion resistance in different media, limiting their application in many desirable applications. Titanium alloys, on the other hand, offer excellent properties, both mechanical and chemical stability, but have a density approximately 2.6 times that of magnesium.

In order to increase the mechanical properties and corrosion resistance of magnesium, as well as to decrease the density of titanium, Mg-33wt%Ti binary material were successfully synthesized by high energy ball milling (HEBM), sintered via hot isostatic pressure (HIP), and then surface modified by plasma electrolytic oxidation (PEO) in phosphate-based electrolyte for corrosion protection. This study focused on two aspects: (i) the processing conditions to obtain the substrate and (ii) the effect of electrolytic plasma oxidation of its surface on the corrosion resistance. For these purposes, scanning electron microscopy (SEM), X-ray diffraction (XRD), and Raman spectroscopy were employed. The corrosion resistance of the coated material was evaluated by electrochemical impedance spectroscopy in a 0.01M sulfate solution. It was found that the surface modification of the binary Mg-Ti material improved the corrosion resistance of the substrate.

Manufacture of Invar Sheets Using a Continuous Electrodeposition Technique for the OLED FMM

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In the producing processes of red-green-blue (RGB)-type organic light emitting diode (OLED) displays, Invar is used as a material for the fine metal mask (FMM), which guides the evaporated diode materials through its small holes onto the correct positions of the substrate glass. Manufacture of Invar thin sheets is an immediate hot issue in the RGB-type OLED display industries. Contrary to the conventional top-down method of pyrometallurgically producing Invar, a bottom-up approach of electroforming is a promising technology for producing very thin FMMs to achieve high-quality images in such displays. The present authors have recently presented that the electroformed Invar via sophisticated heat treatment exhibits the coefficient of thermal expansion (CTE) as low as that of the conventional Invar. The current work has been aimed at investigating the effect of the microstructure evolution on the CTE during heat treatment of the electroformed Invar. Finally, we propose optimal process conditions to produce Invar thin sheets for the OLED FMM.

Influence of microstructure and porosity on bending strength of nanoporous, selective laser-sintered glasses

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Porous glasses are used commercially in medical technology and chemical analysis for separating particles from liquids or gases. These silicate glasses are characterized by open, individually adjustable pore structures in the nanometer range. This pore structure is achieved by thermally induced phase separation of sodium borosilicate glasses and subsequent acidic as well as alkaline leaching (VYCOR® process). Nanoporous glasses can be widely applied due to the direct shaping out of the melt and various post-treatment options, but technical limits are set in terms of geometric complexity. However, additive manufacturing technologies enable the production of complex three-dimensional components, e.g., by selective laser sintering (SLS). In this process, the powdered starting material is selectively compacted layer by layer using scanned laser radiation.

Combining the VYCOR® and SLS processes enables the production of complex glass components with a graded pore system. Microporosity is mainly generated by the SLS process while nanoporosity is obtained by the VYCOR process. However, the resulting bimodal pore system also influences the mechanical stability, which is relevant for use in chemical reaction engineering and filter technology.

Nanoporous samples with porosities in the range of 40–90% are prepared by both the conventional VYCOR® and hybrid SLS-VYCOR® methods to investigate the influence of phase separation, porosity and pore size on mechanical stability (flexural strength). Furthermore, mercury porosimetry, low-temperature nitrogen sorption and scanning electron microscopy are used to quantify the microstructure. A particularly stable combination of porosity and pore sizes is found, where significantly higher mechanical stabilities can be achieved. This increased stability is associated with an ideal ratio of pore wall, pore volume and degree of sintering of the particles.

Effect of a physical vapor deposition film applied on decorative electroplated coatings of plastic substrates

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Hexavalent-chromium-containing compounds are used to provide a protective or decorative coating to metal and plastic parts. However, due to their carcinogenic effect on humans, there is a great need to explore suitable alternatives to these coatings. One possible alternative is to use a hybrid system consisting of a physical vapor deposited thin film on trivalent chromium decorative electroplated coating. In this study, the corrosion mechanisms of a hybrid decorative coating system were investigated. The decorative electroplated coating deposited on ABS plates consisted of copper plus nickel plus microcracked chromium plating obtained from trivalent baths. The electrochemical and corrosion behavior of these trivalent chromium decorative electroplated coatings were studied with and without a physical vapor deposited thin film by polarization curves and electrochemical impedance spectroscopy in a solution of 0.5M NaCl. It was found that the magnetron sputtered physical vapor deposited thin film on top of the decorative electroplated coating appears to produce an unfavorable effect on the corrosion resistance of the conventional electroplated coating. This may be linked to the porosity of the top layer, which allows the penetration of the corrosion media to the exposed electroplated coating. This investigation provides an additional understanding of the corrosion mechanisms of hybrid systems and, thereby, the potential to develop improved systems to control corrosion and offer further environmental, health, and wear resistance to meet engineering application requirements.

Additive Manufacturing of Preforms for Special Glass Fibres made of Al-doped Fused Silica

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The application of additive technologies for manufacturing optical components with complex geometries is currently an international focus of numerous research activities. Different processes such as fused filament fabrication (FFF), laser powder bed fusion (LPBF), and stereolithographic processes (SLA) are being investigated.

Particularly the process-technological advancement of the SLA enables complex optical components to be additively manufactured from fused silica. In the case of fibre preforms, non-axially symmetrical or non-hexagonal fibre structures could be prepared by a newly developed SLA printer. This process consists of several process steps, especially additive green body production and subsequent debinding and gas pressure vitrification. Photosensitive glass suspensions of commercially doped glass powder materials and standard resins are being developed for green body production. An important influence on the process suitability is the preparation of the doped starting powder. Very high purity, defined morphological properties, and the dopant concentration significantly influence the subsequent gas pressure vitrification with regard to undesired crystallisation processes.

In the next process step, the required debinding process was developed on the basis of metrological analyses (SEM, dilatometer, DTA/TG). Thus, the resin matrix of the silicate-rich green bodies could be successfully and completely removed with low defect formation.

The subsequent vitrification process allows compact and transparent fused silica components with a defined aluminium concentration to be produced. The manufactured optical components were analysed with regard to their composition (EPMA) and optical properties (UV–VIS–NIR spectroscopy, shadow casting, etc.). Doped preforms for optical glass fibres as well as lenses and axicons were successfully produced by SLA, and the preforms were processed to fibers. For the first time, optical fiber was produced from Al-doped material made by additive manufacturing. The attenuation of the manufactured glass fibre is 0.9 dB/m and can still be improved by process optimisation, especially with regard to higher material purity.

High-Entropy Alloys: Opportunities, Challenges, and Progress

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High-entropy alloys (HEAs), interchangeably called multi-principal-element alloys (MPEA) and compositionally complex alloys (CCA), offer unique and vast opportunities for designing and discovering material systems with desirable properties. Due to exponential growth in compositions as the number of components increases, there are fundamental challenges in identifying the “sweet spots” in the compositional space with sufficient accuracy. Using data-driven high-throughput methods such as supervised machine learning (ML), HEA solid solutions of face-centered cubic, body-centered cubic, and hexagonal closed packed structures can be predicted with sufficient accuracies for environmental resilience applications. A similar method applied to high-entropy intermetallics (HEI) that are usually the carriers of functional properties, however, encounters the limitations of available datasets. Physics-based and compound-specific models are being developed to explore the complex compositional landscape of HEIs for energy conversion and storage. In particular, the high prediction capability of the models enables the design of ordered BCC (B2) and Heusler (L21) HEI for high-performance properties.

Evolution of the microstructure, mechanical properties, and corrosion resistance of Mg–2.2Gd–2.2Zn–0.2Ca (wt%) alloy by extrusion at various temperatures

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In the present study, the Mg-2Gd-2Zn-0.2Ca (wt%) alloy (GZX220) was cast by gravitational permanent mold casting followed by homogenization at 400 °C for 24 h and extrusion at four different temperatures: 250 °C, 300 °C, 350 °C, and 400 °C. Microstructure analyses were performed by optical (OM) and scanning electron microscopy (SEM). Mechanical properties were investigated by a tensile test at room temperature. Corrosion properties were analyzed by immersion and electrochemical corrosion tests at room temperature in 3.5% NaCl solution. The results showed that the as-cast alloy consisted of α -Mg, Mg-Gd binary, and Mg-Gd-Zn ternary phases. After the homogenization treatment, most of the second-phase particles partially dissolved through the matrix phase. α -Mg grains were considerably refined by extrusion due to dynamic recrystallization (DRX). At low extrusion temperatures, higher basal texture intensities were observed. The extrusion process resulted in a remarkable improvement in the mechanical properties. The strength of the extruded alloys showed a continual decrease with increasing extrusion temperature. The corrosion resistance of the alloy was reduced after homogenization treatment due to the lack of corrosion barrier effect of second phases. The extrusion process led to a significant enhancement of corrosion resistance.

Development of antioxidant films based on oil/water emulsions with sunflower proteins and cellulose nanoparticles

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The goal of this study was to evaluate the structural and functional properties of films produced from emulsions stabilized by sunflower protein concentrates (SFP) with low and high chlorogenic acid content and two different types of cellulose nanoparticles (fibers and crystals), with eugenol also being incorporated in order to provide antioxidant activity to the films. The prepared emulsions were evaluated with respect to their rheological properties, morphology, and zeta potential, while the produced films were characterized with respect to thickness, water vapor permeability, color, morphology, mechanical properties, and content of phenolics. For the emulsified systems, it was observed that the sunflower protein with high contents of chlorogenic acids was able to provide a reduction in the electrostatic repulsion between protein molecules. This provided improvements in protein aggregation, flocculation of oil droplets, and increased viscosity of the emulsions. Nonetheless, both the water vapor permeability of the films and their mechanical properties were affected due to the presence of cracks and micropores of oil droplets. Such adverse effects observed on the prepared polymers were due to lipid–protein interactions and thus could not be overcome by the interaction between cellulose nanoparticles and protein molecules. However, the addition of eugenol provided a significant increase in the antioxidant capacity of the prepared film, indicating their potential for the production of active food packaging.

Assessment of ammonium ions removal from aqueous solutions using zeolite-composite materials derived from fly ash

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Environmental pollution with both inorganic and organic compounds remains a valid topic and requires intensive development of novel methods for their removal. Contamination of groundwaters, rivers, lakes and oceans with *i.a.* ammonium and nitrate (V) ions can lead to significant growth of harmful algae causing eutrophication. Among methods used for removal of ammonium ions like denitrification, which is limited by rather low temperature of regenerated water, adsorption process can be found as a promising approach. In our research we have investigated zeolite NaX from fly ash and its composite with carbon and vermiculite. Materials were characterized in detail by means of XRD, XRF, and N₂ adsorption-desorption. To evaluate the utility of obtained materials, zeolites were subjected to series of adsorption studies to investigate their adsorption properties towards ammonium ions. The effect of initial solution pH and adsorbent dose were also investigated. The optimal conditions for ammonium ions (NH₄⁺) removal were found to be pH of 7.00 and adsorbent dose of 2 g L⁻¹. At these conditions both parent zeolite NaX and zeolite NaX-Vermiculite composite displayed similar adsorption capacities of about 21 mg (NH₄⁺) g⁻¹ and the percentage (NH₄⁺) removal was 41%. On the other hand the NaX-Carbon composite adsorption capacity was significantly lower – 14 mg (NH₄⁺) g⁻¹ and percentage (NH₄⁺) removal of 25%. Such phenomenon can be a result of the distinct surface properties of the materials. The equilibrium of adsorption was obtained relatively fast after 30 min only. The investigated materials can find their future application as efficient adsorbents or additives to mineral-organic fertilizers.

Acknowledgement

The POIR.04.00-00-14E6/18-00 project is carried out within the TEAM-NET programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund

Tailings recycling into fired building bricks and anti-acid bricks

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Recycling mining wastes into building materials is a mean of protecting environment by controlling pollution. The DR Congo copper-belt area is full of copper and cobalt extraction plants. Tons of metallurgical wastes are accumulated with no treatment, despite their heavy metals content and their fine granulometry that have negative effects on health in all seasons. Finding a use for these wastes is a critical environmental issue. The recycling of the wastes (tailings) involves, first, the removal of metals by leaching with acid. The treated tailings could be then used to manufacture bricks by adding clay and glass powder coming from non-recycled glass bottles.

We studied an optimized drying–firing cycle, to manufacture fired building bricks at 800°C. Their characteristics: total linear shrinkage of under 5%, bulk density between 1.7 and 1.9, apparent porosity below 22%, and water absorption resistance smaller than 17%, compressive strength over 12 MPa are well within the required values for fired building bricks [1] and better than those of usual local clay fired bricks.

The addition of glass to the mixtures enhances the physico-chemical and mechanical properties. At 1100°C, anti-acid bricks are produced with a total linear shrinkage under 8%. The vitro-ceramic formed in this process allows the reduction of water absorption (5%) and of apparent porosity (10%). A bulk density between 1.8 and 2 and a compressive strength larger than 17 MPa are reached. The vitro-ceramic formed within the manufactured materials is also responsible for the high acid resistance with a mass loss of under 3.5% [1-3] in solution of sulfuric acid prepared at 2M.

The primary materials (Kakanda tailings), mainly alumino-silicate minerals, the kaolinitic clay and soda-lime glass (alkali >15% by mass), are fully characterized as well as the resulting brick materials.

Characterization and Minimization of the Four-Point Probe for Direct Blood Impedance Measurements in Vacutainer Tube

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Electrical impedance measurement is a promising approach for identifying and characterizing biological tissues based on their electrical properties. This has gained more importance in the diagnosis and detection of malignant and non-malignant conditions of the biological tissues. Using the electrical impedance, the conductivity of the blood in various pathological conditions can also be determined using a four-point probe system. Generally, blood is collected in vacutainer tubes, and using the four-point probe system, the blood sample is taken out from the vacutainer tubes and loaded on a different sample stage or container for impedance measurements. During this procedure, the test sample is exposed to external influences, such as temperature, impurities, and infections of the external container introducing errors and anomalies in the electrical resistance of the blood. This necessitates designing and characterizing the four-point probe system that will enable the direct measurements of the blood in the vacutainer tubes. To fulfil this need, we investigated the three distinct probe geometries for minimized structure and to reduce the errors due to external contamination of the blood. These four-point collinear probes are designed and fabricated with different geometry (i.e., circular, square, and rectangular) of the electrodes. All the probes are fabricated using a flexible single-sided isolating circuit with a copper thickness of 35 μm . The probes are calibrated with three different saline solutions (0.01, 0.05M, and 0.1M) and the accuracy of the probes is determined using 0.01M potassium chloride solution. Results have shown that our designed probe is accurate and offers repeatable and reproducible impedance measurements. This provides a cost-effective solution for direct blood impedance measurements in vacutainer tubes. The probe designs presented here can be easily extended for optimization of the design for real-time impedance measurements and to enhance the quality of collected data.

Therapeutic biomaterials for the stimulation of tissue regeneration

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Tissue-engineered scaffolds have played a decisive role in the repair and regeneration of a diverse range of tissues, including bone. These scaffolds not only provide a supporting matrix for cells, especially in bone tissue engineering, but also provide essential environments for cells to spread, migrate, multiply, and conform to differentiation into a specific lineage. For this, bone scaffolds should be tuned physicochemically to successfully repair and regenerate bone. Unlike conventional scaffolds that temporarily fill defects and need secondary surgery for their replacement and/or removal, promising therapeutic scaffolds have utilized a variety of biological actions that favor and trigger cells, especially stem cells, to carry out relevant therapeutic roles. Bone repair or regeneration is a part of a complex dynamic event that involves many molecules and cells. After scaffold implantation, the therapeutic actions should thus be harmonized with the biological events and even facilitate a better healing process. Key events in the active healing process include mild inflammatory reactions with no tissue rejection, substantial angiogenesis to form blood vessels, recruitment of progenitor/stem cells, and driving of these cells toward osteogenic lineage and finalizing matrix maturation. Therefore, tailoring the scaffolds to aid and stimulate these biological processes is an important milestone for scaffold-based bone engineering. In this talk, we will highlight the designs of therapeutically relevant scaffolds that trigger cellular functions that benefit the repair and regeneration of bone, which will lead to the development of ideal scaffolds for bone engineering.

Imaging cell and tissue physical properties

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There is currently a need to better understand the interactions between physics and biology in tissue repair and regeneration. While the field of microscopy has recently accomplished great advances in imaging 3D tissues at a greater depth with unprecedented resolution, it is still difficult to assess the physical properties of cells and tissues with fluorescent probes.

We recently leveraged optical interferometry imaging techniques such as optical coherence tomography and digital holography microscopy to measure physical properties relevant to the field of tissue engineering and regenerative medicine. In particular, fluid flow and mechanical properties of biomaterials were of great interest as they impact cell proliferation, differentiation and function. We have developed specialist algorithms and methods to measure these properties in 2D and 3D (spheroids, scaffolds) with applications in the field of tissue engineering and regenerative medicine. In addition, we will show how we can measure and relate time-course optical properties of cells and tissue to biologically relevant parameters such as cell activity, a measure of metabolism and viability in cell spheroids, organoids and 3D scaffolds. Finally, despite often being overlooked, the electrical properties of tissues are very informative for barrier-forming tissues with the measure of transepithelial/endothelial resistance (TEER) and cell viability. We will demonstrate a novel label-free non-destructive and quantitative method based on impedance sensing to measure and image these parameters for 3D scaffolds and spheroids.

The development of label-free quantitative monitoring technologies to monitor the physical properties of 3D cell culture, organoids, gels and scaffolds will enable the study of the complex interactions between physics and biology in tissue repair and regeneration.

Microstructured arrays based on self-assembled fibrillar networks for specific cell immobilization

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We established DNA–spider silk conjugates to create hybrid materials. The spider silk moiety enabled self-assembly into nanofibrils controlled by phosphate ions in aqueous buffers, whilst the DNA part enabled DNA-specific fibril labeling [1] or sequence-specific immobilization of DNA–spider silk conjugates [2]. Recently, we developed surface nucleated self-assembly of the DNA-modified recombinant spider silk proteins into immobilized fibril-based networks, which revealed swelling and softening properties of nanohydrogels [3]. The DNA functionalization in the highly hydrated cell repellent networks could be used for a specific cell binding. For this, a mild lipid–DNA incorporation into the cell membrane was employed, which showed high labelling efficiency as well as negligible cytotoxicity. Based on the complementarity of the nucleic acids, highly specific DNA-assisted immobilization of the cells on the nanohydrogels with tuneable cell densities was possible. The designed competitor DNA probes enabled the cell's liftoff on demand. We also employed modification of the nanohydrogels with DNA aptamers capable of binding to cell markers to immobilize different types of cancer cells specifically. The principle of surface-nucleated nanohydrogel self-assembly was further combined with photolithography. Using a positive-tone resist on an amino-reactive substrate, arbitrarily shaped microwells were patterned, the bottom of which served to define the binding of spider silk nucleation sites and the formation of the fibrillar networks. After stripping the sacrificial photoresists, a nanohydrogel micro-structured pattern was achieved, enabling either the DNA-assisted immobilization of DNA-labelled cells or the aptamer–cancer cell marker interactions with high spatial fidelity [4].

References

- [1] M. Humeník & T. Scheibel, *ACS Nano* **2014**, *8*, 1342-1349
- [2] M. Humeník, A. Molina & T. Scheibel, *Biomacromolecules* **2019**, *20*, 347–352
- [3] M. Humeník, T. Preiš, S. Gödrich, G. Papastavrou and T. Scheibel, *Materials Today Bio* **2020**, *6*, 100045
- [4] C. Heinritz, Z. Lamberger, K. Kocourková, A. Minařík; M. Humeník *ACS Nano* **2022**

Soft functional materials by bottom-up 1D assembly of pyrazole dendrons

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Self-assembly of tailored molecular units into well-defined nanostructures is an efficient approach towards new forms of functional soft matter. Dendritic structures, due to their regular branched morphologies and wide possibilities of chemical functionalization, are excellent candidates for the development of complex organizations using a bottom-up self-assembly approach. In fact, some dendrimers, dendrons and dendronized polymers are able to imitate nanostructures found in nature, such as viruses. In this work, novel dendrons with a pyrazole group at their focal point and wedge-shaped or cone-shaped conformations are found to self-assemble into cylindrical aggregates, giving rise to 1D nanostructures with liquid crystalline hexagonal columnar phase behavior. In addition, they form supergels consisting in fibers with a similar mesoscopic organization, adding to the few reported cases of dendritic structures that are able to show behaviors of both liquid crystal and gel. Moreover, these two forms of soft matter are photoluminescent and exhibit the AIE effect, that is, their emission is enhanced by several orders of magnitude upon assembly in the bulk or in solvents.

Investigation of Mechanical Properties in Novel Auxetic Skin Grafts

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Skin graft expansion is essential for treating severe burn injuries requiring skin transplantation across a large area. Skin grafting involves the projection of parallel incisions on a small sample of incised healthy skin, followed by its stretching and surgical implantation at the burn site. Although the majority of split-thickness skin-graft manufacturers claim large expansions, the real expansions are reported to be limited. In this work, a range of unique incision patterns (i.e., AS, HCS, HS, IS, RR, RT, and YS structures) with auxetic properties were tested on a skin simulant material, and the expansion potentials of the resulting skin graft simulants were studied. Mechanical testing and digital image correlation (DIC) were conducted to quantify the nonlinear stress–strain, effective Poisson's ratio, meshing ratio, and induced local strains on the auxetic skin graft simulants. It was observed that the YS skin graft simulant exhibited the highest negative Poisson's ratio, significant areal expansions, the lowest values of maximum induced stresses and strains, and uniform strain distribution, making it a suitable candidate for skin-graft expansion. The expansions were also shown to be sensitive to strain, with increased auxeticity observed at low strains. These innovative findings with auxetic skin graft simulants are anticipated to provide valuable insights for the future development of high-expansion skin grafts.

Influence of Anodization Parameters on The Surface and Corrosion Resistant Characteristics of Titanium Nanotubes Formed on Ti Substrate in Simulated Body Fluids

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Biomaterials are materials that can be used to repair or replace broken or diseased parts of the body, interacting with the biological systems to serve the body for an extended period of time with minimal failure. In this study, titanium (Ti) substrate was used as bio-implant material because it matches several mechanical properties in the human body, including the modulus of elasticity. However, when using bare titanium as an implant treatment, for example, bone fracture, its corrosion resistance is weak. Therefore, an electrochemical anodization process will be conducted to form titanium dioxide nanotubes (TNTs), which will enhance the corrosion resistance. The electrolyte used for anodization was ethylene glycol containing H₂O and ammonium fluoride NH₄F. The anodization experiments were carried out under three different voltages (40V, 50V, 60V) corresponding to three different periods (30 min, 60 min, 90 min). Then, the annealing process was performed at 450 °C for 2 h. After that, electrochemical tests (potentiodynamic polarization measurements) were conducted in simulated body fluid (SBF) to pick the best time that held higher corrosion resistance at different voltages, which was 30 min. Additionally, the optimum voltage value was selected according to the excellent distribution of the TNTs using field emission scanning electron microscopy (FE-SEM) and X-ray diffraction (XRD). The optimum voltage was 50 V because the TNTs were distributed perfectly and the anatase phase existed. Forming TNTs will be a preparation for the next step, which is filling these tubes with an antibiotic (antibacterial) solution and performing drug delivery to the infection, which might harm the implant.

***In-silico* designing bimetallic nanoparticles**

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Nanoparticles composed of more than one metal (nanoalloys) are the materials of choice for many applications. However, determining chemical ordering (mutual positions of different metal atoms) in nanoalloys, which largely defines their properties, is very challenging. We developed a method to determine the lowest-energy chemical (atomic) orderings in bimetallic nanoalloys by first-principles Density Functional Theory (DFT) calculations combined with a Topological approach [1,2]. The method allows one to reliably and efficiently predict the most stable ordering patterns of atoms in bimetallic crystallites containing up to several thousand atoms. So far the applications of the method have been focused on nanoalloys used in catalysis and energy technologies, for which the surface atomic ordering is key for the reactivity. Among the studied systems were bimetallic nanoparticles, such as PtCo [3,4], PtNi [5], CuNi [6], PdRh [7], PdX [1,2] and PtX (X = Au, Ag, Cu) [8]. In this lecture the novel computational method to model chemical orderings will be outlined and its applications will be illustrated by results obtained for technologically-relevant bimetallic nanoparticles. The present modelling method is helpful for accelerating design of tailor-made bimetallic nanoalloys for various technical needs. It also allows deepening general understanding of the chemical bonding in nanoalloys.

References

1. Kozlov, S. M.; Kovács, G.; Ferrando, R.; Neyman, K. M. How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. *Chem. Sci.* 2015, 6, 3868–3880.
2. Kovács, G.; Kozlov, S. M.; Neyman, K. M. Versatile optimization of chemical ordering in bimetallic nanoparticles. *J. Phys. Chem. C* 2017, 121, 10803–10808.
3. Kovács, G.; Kozlov, S. M.; Matolínová, I.; Vorokhta, M.; Matolín, V.; Neyman, K. M. Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. *Phys. Chem. Chem. Phys.* 2015, 17, 28298–28310.
4. Vorokhta, M.; Khalakhan, I.; Václavů, M.; Kovács, G.; Kozlov, S. M.; Kúš, P.; Skála, T.; Tsud, N.; Lavk-ová, J.; Potin, V.; Matolínová, I.; Neyman, K. M.; Matolín, V. Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. *Appl. Surf. Sci.* 2016, 365, 245–251.
5. Khalakhan, I.; Vega, L.; Vorokhta, M.; Skála, T.; Viñes, F.; Yakovlev, Y. V.; Neyman, K. M.; Matolínová, I. Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. *Appl. Catal. B: Environ.* 2020, 264, 118476 (1–9).
6. Wolfbeisser, A.; Kovács, G.; Kozlov, S. M.; Föttinger, K.; Bernardi, J.; Klötzer, B.; Neyman, K. M.; Rupprechter, G. Surface composition changes of CuNi-ZrO₂ catalysts during methane decomposition: An operando NAP-XPS and density functional study. *Catal. Today* 2017, 283, 134–143.
7. Vega, L.; Aleksandrov, H. A.; Neyman, K. M. Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications. *Chin. J. Catal.* 2019, 40, 1749–1757.
8. Vega, L.; Aleksandrov, H. A.; Farris, R.; Bruix, A.; Viñes, F.; Neyman, K. M. Chemical ordering in Pt-Au, Pt-Ag and Pt-Cu nanoparticles from density functional calculations using a topological approach. *Mater. Adv.* 2021, 2, 6589–6602.

Self-Assembling Nanofibrous Viral Microgels as Sprayable Antimicrobials Targeting Multidrug-Resistant Bacteria

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Bacteriophages, or bacterial viruses, are naturally antimicrobial proteinous nanoparticles. We packed half a million self-organized phages, as the sole structural component, to construct soft microparticles, thus creating a virus-exclusive microgel platform that preserved and amplified the natural antimicrobial activity of their nano building blocks. We further developed a high-throughput template method to manufacture superintegrated, single-layered, pure and hybrid phage microgel arrays (at a density of 35,000 microgels/cm², equivalent to 13-billion phages per unit area) as antimicrobial patches, which can be optionally detached to independent microgels, offering applications as high-load delivery vehicles for sprayable phage antimicrobials. The crosslinked phages in each phage-exclusive microgel self-organized to exhibit a highly aligned nanofibrous texture and emit tunable fluorescence that can expand potential applications beyond biocontrol to theranostics and biosensing. Sprays of hybrid microgels loaded with potent virulent phage effectively reduced heavy loads of multidrug-resistant *Escherichia coli* O157:H7 on food products, leading to up to a 6 log reduction in 9 hours and rendering food contaminant free.

Ni-Foam-Graphene-CNTs-SnSeP: An efficient electrocatalyst covering universal pH range and tap water splitting for hydrogen evolution reaction

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The growing demand for renewable energy has to be addressed, and greenfuel generation via water splitting is a game-changing alternative to fossil fuels. The development of rationally designed, cost-effective, noble-metal-free electrocatalysts with high efficiency and long-term stability has been vigorously pursued. Herein, we report a super-hydrophilic bi-ligand metal phosphide (SnSeP) on the surface of a highly porous nickel foam–graphene–carbon nanotube matrix via the facile thermal chemical vapour deposition method. The newly developed electrocatalyst renders superior electrocatalytic performance with long-term stability for a minimum of 10 days at a high current density of 250 mA/cm² in each acidic, basic, and neutral medium, inferring the commercialization of the catalyst toward industrial-grade applications. The excellent electrocatalytic performance is analyzed in terms of a low overpotential of 45 mV, 85 mV, and 135 mV at 10 mA/cm² in acidic, basic, and neutral media, respectively. Moreover, the as-designed catalyst has shown noteworthy performance in the smart utilization of tap water in hydrogen fuel production. This work highlights a new insight in adopting a feasible strategy to develop a cost-effective robust electrocatalyst that is capable enough for the facile usage of tap water, which could be an attractive paradigm of green fuel synthesis via renewable electrochemical energy conversion.

Nanosilica Modification of Epoxy Matrix in Hybrid Basalt-Carbon FRP Bars - Impact on Microstructure and Mechanical Properties

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The global nanotechnology market is still growing, and new and more innovative solutions which use this technology are being implemented. The effect of nanotechnology effect is also seen in the field of Civil Engineering, where new, high-strength, and cost-effective materials are constantly being researched. The article focuses on the influence of nanosilica on the epoxy matrix of hybrid polymer composites reinforced with basalt and carbon fibers. The use of this type of Fiber Reinforced Polymer (FRP) bars in the construction industry is still increasing. Corrosion resistance, strength parameters, and easy and quick assembly at the construction site are advantages compared to traditional reinforcement. Composites also have disadvantages, including sensitivity to elevated temperature and a lower modulus of elasticity. Research into solutions has resulted in the intensive development of a new type of FRP composites.

In this study, the microstructure of two types of bars was analyzed and compared using Scanning Electron Microscopy (SEM): 1) Hybrid Fiber Reinforced Polymer (HFRP), in which 25% of basalt fibers were replaced with carbon fibers to increase the stiffness of the existing Basalt Fiber Reinforced Polymer (BFRP) bars, having better strength properties than popular Glass Fiber Reinforced Polymer (GFRP) bars; 2) Nano-Hybrid Fiber Reinforced Polymer (nHFRP), in which the HFRP was additionally modified with epoxy resin with 3% admixture of nanosilica SiO₂. The admixture was used to increase the glass transition temperature (T_g), and thus shift the limit beyond which the composite strength parameters deteriorate. SEM micrographs show the mechanisms that occur in FRP composites after nanomodification. Mechanical properties of the composite bars were previously determined using ASTM standard testing for transverse shear strength and tensile strength, where the bars were exposed to elevated temperatures. The correlation of the investigated by SEM microstructure parameters with the obtained strength results allowed for the assessment of nanomodification of this type of construction material.

Fabrication of $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ alloy-based hydrogen gas sensor

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Concerning climate stabilization, the decarbonization of our energy systems is the only solution. That is why *green hydrogen* is emerging as an *alternative* to reduce emissions. However, hydrogen shows the issue to be highly flammable and very light, so it has tendency to leak. Therefore, it seems clear that there is a need for early detection of those possible leaks. Transition metal dichalcogenides are a promising material for such an aim, due to their affinity to H atom. In this work, we demonstrate the suitability of ternary $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ -based sensor in order to detect hydrogen. $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ composite flake films via sol-gel nucleation of MoO_3 were grown on different substrates (TiN and Si). X-ray analysis reveals the obtained ternary alloy forming high-quality crystal. The alloy is in accordance with the bands present in the Raman spectrum. Finally, preliminary results reveal that $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ -based transistor could pose a great potential for gas sensor applications.

Abstracts

Poster Exhibition

A1. 3D Printed Scaffolds for Stabilization and Local Therapeutic Delivery in Bone Metastases

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The gold standard of treatment for bone metastases is surgical resection. The defect created by resection can be filled with 3D printed scaffolds with patient-specific geometries. We aim to generate composite implants from stiff (Lactoprene) and sponge-like (LAY-FOMM) polymers loaded with chemotherapeutics for local delivery to prevent tumor recurrence, and to characterize their mechanical integrity. We anticipate these scaffolds will deliver effective doxorubicin (DOX) and cisplatin (CIS) chemotherapy to inhibit breast (MDA-MB-231) and prostate (C4-2B) cancer cell growth. Compression testing was performed on Lactoprene, and Lactoprene-LAYFOMM composite scaffolds. The release of DOX was quantified over a period of 1 week using a fluorescent microplate reader. DOX and CIS were loaded onto scaffolds and were incubated with monolayer cultures of MDA-MB-231 and C4-2B cell lines to determine metabolic activity via alamarBlue assays. Lactoprene and composite scaffolds behaved similarly in terms of compression testing properties. The composite scaffolds were loaded with two differing amounts of DOX to determine the release profile and over 60% was released over 7 days for both groups. A significant reduction in metabolic activity was found with MDA-MB-231 and C4-2B cells treated with scaffolds loaded with DOX or CIS compared to control scaffolds ($p < 0.0001$). We show that composite scaffolds capable of releasing effective doses of chemotherapeutics for local delivery applications can be developed. There is currently an unmet need for enhanced approaches in surgical bone resection. These concerns can be addressed by developing mechanically stable 3D printed scaffolds that can deliver chemotherapeutics to reduce the proliferation of cancer cells *in vitro*.

A2. Femoral stems with lattice structures integration: from concept to part

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Lattice structures are widely used, especially in the medical field, due to their advantages such as being lightweight and effective for osseointegration stimulation. For bone implantation, both the mechanical behaviour and biocompatibility are of major importance. However, lattice structures have limitations in terms of fabrication, additive manufacturing being the most accessible option.

For metal powder additive manufacturing techniques, the location, orientation, and part spacing within the build volume may considerably affect the mechanical characteristics of the product; therefore, two identical designed parts, placed differently into the building volume, might differ in terms of their dimensional accuracy and surface quality.

This work presents an analysis of the mechanical behaviour of additive manufactured lattice structures and the production of an innovative femoral stem with integrated lattice structures, from concept to fabrication. Various femoral stem options are designed and analysed by means of the finite element method, some are chosen for selective laser sintering with PA 2200 material for coarse analysis, and the optimal one is direct metal laser sintered out of CoCr powder, with two different orientations inside the building volume. The metal femoral stems were determined to be dimensionally different despite having an identical digital design.

A3. Stabilization effects of natural antioxidants in PLA/SIS blends

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The appropriate stability of materials is one of the basic conditions for packaging applications. This study presents investigations into the material features supporting thermal resistance. The composition is a poly (lactic acid) (PLA)/styrene-isoprene-styrene copolymer (SIS) blend with 30 % of SIS, by the addition of acrylic acid (AA) improved with natural antioxidants and vanillic and caffeic acids. It proves the good oxidation strength by which it may be successfully used in the production of food packaging, beverage bottles, toys, or medical items.

The chemiluminescence measurements demonstrate good oxidation durability, which makes a difference to the stabilization effects of additives. The evaluation of OOT values for the CL nonisothermal determinations for all compositions and doses places the thermal stability of PLA/SIS 30 compound in the following sequence: none vanillic acid caffeic acid Irganox 1076. The values of activation energies mirror the contribution of used antioxidants to the protection of polymer materials. FTIR investigation reveals a peculiar feature of the stabilized PLA/SIS 30 blend—the identification of additive capacity—which demonstrates the antirad efficiency. For all systems, it was observed that both vanillic acid and caffeic acid exert a nucleating effect in PLA systems, as compared with control. The degree of crystallinity increased as the cold crystallization enthalpy decreased and the glass transition increased.

This study emphasizes the versatility of natural antioxidants for the stabilization of polymer materials with comparable effects with respect to synthesis compounds that are often preferred in the production of packaging products.

A4. TiO₂ films synthesized by sol–gel method at low temperature for photovoltaic applications

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This work is based on the preparation of titanium oxide (TiO₂) films deposited on glass through the spin-coating technique in order to use them as electron-selective contacts in the manufacture of solar cells.

To this end, a study has been carried out using different titanium precursors and concentrations. Films with different thicknesses and with different synthesis temperatures were grown and were subsequently subjected to different heat treatments to increase their crystallinity.

It has been observed, by means of optical and structural characterization, that, depending on the conditions of preparation used, the properties of the materials obtained are different.

Through transmittance measurements in the UV–Vis range, it was observed that the films prepared under conditions of low concentrations and high thicknesses show lower transparency (65% in the visible region).

There are differences between the energy gap values of the films, ranging from 3.184 eV to 3.713 eV. As the thickness increases for the same concentration of titanium precursor, its value decreases. The same happens when the concentration of the titanium precursor increases, but the value of the energy gap increases when the temperature of the synthesis is higher.

Crystallinity is only observed when the heat treatments are above 400 °C, which corresponds to the anatase phase of TiO₂.

A5. Organophilized montmorillonites as fillers for silicone pressure-sensitive adhesives

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The aim of the work is an organophilization of sodium montmorillonite with selected quaternary ammonium compounds and applied the clays as fillers to silicone pressure-sensitive adhesives (Si-PSA) for special applications. Organophilized montmorillonites (OMMTs) were obtained in the methanol or aqueous slurry by stepwise addition of the compounds: tetraethylammonium bromide—TeBr; 2-methacryloxyethylammonium chloride—MOA; cetyltrimethylammonium bromide—CTAB; Tricaprylmethylammonium chloride (Aliquat 336)—A336; and dimethyloctadecylo(3-methoxilo)ammonium chloride—D. OMMTs were characterized using XRD, TGA, and FTIR-ATR analysis, as well as particles size was determined with Masterisizer. All studies confirmed intercalation of MMT pellets. After the addition of aluminosilicate fillers in amount 0.1 pph to silicone resin (type MQ—SilGrip PSA595) with 1,5 pph of cross-linker (2-4-dichlorobenzoyl peroxide-DCLBPO) viscosity of the composition was measured during week of storage. The composition was applied on a polyester film with a thickness of 50 µm using a semi-automatic PSAT coater. After drying the cross-linked adhesive film were pulled out and secured with film tape to obtain an adhesive tape with an adhesive grammage of 45 g/m². Adhesion, tack, and shear adhesion failure tests (SAFT) were performed for the samples. OMMT addition to the composition decreased its viscosity facilitating application on the liner. SAFT results revealed that some of the OMMT, especially OMMT-MOA and OMMT-D increased thermal stability of Si-PSA.

SPECSIL tapes are materials developed as part of research in the project from the Lider program No. LIDER/9/0028 /L-11/19/NCBR/2020 financed by the National Center for Research and Development.

A6. Microstructural evolution occurring during sintering of Ni-SiC composite material

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The properties of metal–ceramic composites depend on many factors. Among others, the type of matrix material and its share in volume, and primarily the type, form, size, orientation and distribution method of the reinforcing phase in the composite, can be distinguished. Equally important is the type and quality of the bonding between the metal and the ceramic at the interface. The processing conditions also seem to be crucial for further exploitation of the composite.

This paper explores the technological aspects of the interface formation in the nickel–silicon carbide composite during the sintering process. Nickel matrix composite with 20%vol. of SiC particles as the reinforcing phase was fabricated by the spark plasma sintering technique. The sintering tests were conducted in variable process conditions. The strong interaction between individual components depending on the sintering parameters was revealed. To identify the microstructural evolution, scanning electron microscopy, energy-dispersive spectroscopy, transmission electron microscopy, X-ray diffraction and Raman spectroscopy were used. The silicon carbide decomposition process progresses with the extension of the sintering time. As the final product of the observed reaction, new phases from the Ni–Si system and free carbon were detected.

A7. The role of imperfections in numerical homogenization of multi-layered panels with a corrugated core

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Multi-layered panels with a corrugated core are usually thin plates composed of very thin layers. One of the most popular examples of such plates is corrugated cardboard, which is an ecological material that is widely used in the packaging industry. To determine the behavior of cardboard, it is necessary to know its strength parameters from several basic laboratory tests, e.g., edge crush resistance, bending, shear, torsional stiffness and many others. Correctly calculating these parameters is crucial as they are often used to analytically determine the load capacity of corrugated board packaging. An additional factor that must be taken into account for the numerical simulation of the behavior of laboratory samples is the initial imperfections, which are of great importance in the compression of the cardboard layers. In the present communication through the use of the finite element method (FEM), the initial global stiffness matrix of the detailed model was determined, which, after condensation, was utilized in the homogenization process. The homogenization method based on elastic strain energy equivalence transformed the 3D model of the corrugated board into an equivalent plate with effective parameters. The method was verified using experimental data and data from the literature. Satisfactory compliance with the experimental data was obtained.

A8. Thermal stability of copper based layers reinforced by carbon nanoforms

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Electronics belong to one of the fastest growing industries, and its main features are the constant miniaturization of components and their high integration. This is achieved, inter alia, by the use of various techniques to connect various materials that play a key role in electronic devices, shaping their functionality, reliability, and scope of application. The developed new copper-based thermally conductive layers doped with various forms of carbon are characterized by a rapid dissipation of heat generated in electrical systems. The paper presents the influence of the carbon nanoforms (diamond, graphene, and carbon nanotubes) on the microstructure and thermal stability of copper based layers. Measurements of the thermal stability of the tested materials were carried out on the basis of thermogravimetric tests Tg/DSC in a protective atmosphere in the temperature range of RT—850°C. After the annealing process, scanning electron microscopy was used to observe changes that occurred in the structure of the layer. The Cu/C layers were also characterized via Raman spectroscopy to obtain the graphene peak and its variation according to the different temperatures. X-ray diffraction tests were also performed to identify the carbon forms in the structure of the copper nanoparticles. Thermal studies have shown that copper-based layers reinforced with carbon nanoforms are characterized by stability up to 850°C. The microstructural observation confirmed that copper oxides of different morphology were formed on the surface.

A9. Characterization of solids wetting by aqueous solutions of ethanol and surfactin mixture

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Wetting is a very important phenomenon which describes the force balance between adhesion and cohesion. It results from intermolecular interactions between the solid surface and the liquid. Both adhesion and wetting of liquids can be modified by adding surfactants or biosurfactants to the solutions. Moreover, by the addition of short chain alcohols, such as ethanol, it is possible to influence the hydration of the head and tail of the surfactants or the structure of water, and, in consequence, influence the adhesion, aggregation, and adsorption properties of the surfactants.

The aim of this study was to determine ethanol (ET) influence on surfactin (SF) adhesion and wetting properties. For this purpose, the contact angle measurements were conducted using aqueous solutions of SF and ET mixture on the surfaces of polytetrafluoroethylene (PTFE), poly(methyl methacrylate) (PMMA), and quartz. The obtained results were analyzed in regards of the surface tension components and parameters of the appropriate solids, water, ET, and SF in respect to its head and tail surface tension. Through the thermodynamic analysis, it was possible to consider adsorption of ET and SF at the solid–solution interface by taking into account the dependencies between adhesion, work of adhesion, and surface tension. From the comparison of the ET and SF adsorption at the PTFE–water and water–air interfaces, it resulted that the adsorption of both substrates at the PTFE–water interface was smaller than that at the water–air one. For PMMA, it could be stated that adsorption at PMMA–air and PMMA–water interfaces was smaller than that at water–air one, which suggests that SF molecules are oriented parallel to the interface independently of SF or ET concentration. For quartz, the SF molecules coverage of the quartz–air and quartz–water interfaces, as well as the water–air one decreased with increasing ET concentration.

A10. The stability consequence promoted by oxide traces on the degradation of poly(e-caprolactone)

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The stability of polymer materials is essentially determined by the molecular structure and the presence of additives and impurities. While the antioxidant protects the material against its degradation, the oxide traces promote oxidation. When a polymer substrate is subjected to damage by the thermal treatment of an accelerated degradation by g-exposure, the molecular scission generates fragments, which may be oxidized by the diffused oxygen. The traces of catalysts that may be incorporated in the polymer materials initiate a faster oxidation that influences the material shelf life. This study presents the behavior of poly(e-caprolactone), (PCL) loaded with 2 wt% PbTiO_3 previously doped with foreign atoms (Cr, Nd, Mg, Mn, Ti). The concentration of these doping atoms placed in the corner of a perovskite structure was 0.1 mol. The investigation procedure, chemiluminescence, reveals the acceleration of the degradation of PCL. The contribution of the metallic traces existing in the structure of PbTiO_3 powder is characterized by the activation energies (E_a) involved in the propagation of oxidation. These E_a values are different from one dopant to the other, while the pre-irradiation emphasizes the pro-oxidation effect on the propagation rates. The free radicals are involved in a faster oxidation when the polymer substrate is heated at superior rates. The comparison of the oxidation levels at the extended period of heating and irradiation indicates the sustained activities of metallic traces acting in oxide powder fillers, especially at temperatures exceeding 150 °C. The considerations for material durability are presented.

A11. Characterization of X-type zeolite composites derived from fly ash

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The zeolite X composites, zeolite-carbon (NaX-C) and zeolite-vermiculite (NaX-Ver), prepared from fly ash using hydrothermal method were characterized. The determination of selected characteristics included mineralogical composition (XRD), structural characterization (SEM) as well as selected physico-chemical properties including pH, pH point of zero charge (pHpzc), content of elements and polycyclic aromatic hydrocarbons, chemical structure (FTIR spectroscopy), chemical composition (XPS), textural parameters-BET surface area.

Zeolite X was the main component in the NaX-C, while vermiculite in NaX-Ver. The ratio Si/Al in case of the NaX-Ver was about 1.3 times higher compared to NaX-C. The BET surface area of examined materials showed a type IV isotherm with hysteresis loop of type H3. The registered visible peak at around 1135 cm^{-1} may be attributed to the stretching vibration of C-OH which can be associated with the presence of coal in the composition of the samples.

Based on conducted characterization of zeolites composites, it could be concluded that they have a great potential as an innovative materials for application in many areas including civil engineering, environment engineering and agriculture. Additionally, the synthesis of zeolite from fly ash is one of the effective and promising technological for management of fly ash which are considered as a waste material.

Acknowledgement

The POIR.04.04.00-00-14E6/18-00 project is carried out within the TEAM-NET programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund

A12. CO₂ adsorption reactions of synthetic calcium aluminoferrite compounds

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In this study, we investigated a mechanism of carbonation reaction by CO₂ capture through the synthesis of CaO-Al₂O₃-Fe₂O₃ compounds. As for the composition of the sintered calcium aluminoferrite (SCAF), the proportions of CF-based product and CA-based product were high at 87.3% and 64.6% at a sintering temperature of 1000°C and 1100°C, respectively. In addition, in the process of both dry and wet carbonation, the carbonation reaction occurred in the synthetic SCAF regardless of the sintering temperature conditions. In particular, in the wet carbonation method, CAH and CAFH, which are hydrates, were produced for up to 1 hour of the reaction time with CO₂, but from 3 hours of reaction time, carbo compounds such as calcium carboaluminate and calcium carboaluminoferrite compounds were produced. That is, with increasing reaction time, the carbo reaction becomes more active in the process. Therefore, SCAF synthesized in this study easily produced carbo compound through carbonation reaction and formed carbonates by reaction with CO₂. Thus, it is expected that the compounds can be effectively utilized as an excellent material for CO₂ capture capable of CO₂ absorption and fixation.

A13. Salt resistance of cement mortar using modified sulfur with slaked lime

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Recently, a huge amount of sulfur has been produced as a byproduct of petroleum refining processes, and bio-sulfur was obtained from a landfill site in Korea. Sulfur mortar and/or concrete is made of cement paste with sulfur, which has advantages including reducing CO₂ emissions from the cement industry as well as utilizing surplus sulfur. In general, sulfur is in a solid state at room temperature, and in order to use it in cement mortar and/or concrete, it must be converted into water-soluble sulfur. In this study, sulfur was modified by using slaked lime, converted into water-soluble sulfur and used in cement mortar. The main components of slaked-lime-modified sulfur were CaSO_x and CaS under constant chemical reaction conditions. The salt resistance of cement mortar with modified sulfur by slaked lime was experimentally investigated. The resistance of the chemical and sodium ability of cement mortar with the modified sulfur were evaluated using SEM and XRD analysis. The structure of cement mortar with the modified sulfur shows that it has dense microparticles and is hard enough to resist chemical and sodium intrusion. From the test results, it was found that the performance was improved by more than 120% compared to the salt damage resistance of general OPC mortar.

A14. Synthesis of $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ by multiple calcination and hydration properties of synthetic $12\text{CaO}\times 7\text{Al}_2\text{O}_3$

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Among cement-based materials, $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ is a representative calcium aluminate-based compound, and when added to Portland cement, it exhibits super-quick hardness and rapid hardening properties by precipitating a large amount of $3\text{CaO}\cdot\text{Al}_2\text{O}_3\cdot 6\text{H}_2\text{O}$ in hexagonal plate-like flakes at early hydration. However, $3\text{CaO}\cdot\text{Al}_2\text{O}_3\cdot 6\text{H}_2\text{O}$, which is crystallized as the final hydrate of $12\text{CaO}\times 7\text{Al}_2\text{O}_3$, has poor strength development. If gypsum is properly added to this, Ettringite and Monosulfate are formed, which can improve strength development. Therefore, it is used for the manufacture of various special cements. However, since $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ is a metastable phase that exists between $3\text{CaO}\times \text{Al}_2\text{O}_3$ and $\text{CaO}\times \text{Al}_2\text{O}_3$ in composition, it is mainly prepared by a melting method. In this study, it is judged that the hydration-synthesis method of $3\text{CaO}\cdot\text{Al}_2\text{O}_3$, which is a similar system, can be manufactured without going through the melting process.

Limestone and alumina were used as raw materials, and wet mixing was performed according to the mole ratios of $12\text{CaO}\times 7\text{Al}_2\text{O}_3$. The primary calcination was carried out at temperature of 1,000 °C and time of 1 h, and after the primary calcination, resultant of primary calcination was hydrated with H_2O and secondary calcination at 1,000 °C and 1 h. The synthesis yield of $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ after final calcination was 86%. Gypsum was used to control the hydration rate of the synthesized $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ and the $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ with gypsum 5, 10, 15, 20% compared to OPC, and were experimented for hydration properties. As $12\text{CaO}\times 7\text{Al}_2\text{O}_3$ with gypsum amount increased, it could be confirmed that the amount of ettringite increased, and it was very slow monosulfate formation by ettringite consumption.

A15. Morphological studies of needle-free electrospun PAN/Daemonorops draco nanofiber mats for possible medical applications

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The novel bio-based materials are of great interest and the field of green composites is continuously developing. Daemonorops draco (DD), commonly known as "Dragon's blood", is a biomaterial which is a renewable and environmentally friendly source [1]. The resin of the plant species *D. draco* is known since ancient times and is used as a natural remedy. *D. draco* has a wide range of potential applications, including anti-microbial, anti-viral, wound healing, anti-tumor, anti-cancer, and anti-oxidant applications [2,3,4]. In this work, PAN/ Daemonorops draco (DR) nanofiber mats were prepared by needle-free electrospinning technique from low toxic solvent dimethyl sulfoxide (DMSO). The nanofiber mats were oxidatively stabilized at 280 °C and then carbonized at 800 °C in argon. In addition, the chemical and surface morphological properties of nanofiber mats prepared of PAN/DD nanofiber mats were investigated using CLSM, SEM, AFM, and FTIR. It was found that the 5% addition of DD in PAN led to increase of nanofiber diameters compared to pure PAN nanofiber mats. The nanofiber diameter increased after stabilization and carbonization. Moreover, carbonized nanofiber mats showed stable morphology of nanofibers with straight nanofibers without large contraction.

A16. Surface Morphological and Thermal Aging Analysis of Polymer Modified Agbabu Natural Bitumen

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Bitumen's premature failure resulting in road pavement faults from oxidative aging has necessitated an investigation into the microstructural morphologies of polymer-modified Agbabu Natural Bitumen (ANB) samples. This, as well as the effects of aging on modified ANBs chemical compositions and physical properties, was used to explore the possibility of the elongation of pavement service life. Raw ANB sample was purified and the resulting base sample was modified with 2, 4, and 6wt.% percentage compositions for each of High Density Polyethylene (HDPE), Polyethylenevinyl-acetate (PEVA), Polystyrene-co-butadiene (PSCB), and Polyphosphoric acid (PPA) using melt-blend technique. Pressure Scanning Electron Microscopy (PSEM) was used to investigate the morphological changes. Base and 6wt.% polymer modified base samples were studied for long-term aging at 60 °C to understand its effects on chemical and physical compositions of samples. PSEM analysis revealed good compatibilities between all the polymers and the base bitumen at various percentage compositions except PSCB, which is only compatible at 2wt.%. Penetration values reduced and softening points increased for the base and modified base samples due, generally, to thermal aging. Additionally, thermal aging effects on chemical composition of base and 6wt.% modified base samples were found to be faster in the base sample than in the modified base samples at various aging periods. We, thus, concluded that the use of PEVA, HDPE, and PPA for modification at these three weight percentages is recommended but PSCB at 2wt.% is recommended due to poor compatibilities at 4 and 6wt.%.

A17. Colorimetric and thermoplasmonic dual-mode detection of C-reactive protein based on aptamer conjugated gold nanoparticles

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Human C-reactive protein (CRP) is a routinely used biomarker to evaluate infection or inflammatory processes in the body and is a reliable predictive marker of cardiovascular diseases. CRP detection is a multi-step, time-consuming process that requires a specialized laboratory with skilled personnel. In this study, we address this issue by developing a new dual detection method for CRP biomarker. Specifically, this method is based on colorimetric and thermoplasmonic detection of CRP in the presence of aptamer conjugated gold nanoparticles (AuNPs).

For colorimetric detection of CRP, citrate-coated AuNPs are conjugated with an aptamer presenting a high affinity for CRP. In the presence of the target analyte, the aptamer detaches from the AuNPs surface and strongly binds to CRP. Uncoated AuNPs are subsequently affected by the NaCl from the reaction medium, leading to their aggregation. The aggregation degree is correlated with the detected CRP concentration and is easily observed by the naked eye as a color change in the colloidal solution. Using a UV-Vis spectrometer the AuNPs aggregation ratio relative to individual AuNPs in the solution can be accurately measured.

Aggregated AuNPs exhibit photothermal properties under laser irradiation, also allowing quantitative CRP detection using an IR thermal camera. The detection of different concentrations of CRP leads to different amounts of aggregated AuNPs. Under laser irradiation, these aggregates present a different light-to-heat conversion efficiency resulting, therefore, in different temperature increments, as a function of detected CRP concentration.

After rigorous characterization, optimization, and investigation of different setups, we demonstrate that this colorimetric/thermoplasmonic dual-mode CRP biosensing method is able to provide an inexpensive, rapid, selective, and highly sensitive detection of CRP, suitable for future point-of-care testing.

Acknowledgment

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1592, within PNCDI III.

A18. Effects on the H gas sensor-based $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ alloy driven by Ga and In nanoparticles

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Gallium and indium nanoparticles (NPs) have attracted a lot of interest in recent decades due to their potential applications in many research areas, such as optoelectronics, catalysis, and flexible electronics, among others [1,2], since they provide a wide tunability of the plasmon resonance energy from the UV to the IR spectral region. This resonance is controlled by the size, shape, interdistance, and refractive index of the surrounding media [3]. Interestingly, these NPs can be evaporated forming different alloy compositions from the hybridization to the eutectic phase [4]. Moreover, the capability of the tunable resonance of the NPs with the band gap of certain materials, such as ternary $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$, makes them a good tandem for developing electronics or optoelectronics sensors.

In this work we use Joule-effect thermal evaporation to produce Ga and In NPs on different substrates based on $\text{MoTe}_{2(1-x)}\text{Se}_{2x}$ alloys, which is a promising material due to their affinity to the H atom [5]. This investigation aims to explore the benefits and limits of these NPs in new platforms for optical or electrical gas sensing devices. We have characterized the surface morphology through scanning electron microscopy. The optical properties were determined by ellipsometry, photoluminescence, and Raman spectroscopy, whereas the electrical properties were determined by I/V characterization.

References

1. A. García Marín et al., Biosens. Bioelectron. 74 (2015) 1069
2. Y. Kumamoto et al., ACS Photonics 1(2014) 598
3. S. Catalan et al., Nano Futures 2 (2018) 041001
4. N. Gordillo et al., Nanotechnology 30 (2019) 475705
5. A. Fernandez-García et al., Applied Surface Science 546 (2021) 149076

A19. Composite TiO₂-based photocatalysis

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TiO₂ is the most studied photocatalyst because of its non-toxicity, chemical stability, and affordability. However, the problem with TiO₂ is its low activity in the visible region of the spectrum. In this study, we focused on the preparation of composite photocatalytic materials with altered light-absorption properties. TiO₂ P25 and various metal oxides were mechanically joined by ball-milling and immobilized on glass plates. The prepared samples were evaluated based on their ability to degrade NO in gas phase. The formation of undesirable byproducts was also investigated. The four best-performing composites were later chosen, characterized, and further evaluated under various conditions in both gas and aqueous phase. According to their performance, the metal oxide additives can be divided into three groups. P25/Fe₂O₃ showed the best results—an increase in overall deNO_x activity under ISO conditions and altered selectivity (less NO₂ is formed) under both real outdoor and real indoor conditions. On the other hand, P25/V₂O₅ composite showed negligible photocatalytic activity. The intermediate group includes P25/WO₃ and P25/ZnO photocatalysts, whose performances are similar to those of pristine P25. The aqueous experiments proved that close contact between the parts of the composite is necessary for a successful energy transfer.

A20. Highly Efficient C-containing TiO₂ Layers for the Photocatalytic Degradation of Chlorinated Pollutants

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TiO₂ nanoparticles are suitable building-block nanostructures for the synthesis of porous functional thin films. Here, we report the preparation of films using brookite, P25 titania, and anatase pristine nanoparticles and of nanocomposite layers combining anatase nanoparticles and multi-walled carbon nanotubes (MWCNTs) at various concentrations. The structure and phase composition of the layers were characterized by X-ray diffraction and Raman spectroscopy. Their morphology and texture properties were determined by scanning electron microscopy and krypton adsorption experiments, respectively. Additionally to strong absorption in the UV range, the composites exhibited light absorption in the visible range as well. The photocatalytic performance of the layers was tested in the degradation of aqueous solutions of 4-chlorophenol, serving as a model of an eco-persistent pollutant. Besides the determination of the decrease in the concentration of 4-chlorophenol, the formation of intermediate degradation products, namely hydroquinone and benzoquinone, was also followed. The presence of MWCNTs had a beneficial effect on the photocatalytic performance, a marked increase in the photocatalytic degradation rate constant being observed even at very low concentrations of MWCNTs. Compared to a P25 reference layer, the first-order rate reaction constant increased by about 100% for the composite films containing MWCNTs at concentrations above 0.6 wt%. The key parameters for the enhancement of the photocatalytic performance are discussed. The presence of carbon nanotubes beneficially influences the degradation of 4-chlorophenol by an attack of the primarily photoproduced hydroxyl radicals onto the 4-chlorophenol molecules. The degradation due to the direct charge transfer is practically not influenced at all.

A21. Synthesis and characterisation of MAX phase Ti_3AlC_2 by pressureless sintering

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MAX phases materials have the potential to bridge the gap between metallic and ceramic materials owing to their excellent properties like good machinability, thermal conductivity, high temperature oxidation, corrosion resistance, low density, low thermal expansion coefficient, etc. The present study emphasises the synthesis of layered ternary carbide Ti_3AlC_2 by mixing the TiH_2 , Al, and TiC powders in a planetary ball mill followed by pressureless sintering in flowing Argon (Ar) atmosphere. The sintering process is carried out in two steps: i) decomposition of TiH_2 to Ti which leads to solid-liquid reaction of Ti and molten Al, and ii) Ti-Al compounds formed by step 1 react with TiC to synthesis MAX phase Ti_3AlC_2 . The mixed precursor powders were cold pressed and annealed at 750°C for 2 hours at a ramp rate of $10^\circ\text{C}/\text{minute}$ in step 1. Step 2 includes the heat treatment of annealed samples at a ramp rate of $10^\circ\text{C}/\text{minute}$ to 1250°C for 5 hours in a tube furnace under flowing Ar. The processed Ti_3AlC_2 samples were analysed by X-ray diffraction (XRD), Raman Spectroscopy for phase identification, followed by Scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS) to investigate the morphology and quantify different phase constituents present. Differential Scanning Calorimetry (DSC) was performed to study the thermal analysis of Ti_3AlC_2 phase up to 1400°C in Ar atmosphere. The results indicated that the synthesised Ti_3AlC_2 have high purity along with TiC as a minimal impurity. DSC results revealed that Ti_3AlC_2 phase does not undergo decomposition up to 1400°C in Ar atmosphere. Thus, this study provides a beneficial approach to low temperature synthesis of high-purity Ti_3AlC_2 materials and understanding the thermal behaviour of Ti_3AlC_2 for high-temperature applications.

A22. Investigation of the relationship between the change in microstructure and mechanical characteristics of dissimilar welds

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The present study investigates the relationship between the change in microstructure and mechanical characteristics of various dissimilar welded stainless steels and a standard structural steel. It refers to a weld joining two materials from different alloy systems commonly used in heat exchangers, pressure vessels, and power plant systems. It is clear that maintaining the integrity of such welds is critical to safety issues. Therefore, detailed microscopic and experimental studies were performed to evaluate the relationship between these welds. The microscopic analysis did not reveal the presence of any weld defects such as porosity or cracks. Changes in welds were evaluated after hardness and tensile tests. The hardness profiles revealed differences between austenitic and martensitic steel welds that later showed extremely high values in the heat-affected zone, which caused fractures in this zone during a tensile test. The welds of all austenitic steel grades withstood the tensile test with fractures observed in the base metal zone. The achieved results revealed that the higher hardness of the martensitic phase is closely related to the formation of an untempered coarse martensitic structure and higher carbon content.

A23. Enhancement of electromagnetic wave shielding effectiveness by carbon microcoils incorporation into carbon paste for commercial heating film

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Carbon microcoils (CMCs) were formed on stainless steel substrate using C_2H_2 + SF_6 gas flow under thermal chemical vapor deposition system. The manipulation of SF_6 gas flow rate, as well as SF_6 gas flow injection time, was carried out to obtain the controllable CMCs. The change of CMCs geometries according to SF_6 gas flow injection time, instead of SF_6 gas flow rate, was remarkable. In addition, the electromagnetic wave shielding effectiveness (SE) of the heating film made by CMCs incorporated carbon paste thin film was investigated across the operating frequencies in the 8.0–12.0 GHz range. The measured results were compared with those for the commercial heating film made by the native carbon paste thin film. Although the electrical conductivity of the native carbon paste was lowered by the incorporation of CMCs, the total SE values of the manufactured heating film increased following the CMCs incorporation. Considering the thickness of the thin film in the heating film, the presently measured values seemed to rank in the top tier among the previously reported total SE values. This dramatic improvement of total SE values was thought to be ascribed to the intrinsic characteristics of CMCs and the numerous cross-points of tiny-sized carbon nanofibers contributing to the absorption SE in the thin film.

A24. Microstructure and mechanical property assessment of plasma tempered aluminized Indian RAFM steels

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Indian Reduced Activated Ferritic Martensitic (IN-RAFM) steels are structural materials for the blanket module in nuclear fusion applications. Critical issues, such as liquid metal corrosion of RAFM steel, tritium permeation, and magneto hydrodynamic drag generation due to flowing Pb–17Li, have already been reported for the test blanket module. To mitigate these problems, aluminized coatings ($\text{FeAl} + \alpha\text{-Al}_2\text{O}_3$) with novel plasma assisted heat treatments have been widely reported for the surrogate material 9Cr-1Mo steel. However, the coatings on RAFM steel and its effects on microstructures and mechanical properties are scarcely reported.

In order to investigate this, an aluminizing process of RAFM steel followed by tensile tests were carried out in this study. In-RAFM steel (9Cr-1.4W-0.06Ta) samples were hot dipped in a molten bath of 93%Al & 7%Si at 730 °C. These samples were then subjected to heat treatments in air and plasma environment (100% O₂) to study the transformation of $\theta\text{-Al}_2\text{O}_3$ to $\alpha\text{-Al}_2\text{O}_3$. The coated samples were characterized with X-ray diffraction and scanning electron microscopy (SEM) to correlate the phase transformation in microstructure. Subsequently, tensile tests of coated samples at room temperature and 550°C, and a comparative analysis of both is done with respect to substrate steel. At room temperature, mechanical tests revealed a higher strength in case of thermally tempered specimens with around ~720 MPa, 25% elongation; whereas plasma tempered and substrate steel strength was found around ~550 MPa, 25% elongation and ~600 MPa, 28% elongation, respectively. A similar trend was observed at high temperature (550 °C). The outcomes are promising as the effect of coating is minimal on tensile strength in case of plasma tempering. In addition, it also motivates the scientific community to conduct extensive research for the implication of coatings for fusion applications.

A25. Aluminium TIG welding: AC versus DC

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This study compares two ways to weld a aluminium. The tungsten inert gas (TIG) welding process was chosen. It has three options for welding current: direct current positive electrode (DCEP), DC negative electrode (DCEN), and alternating current (AC). Every method has pros and cons and is used in the welding of ferrous or non-ferrous metals. Generally, welding manuals recommend that DC is used for TIG welding of mild or stainless steel while AC for is used for welding aluminium. Aluminium, when exposed to air, forms an oxide layer that melts at a higher temperature than base metal. An AC positive cycle where the current flows from base metal to the electrode removes surface oxides more effectively than during a negative cycle. The positive cycle acts as a surface scrub, breaking up oxides while the necessary weld penetration is achieved during the negative cycle. Both cycles work to ensure high-quality integral welds. Cleaning the weld area with a stainless-steel brush is mandatory to assure it. The control of the heat input is another challenge in aluminium TIG AC welding. However, in the case of DC, these processes are performed without the above-mentioned problems. Good, deep welds are obtained in one pass. This operation not only creates a stronger weld but also reduces the time required. DC welding finds its application in repairing deep pits and gouges in aluminium products; a pit or cavity is quickly filled with molten metal keeping the filler in the right place, ensuring solidification of the joint, which needs to be smoothed afterwards, and then the part is like new. This method makes it possible to repair expensive machined parts that are slightly damaged. Even though AC has a surface-scrubbing effect which breaks up the oxide layer, providing the possibility to obtain good welds, unlike DC current, it cannot produce integral welds.

A26. Rheological study of AlSi9Cu3 aluminium alloy in a semi-solid state

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Several routes have been developed to obtain materials in a semi-solid state with the aim of obtaining components with very good structural integrity. Currently, some of them are being oriented to obtain aluminium alloys with a globular microstructure capable of being used in additive manufacturing techniques. The good mechanical properties of semisolid metal (SSM) can make the deposition of a metal stream a practical process for forming 3D-printed parts. Compared with fully molten metals, the semisolid slurries can exhibit special improved rheological properties which provide help in the control of viscosity and benefit for laminar flow. In a semi-solid state, aluminium alloys can show rheological characteristics comparable to that of polymers, so semisolid processing is one of the currently considered routes for additive manufacturing with metallic materials. In this work, an approximation of the rheological control of AlSi9Cu3 aluminium alloy, for its subsequent 3D printing, was carried out. A continuous cooling rheometer was designed and used to evaluate the influence of different process parameters on the variation of the dynamic viscosity of the alloy.

A27. High-Temperature Composite Materials for Ferrous and Non-Ferrous Metallurgy

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The method of obtaining high-temperature composites based on the interaction of an active chemical mixture with the ingredients of the charge under certain conditions has been developed. High-temperature materials for various purposes have been tested at the enterprises of ferrous and non-ferrous metallurgy.

ArcelorMittal Temirtau JSC has hosted a series of tests on thermal insulation/exothermal mixtures. It has been established that the use of heat-insulating and exothermic mixes for thermal insulation of iron mirror in iron ladles increases the lining durability, reduces the formation of tare build-up, facilitates the processing of ladles in the mixer department, increases the productivity of iron ladles. New ramming mass facilitates increasing durability and overhaul life of the main, transport and swinging chutes of the Blast Furnace Shop. The use of the experimental taphole mix allowed to increase the service life of the machine designed to plug the blast furnace taphole with the refractory filler; to facilitate the casthouse work on preparing the taphole for the next discharge and charging the machine with the taphole-closing mix, as well as the discharge control; to avoid heating the taphole mix in the heater in winter period. Pilot tests of concrete mix for insulation/lining of main and transport chutes aspiration covers showed an increase in the cover durability up to 10% on average. This factor contributed to an increase in the service life of the units, reduction of operating costs and, ultimately, obtaining economic effect.

Compositions and production technology were developed and new high-temperature chemically resistant composite materials have been obtained for non-ferrous metallurgy. Experimental batches of high alumina carbide-silicon composite materials were successfully tested at the Zhezkazgan smelter of Kazakhmys Smelting LLP. The tested material is suitable for concreting of the anode furnace neck.

Refractory materials of various composition were produced using rice husk as a source of silica-containing phase.

A28. Preparation and characterization of biocomposites using waste cooking oil and spent coffee grounds

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Polymer composites reinforced with fibers from renewable sources present a wide variety of applications. However, for a composite to be 100% renewable, not only the reinforcement but also the polymeric matrix should be bio-based. Therefore, in this work, a 100% renewable composite was developed, based on an epoxy matrix produced from residual (frying) soybean oil and reinforced with spent coffee grounds (SCG). SCG underwent alkaline treatment in order to decrease its hydrophilicity and increase the interfacial interaction with the polymeric matrix. The effects of variations in the amount of curing agent and time and in the SCG mass fraction were evaluated. The use of SCG improved the thermal stability and mechanical properties, indicating compatibility and good interaction between the polymeric matrix and reinforcement. The addition of SCG provided increases in the glass transition temperature, density, porosity, water absorption, tensile strength, and elasticity modulus. The composites prepared with a molar ratio of maleic anhydride 1:1.2, SCG mass fraction of 35%, and 8 h curing time were those that presented the best mechanical properties. A comparison with a preliminary study [1] indicated that increasing the curing time led to a decrease in porosity and increase in density and tensile strength, with the latter being higher or similar to other values reported in the literature on biocomposites. Our results confirm the feasibility of obtaining a truly bio-based composite employing only residual bio-based materials.

References

[1] E. R. T. Tarazona, L. S. Oliveira, J. C. Rubio and A. S. Franca, "Preparation, preliminary characterization and mechanical properties of epoxy composites reinforced with spent coffee grounds," *8th International Conference on Mechanical and Aerospace Engineering (ICMAE)*, 2017, pp. 21-24, (2017).

A29. Biopolymers in road material engineering

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Biopolymers are a group of macromolecular organic compounds (polymers) produced by living organisms. These are the components of the cell building blocks or intercellular areas. Due to their chemical structure, biopolymers are divided into three basic groups: (I) polysaccharides, (II) polynucleotides, and (III) polypeptides. In construction material engineering, polymers are a very important component used for the modification of asphalt binders or concretes. Polymer-modified asphalts (PMA) are materials consisting of an asphalt matrix and one or more polymers. The use of polymers in the modification of asphalt binders allows the obtainment of asphalt mixtures with increased resistance to rutting and thermal cracking. Currently, several synthetic polymers and copolymers such as SBS (styrene–butadiene–styrene), SIS (styrene–isoprene–styrene), PE (polyethylene), or PP (polypropylene) are used in the modification of asphalt binders. In recent years, there has been a continuous increase in the interest in environmentally friendly materials in road material engineering, so the main objective of this study was the application of selected biopolymers from the polysaccharide group in the modification of commercial road bitumen binder. The research included the analysis of physical properties such as the penetration, softening point, and viscosity of asphalts modified with selected biopolymers. Moreover, their interactions with mineral aggregates were analysed on the basis of surface energies. To analyse the chemical changes in the asphalt binders after modification, Fourier transform infrared spectroscopy was used. The study indicated that selected biopolymers from the polysaccharide group are compatible with the asphalt matrix and can be used to produce PMAs.

A30. Synthesis and properties of chitosan derivatives containing Schiff bases, grafted with polycaprolactone

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Recently, due to its wide range of applications and interesting properties the attention of scientific researchers has been attracted by modifications of natural polymers, including such polysaccharides as chitosan, carrageenan, or alginates. Chitosan (CS) is an extremely useful, readily available bioactive polymer, which is characterized by the fact that it is a renewable, non-toxic, edible, and above all biocompatibility, additionally it shows several advantageous biological properties, such as antimicrobial, and hemostatic activities, and promotes wound healing.

Among the substituted biopolymers, particularly noteworthy are the Schiff-bases obtained by the reactions of the free amino groups of chitosan with an active carbonyl compound, such as aldehyde or ketone. In the present study synthesized and characterized two chitosan-based Schiff-based compounds from the reaction of chitosan with different aldehydes, i.e., 2-pyridinecarboxaldehyde and 4-formylbenzene-1,3-disulfonic acid disodium.

In the next stage of research, it was decided to graft these materials with poly(caprolactone) (PCL). The obtained copolymers showed reduced hydrophobicity compared to the starting chitosan, with presence of antibacterial Schiff-based groups. The grafted copolymer also showed increased antibacterial activity, and was suitable both alone and in the form of carrageenan blends for use as a carrier of standard biologically active substances. For these reasons, this bioresorbable copolymers seems to be a promising ingredient of many cosmetic and dermatological formulations to be used in the form of a microgel, as a carrier of selected vitamins or enzymes, and at the same time as an bacteriostatic agent.

This research was funded by the NATIONAL SCIENCE CENTER POLAND, grant number UMO-2019/33/B/ST5/00743: "Bioresorbable polymers and polymer blends with bactericidal properties for use in cosmetics and dermatology".

A31. 3D printing of silk/polycaprolactone composite scaffolds

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Silk protein is a biocompatible material with good mechanical properties, suitable for the development of 3D scaffolds and tissue engineering applications. The conformational transition of the secondary structure of silk fibroin due to shear stress complicates its processability using 3D printing techniques. Therefore, the solution of fibroin with polycaprolactone (PCL) in hexafluoroisopropanol as a good solvent and dimethylsulfoxid as a poor solvent were prepared. From these mixtures, 3D objects were prepared by extrusion printing and the arrangements of macromolecules in the printouts were analyzed. Using atomic force microscopy (AFM), we observed formation of polycaprolactone spherulites which were disrupted by the incorporated fibroin in the form of nano- to micro-particulate structures. The organization of the lamellae of the PCL spherulites and topography of the printed structures was rearranged by a phase separation process caused by the poor solvent in the printing dope. Resulting PCL/Fibroin scaffolds revealed good biocompatibility and mechanical stability.

ACKNOWLEDGMENT

This work was financially supported by the project funded by Czech Science Foundation (Project No. 22-33307S) and project OP-RDE Junior Grant of Tomas Bata University in Zlín, Reg. No. CZ.02.2.69/0.0/0.0/19_073/0016941. The authors thank Prof. Thomas Scheibel, Chairholder of Department Biomaterials, University Bayreuth and Assoc. Prof. Aleš Mráček head of Department of Physics and Materials Engineering, Tomas Bata University in Zlín for providing the facility to conduct this research.

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A32. The course of synthesis and properties of bioresorbable antibacterial copolymers intended for cosmetological application

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Cosmetic and personal care products frequently contain biologically active substances that are often unstable due to sensitivity to temperature, light, or oxidation. This phenomenon means that many of the valuable ingredients contained in cosmetic formulations lose their activity to a large extent during storage or use. Thus, carriers in the form of polymeric microspheres or microcapsules have been proposed to protect against degradation, and simultaneously also to direct and control the release of active ingredients. They are incorporated into skincare formulations to enable the controlled and targeted delivery of bioactive compounds and to enhance the penetration.

The presented work explores the synthesis and properties of a group of polymers that not only meet the above requirements but also show antibacterial and antifungal properties. Using these materials in the form of cosmetic ingredients can allow a reduction in or even elimination of parabens, one of the most controversial ingredients in skincare products currently commonly used in cosmetic formulations. The presented copolymers belong to different classes of biodegradable aliphatic polymers obtained both by polycondensation and ROP. However, they all contain amino groups in the main or side chain. These are poly(esteramines) additionally containing hydroxyl groups, obtained during polycondensation of tartaric acid derivatives with diethanolamine as well as poly(amidoamines) synthesized by polycondensation of sebacic acid derivatives and norspermidine or spermidine derivatives. These copolymers were compared with copolyestercarbonates with side chains containing salts of a quaternary amine, synthesized by chemical modifications of the prepolymers previously obtained by the ROP reaction of L-lactide and a trimethylcarbonate derivative. The physico-chemical properties and activity against selected strains of bacteria and fungi of the final selected copolymers are also presented.

This research was funded by the NATIONAL SCIENCE CENTER POLAND, grant number UMO-2019/33/B/ST5/00743.

A33. Indirect measurements of the electrocaloric effect in $\text{Pb}_5\text{Ge}_3\text{O}_{11}:\text{Ba}$ single crystals

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The electrocaloric effect (ECE) of ferroelectrics is a coupling of electrical and thermal properties which results in an adiabatic temperature change dT in response to an externally applied electric field dE . It is relatively new and a challenging research topic in the field of ferroelectric materials. This phenomenon has attracted large amounts of attention due to its potential use in environmentally friendly solid-state cooling applications. Thus, potential expectations of the EC effect in cooling micro-devices are enlivened by searching for new, more efficient materials.

In this work, we study the ECE by the indirect method for the $(\text{Pb}_{5-x}\text{Ba}_x)\text{Ge}_3\text{O}_{11}$ (pure and doped with $x=0.1$ and 0.2 of Ba) single crystals.

The ECE was characterized via P – T curves under different electric fields. For all of the samples, the experiments have been carried out in room temperature through the phase transition region and in the paraelectric phase. The temperature dependences of polarization for different electric fields were deduced from the upper branches of the hysteresis loops, whereas the values of electrocaloric temperature change (ΔT) were obtained using the Maxwell relations, i.e., from the numerical differentiation of the polarisation versus temperature.

A34. $\text{Cs}_2(\text{Na}_x\text{Ag}_{1-x})\text{BiCl}_6$ Nanocrystals: A New Class of Alloyed Double Perovskite with Tunable Band Gap

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Lead halide perovskites (LHPs) have become champion photoactive semiconductors for their applications in optoelectronic devices. To resolve the main issues regarding instability and toxicity of LHPs, there is a recent surge in research toward alternative lead-free double perovskites with elpasolite structure and visible band gaps. Double perovskite $\text{Cs}_2\text{AgBiCl}_6$ nanocrystals (NCs) are absorbed in the ultra violet region and have an indirect band gap due to the fact that the region is weakly photoluminescent. Herein, we describe the synthesis of a series of alloyed double perovskite ($\text{Cs}_2\text{Na}_x\text{Ag}_{1-x}\text{BiCl}_6$) NCs. This synthesis provides useful way to make new materials with enhanced photoluminescence and tunable band gaps by alloying an alkali metal (Na) into $\text{Cs}_2\text{AgBiCl}_6$. The tuning of bandgap has been further explored by electronic structure calculation under the framework of density functional theory (DFT). The electronic structure calculation confirms that the increase in bandgap is due to reduction in Ag contribution near valence band maxima (VBM) on incorporation of Na in place of Ag. These alloyed double perovskites are potential candidates for making high-performance photodetectors.

B1. Characterization of biocompatible coatings for polymer-made implants

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Polyethylene terephthalate (PET) is a polymer used in medicine for the production of blood vessels, artificial organs, and temporary tendons. However, the passivity of the surface results in poor compatibility with human tissues, leading to the rejection of the implant. Therefore, in order to improve the compatibility of the polymer, thin films of biological substances are deposited on its surface. One of them could be phospholipid - 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC), which is the main building component of most biomembranes. Additionally, an active substance such as cyclosporin A (CsA), which is widely used in medicine to prevent implant/transplant rejection, can be used. However, the administration of this drug has many side effects including lipid peroxidation, which leads to damage to the cell membrane integrity. In order to reduce these undesirable effects, it is necessary to use an antioxidant. One of them is lauryl gallate (LG), which can eliminate free radicals, protecting phospholipids against peroxidation.

The aim of the study was to investigate the properties of Langmuir and Langmuir–Blodgett (LB) monolayers containing biological and bioactive substances. In order to determine the miscibility, physical state, packing, and ordering, the Langmuir technique coupled with a surface potential (ΔV) meter (SPOT) was used. The monolayers were then transferred onto PET using the Langmuir–Blodgett (LB) trough. The LB films were characterized using secondary ion mass spectrometry with a time-of-flight analyzer (TOF-SIMS), atomic force microscopy (AFM), and wettability measurements with an estimation of the surface free energy.

The conducted tests showed that the obtained monolayers were homogeneous. The ΔV -A isotherms proved that the orientation/conformation of the molecules changed during compression. The results acquired by means of TOF-SIMS and AFM techniques as well as wettability tests confirmed the presence of monolayers on the polymer support as well as their organization, ordering, and interactions.

B2. Non-standard structural materials to reduce vibration amplitudes

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The non-standard structural materials to reduce vibration amplitudes for high-frequency excitation of mechanical systems above 2000 Hz are an object of research. The principle of reducing vibration amplitudes by increasing the weight and stiffness is one of the past design approaches. Mechanical machines systems consist mainly of components made of materials such as steel, which has low material damping. Reducing vibration amplitudes through the use of high material damping is an effective approach, mainly in the resonance regions. However, the materials with high material damping have low stiffness. Therefore, the use of materials with a combination of high stiffness and high material damping is suitable. We provide approaches such as the use of polymer particle composites and viscoelastic materials as fillers for hollow components, and the use of layered foam structured composites and particles as passive dampers. These applications compare the original state before and after the use of non-standard structural materials. The comparison is through the time records of oscillation amplitudes, frequency spectrum, acoustic emission, and resonance curves. The measurements of these characteristics are in the frequency band up to 60 kHz, and the acoustic signal in band 60kHz up to 300kHz. The benefits can be stated as favourable with a reduction of amplitudes by an average of 30% up to 70%.

B3. Kinetics and isotherms of adsorption of Phenol and Chlorophenol by four types of activated carbon

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The adsorption on activated carbon is universally used to remove traces of many organic compounds present in water. The aims of this paper are to study the kinetics and adsorption isotherms of two organic micropollutants (Phenol, 4-Chlorophenol) by four types of powdered activated carbon (PAC). The powdered activated carbons were previously characterized by fluorescence X to determine chemical composition, specific surface area S_{BET} , porosity; grain size, ash content, and total acidity. The pH and ionic strength effects were tested to determine their influence on the adsorption capacity. The overall results showed that the adsorption kinetics of all the solutes were very fast. Modeling of adsorption isotherm and kinetic data are the key to predicting and comparing adsorption performance. In this study, three models have been selected to describe the data adsorptions, Langmuir's and Freundlich's isotherm models and Adams–Bohart kinetic model. The correlation coefficient (r^2) indicated that the three models exhibited comparable integrity to fit the experimental data.

B4. Modified POSS nanoparticles for the stabilization of styrene-isoprene-styrene triblock copolymer

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The modification of polyhedral POSS nanoparticles by the presence of different substituents in the benzene ring attached to the polyhedral oligomeric silsequioxane (POSS) structure changes the thermal and radiation stabilities of polymers, for example, styrene-isoprene-styrene triblock copolymer (SIS) used as packaging material. The inspection of differences that exist between the seven hybrids consisting of SIS and modified POSS with benzene rings where CH₃, OCH₃, F and Cl are present indicates the influence of the electronic density on the degradation of inorganic filler and, consequently, the different protection effects against oxidation. The isothermal chemiluminescence determinations show that the pristine polymer is stabilized by all POSS structures, while the nonisothermal chemiluminescence measurements reveal the differentiated decrease in the oxidation start temperature after g-irradiation at 50 kGy. The existence of various substituents in the POSS configurations enables the selection of a suitable filler for the lowest oxidation rate. The protection efficiency of the modified POSS filler is more evident at temperatures exceeding 150 °C, when the electronic effect of substituents becomes evident in the evolution of thermal degradation. If the temperatures characterizing the start of oxidation in SIS/POSS hybrids are different for the seven compounds acting as stabilizers in unirradiated samples, the 50 kGy irradiated patterns present about the same temperature for the oxidative degradation, illustrating severe damage to the fillers.

B5. Microfibrils from oil palm trunk: Effect of delignification and fibrillation technique

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Oil palm trunks represent a potential raw material for the preparation of cellulose nanofibers (CNF). The manufacturing of CNF has typically involved the pretreatment and the mechanical fibrillation stage. However, the different methods used will be affecting the resulting CNF from OPT. In order to understand the effect, this study was done to apply less severe delignification and fibrillation techniques to OPT and then further investigate their influence on fibril properties. Morphology analyses showed less severe delignification and fibrillation techniques resulting in rougher surface, low interfacial adhesion, and higher fiber diameter. However, particle size distribution was found comparable between B-H-OPT and A-MH-OPT. FTIR analysis showed minor changes in the chemical compositions following the alkaline treatment and the bleaching process, whereas the samples subjected to mechanical treatment only remained similar. Rheology analysis exhibited the less viscous characteristics of less severe delignification and fibrillation techniques. Less negative zeta-potential after alkali treatment and more negative zeta after oxidation were detected lower electrophoretic mobility while only a slight decrease in zeta potential value after mechanical treatment. TGA analyses showed OPT began to decompose at 253 °C, while less severe delignification exhibited lower thermal stability.

B6. Fabrication of Cross-Linked PMMA/SnO₂ Nanocomposites for Highly Efficient Removal of Chromium (III) from Wastewater

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In recent times, developments in polymer application properties have required the design of different polymer structures more than ever. Cross-linked polymers (CPs) could be considered a good candidate material for potential applications when used in conjunction with nanoparticles. Crosslinked polymethyl methacrylate nanocomposites are considered to be one of the most commonly polymeric adsorbents due to their varied and simple modification methods. A new class of CPMMA/SnO₂(a–d) nanocomposites have been fabricated as surface-selective adsorbents of Cr (III) with a good yield and different loading of SnO₂ nanoparticles. The morphology, molecular structures, and thermal stability of the new cross-linked polymers were examined using a scanning electron microscope (SEM), the Fourier Transform Infrared method (FTIR), X-ray diffraction (XRD), and Thermogravimetric Analysis (TGA). The adsorption study of C-PMMA/SnO₂ was investigated, and an efficient level of adsorption for Cr (III) cations was detected. To evaluate the potential for the new polymers to be used as adsorbents against Cr (III) ions, the contact time, the initial concentration of Cr (III), and the effects of pH were studied. The introduction of SnO₂ into the polymer network enhanced the efficiency of the adsorption of heavy metals. The C-PMMA/SnO₂ is highly efficient at removing Cr (III) ions in wastewater samples at pH 6 for one hour. The adsorption study demonstrated that the adsorption capacity of C-PMMA/SnO₂c for Cr (III) was 1.76 mg /g, and its adsorption isotherm agreed with the Langmuir adsorption model.

B7. Characterization of Ni-B/MoS₂ composite coatings produced by chemical reduction method using a sediment deposition technique

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Results of research on composite coatings with a nickel boron matrix and molybdenum sulfide as the dispersion phase, produced by the chemical reduction method on a carbon steel substrate, are presented.

Molybdenum sulfide in the form of powder (<90 nm) was used as a dispersion phase. The coatings were deposited from a bath at different concentrations of dispersion phase, namely 0.1; 0.3; 0.5; and 1.0 g/dm³. Composite coatings Ni-B/MoS₂ were produced using a sediment deposition technique. Surface morphology and topography were examined using the scanning electron microscopy (SEM) and light microscopy. Characterization of the structure of the produced materials was performed using X-ray diffraction analysis. Thickness of obtained coatings was examined using X-ray fluorescence spectrometry. Additionally, the mechanical properties of obtained coatings were determined by a Depth Sensing Indentation (DSI) method. Adhesion of the produced coating to carbon steel substrate was tested by scratch test method.

Acknowledgements:

The project "New electroless Ni-B/B and Ni-B/MoS₂ composite coatings with improved mechanical properties" benefits from a EUR 200 000 grant from Norway. The aim of the Small Grant Scheme (SGS) call is to support applied research projects led by female scientists in technical sciences.

B8. Effective Electromagnetic Shielding with Graphene Epoxy Composites in the Extended THF Band: Fabrication, Measurement Procedures, and Data Analysis

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We report on the fabrication, characterization, and measurement of the THz characteristics of graphene composites in the THF band. The composites, containing low percent-by-weight fractions (wt.%) of graphene from 0.8wt.% to 1.2wt.%, were prepared from commercially available graphene by mixing it with epoxy using a high-shear-speed mixer.

EM shielding properties of the composites in the extended THF band from 0.25 to 4.00 THz were investigated using THz-time domain spectroscopy (THz-TDS). Based on the measured transmission and reflection coefficients, the shielding effectiveness parameters of reflection (SE_R) and transmission (SE_T) were calculated to determine the shielding effectiveness of absorption (SE_A). The procedure comprised each of the weight fractions of graphene.

While the SE_R was found to be less than ~ 0.6 dB within the measured frequency range and for all the samples, the SE_T and SE_A were found to be substantially higher, firmly above ~ 70 dB with a graphene loading of 1.2wt.% at the frequency $f=1.6$ THz. Such unexpectedly high total shielding effectiveness resulted mostly from absorption due to the measured low absolute values of SE_R .

The fact that a simple EM energy redirection via conduction-based reflection was not the primary energy loss mechanism is favorable from the point of view of EMI shielding because, contrary to metal-based conducting coatings or metallic nanocomposites, the graphene-based epoxy materials do not spread the unwanted EM radiation from one place to another. Additionally, they have low weights.

By performing Beer–Lambert calculations, we show that even a thin-film or spray coating with a thickness in the few-hundred-micrometer range of lightweight, non-conducting and non-reflecting graphene epoxy composites can be sufficient for blocking THz radiation in many practical applications, wherein the shielding of EM by ~ 20 – 30 dB is typically sufficient. Thus, the fabricated composites can be successfully used as effective ultra-thin stealth materials.

B9. Evaluating Adipose Stromal Cell Seeded Polyurethane Polymers as Tissue Engineered Implantable Ligament Substitutes

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INTRODUCTION: Anterior cruciate ligament (ACL) provides stability to the knee joint and is commonly injured during high-impact activities, with almost 250,000 injuries in the US and Canada. Due to poor self-healing, surgical reconstruction with autograft is often required, but it fails to restore its biomechanical functions, leading to re-injury. To overcome this, biomaterials, such as elastic polyurethane and polyvinyl alcohol copolymers, that are reinforced with stem cells are being studied as an ACL graft substitute. These biocompatible polymers can be 3D-bioprinted using additive manufacturing. Heterogenous adipose stromal cells (ASCs) are abundant, easy to harvest, and have minimal donor-site morbidity. This study aims to characterize LayFomm60 and LayFelt for tendon tissue engineering as they are flexible and display surface micropatterning. We hypothesize that biophysical scaffold properties may drive ASC tenogenic differentiation and matrix deposition to act as a tissue substitute.

METHODS: Swelling assay and degradation profile of LayFomm60 and LayFelt filaments were performed over 90 days. Tensile testing for young's modulus (E), ultimate tensile strength (UTS), and strain at failure (ϵ_f) of 3D-printed scaffolds were determined. Human ASCs were seeded on the scaffolds for 7 days to evaluate cell viability (LIVE/DEAD assay), metabolic activity (Alamar Blue assay), and tenogenic gene expression (Collagen type I, Collagen type 3, and scleraxis).

RESULTS: Layfomm60 had much higher ϵ_f but lower UTS and E, and LayFelt showed lower UTS, E, and ϵ_f , compared to native ACL. ASCs on both Layfomm60 and LayFelt showed cell viability of 100% and remained metabolically active. Scleraxis, one of the early tenogenic markers, was increased 2.5-fold on LayFomm60 and 1.5-fold on LayFelt compared to undifferentiated ASCs, indicating material-driven tenogenic differentiation.

CONCLUSIONS: LayFomm60 co-printed with a rigid material, such as PLA, and seeded with cells and cultured for longer time points such as 14 and 21 days may create a biomechanically viable ACL graft substitute.

B10. Assessment of ammonium ions removal from aqueous solutions using zeolite-composite materials derived from fly ash

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Environmental pollution with both inorganic and organic compounds remains a valid topic and requires intensive development of novel methods for their removal. Contamination of groundwaters, rivers, lakes and oceans with *i.a.* ammonium and nitrate (V) ions can lead to significant growth of harmful algae causing eutrophication. Among methods used for removal of ammonium ions like denitrification, which is limited by rather low temperature of regenerated water, adsorption process can be found as a promising approach. In our research we have investigated zeolite NaX from fly ash and its composite with carbon and vermiculite. Materials were characterized in detail by means of XRD, XRF, and N₂ adsorption-desorption. To evaluate the utility of obtained materials, zeolites were subjected to series of adsorption studies to investigate their adsorption properties towards ammonium ions. The effect of initial solution pH and adsorbent dose were also investigated. The optimal conditions for ammonium ions (NH₄⁺) removal were found to be pH of 7.00 and adsorbent dose of 2 g L⁻¹. At these conditions both parent zeolite NaX and zeolite NaX-Vermiculite composite displayed similar adsorption capacities of about 21 mg (NH₄⁺) g⁻¹ and the percentage (NH₄⁺) removal was 41%. On the other hand the NaX-Carbon composite adsorption capacity was significantly lower – 14 mg (NH₄⁺) g⁻¹ and percentage (NH₄⁺) removal of 25%. Such phenomenon can be a result of the distinct surface properties of the materials. The equilibrium of adsorption was obtained relatively fast after 30 min only. The investigated materials can find their future application as efficient adsorbents or additives to mineral-organic fertilizers.

Acknowledgement

The POIR.04.00-00-14E6/18-00 project is carried out within the TEAM-NET programme of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund

B11. Characteristics of hybrid chitosan-bioglass coatings deposited on plasma activated PEEK polymer

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Polyether ether ketone (PEEK) is biocompatible, chemically and physically stable, and is a radiolucent polymer that exhibits a similar elastic modulus to normal human bone, making it an attractive orthopedic implant material. However, PEEK is biologically inert, preventing enough strong bonding with the surrounding bone tissue when it is implanted *in vivo*. Surface modification and composite preparation are two main strategies to improve the bioactivity of PEEK.

In this study, we prepared and investigated plasma activated PEEK surfaces with embedded bioglass, chitosan, and chitosan-bioglass mixed layers applying dip coating/from solution hybrid coating technique. The obtained surfaces were investigated in terms of wettability and surface free energy changes. Moreover, FTIR (Fourier Transformation Infrared Spectrometry) and SIMS (Secondary Ion Mass Spectrometry) has been applied to establish and control coatings composition. Simultaneously the structure of coatings has been visualised with aid of SEM (Scanning Electron Microscopy). Finally, the obtained systems were incubated in SBF (Simulated Body Fluid) to verify the modifications influence on the bioactivity/biocompatibility of PEEK surface.

For the preparation of bioactive PEEK composites, the main challenge is to keep the excellent mechanical properties of PEEK when impregnating bioactive materials, thus all conducted modifications affected only its upper surface. The development of PEEK composites covered with nano/micro-sized bioactive materials/films may provide an effective way to obtain both mechanical and biological benefits.

B12. Synthesis and Characterisation of Bipyridine-Based Polyaminal Network for Carbon Dioxide Capture

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In order to respond the high demand for decreasing the amount of CO₂ in the atmosphere, a new polyaminal-based polymer network (Bipy-PAN) was designed and successfully prepared through one-pot polycondensation reaction of melamine and ,2'-[Bipyridine]-5,5'- dicarbaldehyde. The formation of the polymer structure was confirmed by FT-IR, solid-state ¹³C NMR, powder X-ray diffraction. The porous properties of the polymeric structure were confirmed by field-emission scanning electron microscope and N₂ adsorption-desorption methods at 77 K. The efficiency of CO₂ capture will be discussed in detail.

References:

- Liu, C.; Xia, M.; Zhang, M.; Yuan, K.; Hu, F.; Yu, G.; Jian, X. *Polymer* 2020, 194, 122401.
Yang, G.; Han, H.; Du, C.; Luo, Z.; Wang, Y. *Polymer* 2010, 51, 6193–6202.
Rong, M.; Yang, L.; Wang, L.; Yu, J.; Qu, H.; Liu, H. J. *Colloid Interface Sci.* 2019, 548, 265–274.
Hou, S.; Tan, B. *Macromolecules* 2018, 51, 2923–2931
McMurry, J. *Organic Chemistry*, 8th ed.; Cengage Learning: Toronto, ON, Canada.
Ibrahim, M.; Tashkandi, N.; Hadjichristidis, N.; Alkayal, N.. *Polymers*, 2022, 14, 1136.

B13. Influence of substrate temperature and gas environment on the structure of Cu₃N thin films as solar absorber deposited by reactive magnetron sputtering

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Copper nitride film is a metastable semiconductor material with an anti-ReO₃ type crystal structure where the face-center-cubic close packed sites are vacant and Cu atoms occupy the center of the cubic edges, forming linear bonds with two nearest N anions. The Cu₃N material is attracting increasing interest as absorber for photovoltaic applications due to its non-toxicity and earth abundance and, besides, its band gap energy can be easily tunable in the range 1.4 to 1.8 eV. This material can be easily doped both p and n type to establish a heterojunction and presents good stability. Therefore, the control of its structure is a hot topic for the development of solar cells. In this work, Cu₃N films were fabricated by reactive magnetron sputtering, from a commercial 3-inch diameter Cu metallic target (purity: 99.99%) on Corning Glass substrate. The films were deposited at room temperature (RT) and 100 °C, at 50W of RF power, by controlling the nitrogen partial pressure, $R=[N_2]/([Ar]+[N_2])$, between 0.8 and 1.0. The total gas flow was 30 sccm, while the pure nitrogen flux was set to 20 sccm. The different working pressures used were 3.5 Pa and 5 Pa. The aim of this work is to determine the morphology, the chemical stoichiometry, and the crystallographic structure of the sputtered Cu₃N thin films as function of both the substrate temperature and the gas environment, evaluating its physical properties related to photovoltaic applications. For this purpose, X-Ray diffraction (XRD) measurements, Atomic Force Microscopy (AFM) analysis, and scanning electron microscopy SEM-EDS techniques are used.

B14. Surface engineering with metal to design heterojunctions for efficient photoelectrochemical ethanol oxidation

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The increase in global energy demand and severe climate change resulting from the impact of fossil fuels has led researchers to find alternative sources of energy.^[1] The implementation of fuel cells based on biofuel ethanol may be one of the promising, efficient and clean alternatives of renewable energy to meet the future energy demand.^[2] The implementation of direct ethanol fuel cells requires an active and durable catalyst for an efficient-energy conversion of ethanol.^[3] Photoelectrochemical processes have also received huge attention for the utilization of solar energy for the energy-harvesting processes.^[4] Metal oxides and carbon-based materials are a huge attraction to develop cost-effective catalysts due to their high stability, abundance, and tunable band edges. Their surface can be modified via decoration with metals or making heterostructures with other oxides.^[5] In the present work, we have explored the effect of the decoration of metal on the metal oxide and carbon nitride structure for their application as a catalyst for the ethanol oxidation process. The photoelectrocatalytic activity of the prepared catalysts have also been explored to utilize sunlight.

B15. NIR fluorescent hybrid microcapsules as efficient delivery agents for controlled in vitro Avastin drug release

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There is a pressing clinical need for researchers and the pharmaceutical industry to develop new strategies to prevent and combat diabetic retinopathy (D.R.), a common complication of diabetes leading to blindness due to retinal and optical nerve damage. Hence, we propose a novel model of hybrid polymeric microcapsules able to encapsulate two FDA-approved molecules as delivery vehicles able to transport therapeutic molecules into human retina cells. Specifically, Indocyanine Green (ICG), an NIR fluorophore with excellent thermal properties, was encapsulated between the polyelectrolytes layers with a loading efficiency of 75%, and Avastin drug, an anti-VEGF therapeutic molecule currently used in the treatment of D.R., was successfully grafted onto the microcapsule surface with 97% efficiency. The microcapsules of 4.5 μm , revealed by SEM images, were synthesized via a layer-by-layer deposition approach on a calcium carbonate template core. First, we proved the capacity of microcapsules to operate as effective photo-therapeutic agents by generating heat under NIR laser irradiation in solution, following the evaluation in human retina cells. We achieved real-time temperature monitoring images of the microcapsules within human retina cells in order to monitor and perform in vitro controlled release of the Avastin drug under laser irradiation. The release of Avastin drug as well as the cytotoxicity of the hybrid microcapsules before and after in vitro laser irradiation was analyzed directly by non-invasive re-scanning confocal fluorescent microscopy images and WST-1 assay. Based on the obtained results, the developed hybrid microcapsules form effective laser-induced microheaters that cause the rupture of the microcapsules and can be used to perform photoinduced release of therapeutic molecules inside retina cells.

Funding: This research was funded by the Romanian National Authority for Scientific Research, CNDS-UEFISCDI, project number PN-III-P2.1-PED-2019-4558. Daria Stoia acknowledges financial support from the Special Scholarship for Scientific Activity grant awarded by STAR-UBB (Babes-Bolyai University), contract number 36605/02.12.2021.

B16. Omniphobic Spray Coating with a Repel-and-Kill Mechanism Prevents Contamination by Drug-Resistant Bacteria and Viruses on High-Touch Surfaces

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The transmission of infectious diseases is a major public health challenge worldwide, accounting for substantial morbidity rates and economic losses. Among the various modes of pathogen transfer, contaminated surfaces in high-touch environments play a key role in the transmission of infectious diseases, specifically in healthcare settings. The inefficiencies of the current intervention methods rely on the use of biocides that aggravate the rapid emergence of antimicrobial resistance and pose harmful health effects. To address this area of need, we developed a universal, dual-functional, and easily scalable omniphobic spray coating that is applicable on various substrates such as glass, textile, stainless steel, polystyrene, and paper. The spray coating induces a “repel and kill” effect against both bacteria and viruses, resulting in a significant decrease in cross-contamination and contamination of surfaces. Pathogen tests against societally relevant pathogens including *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Phi6* (a bacterial virus often used as a surrogate for SARS-CoV-2) reveal an over three-log (99.9%) reduction in pathogen adhesion on coated surfaces. Studies of pathogen transfer under real-life conditions reveal that an uncoated contaminated glove transfers pathogens to more than 50 subsequent surfaces, while a spray-coated glove picks up 10^4 (over 99.99%) fewer pathogens upon first contact and transfers zero pathogens after the second touch. The developed coating provides excellent stability and robustness under harsh conditions, and its remarkable anti-pathogen properties combined with its ease of implementation onto various substrates substantiate its use for the prevention of surface-mediated pathogen transmission.

B17. Composite copper/carbon phase coatings for potential applications in electronics

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The presented work evolves around research dedicated to deposition of composite coatings with dispersion phase of different forms of carbon nanoparticles embedded in copper matrix for potential applications in electronics, such as electric car IZERA.

The composite Cu/C coatings, as well as copper coatings without addition of dispersion phase, obtained for comparative purposes, were deposited on a steel substrate using electrochemical reduction method. Two types of matrixes were used in coatings preparation: micro- and nanostructured, as well as three kinds of carbonous dispersion phase: carbon nanotubes, graphene, or nanodiamond. Coatings were deposited using varying stirring speeds and current densities at room temperature.

Structure, composition, and mechanical properties along with morphology and thickness of obtained layers were investigated to determine influence of applied conditions. For this purpose, a variety of techniques, i.e., X-ray powder diffraction, scanning electron microscopy equipped with energy-dispersive X-ray spectrometer, X-ray fluorescence spectrometry, and the Vickers hardness or scratch test method, were utilized.

Changes in current density and incorporation of differing dispersion phases were determined to influence coatings thickness, morphology, topography, etc.

Acknowledgements

The presented research was financed by the earmarked grants awarded by Łukasiewicz Center, grand contract no 2/Ł-IMP/Ct/2021.

B18. Photocatalytic NO_x abatement: The effect of high air-flow velocity

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In the literature, the abatement of nitrogen oxide (NO_x) emissions by photocatalysis is rarely carried out under real-world air-flow velocities. Here, we investigated the ability of two commercial photocatalysts, Aeroxide[®] TiO₂ P25 (Evonik Industries, Germany) and FN NANO[®]2 (Advanced Materials-JTJ, Czech Republic). P25 contains 88% anatase and 12% rutile, and FN 2 contains 13% of the binder. The degradation of NO_x pollutants NO and NO₂ (0.1 and 1.0 ppmv) under air-flow velocities ranging from 0.02 to 0.7 m s⁻¹ was tested. At these velocities, the photocatalytic efficiency was determined for various slit heights (5–25 mm) and air-flow rates (1500–11 000 cm³ min⁻¹). The photocatalysts achieved substantial NO and NO₂ abatement. The pollutant conversion decreased as the air-flow velocity increased, with the highest conversion (80%) occurring at 0.1 m s⁻¹. The NO_x conversions were slightly higher for NO than for NO₂, and significantly higher for the NO concentration of 0.1 ppmv. The slit height had a negligible effect, indicating that there was a substantial degree of mixing in the direction perpendicular to the flow; this means that the flow cannot be laminar in nature as the ISO standard (22197-1:2016) states. This finding is supported by the nanoindentation technique showing that the surface roughness contributed to the formation of vortexes and enhancement of the mass transport. To the best of our knowledge, this is the first study to test commercial photocatalysts under such a wide range of air velocities and, in doing so, it has identified considerable implications for outdoor air purification.

B19. Photocatalytic Degradation of Halogenated Phenols: Experimental, DFT and Antibacterial Study

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Halogenated phenols represent an important group of industrial pollutants due to their toxicity and low biodegradability. In this work, the degradation of 4-chlorophenol (4-CP) and 4-bromophenol (4-BP) by heterogeneous photocatalysis using different sizes and allotropes of TiO_2 was investigated. The physico-chemical properties of a wide range of photocatalyst nanoparticles with a nominal crystallite size ranging from 5 to 800 nm were correlated with their photocatalytic activity. The increase in anatase particle size led to the enhancement of the degradation rate of 4-CP and 4-BP while the rutile behaviour was the opposite. Moreover, the larger nanoparticles directed the degradation mechanism, as the formation of hydroxylated aromatic products (4-chlorocatechol, 4-bromocatechol) was observed only for them. This finding is supported by the analysis of the total organic carbon content as its direct decrease was found for the smaller ones (and reference P25). Based on the DFT model, by employing OH radical attack, an alternative reaction pathway leading to either direct decarboxylation or hydroxylation was proposed. The bactericidal properties of the nanoparticles and chemical substances of Gram-positive and Gram-negative bacteria, including multiresistant strains, were successfully demonstrated. The participation of hydroxyl radicals in the degradation was assessed with a radical scavenger. The presented results demonstrate that not only the crystalline form/chemical constitution of the photocatalyst but also other properties are important in its performance and should be considered in the development of photocatalytic applications.

B20. Microfluidic platform for inline photocatalytic reduction of Cr(VI) using nanosized titanium dioxide

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Hexavalent chromium (Cr(VI)) is a toxic heavy metal ion as a wastewater by-product from various industries, such as leather tanning, refractory production, metal plating, pigmentation, and electroplating. The Cr(VI) is a strong oxidizing agent which causes an adverse effect on living organisms as it has a teratogenic and carcinogenic effect on human health. Several techniques, such as solvent extraction, chemical precipitation, ion exchange, reverse osmosis, adsorption, and photocatalytic reduction have been reported to eliminate Cr(VI) from industrial waste. Using photocatalytic reduction of Cr(VI) seems a practical and cleaner approach because it is a solar-light-driven process that reduces the cost considerably. However, the conventional batch photocatalytic reduction process suffers from low mass transfer efficiency and non-uniform light management resulting in low photon transfer efficiency, which can be overcome by using microfluidic technology termed as the *inline photocatalysis* process. Our study indicates that the microreactor design is crucial in determining the overall efficiency of a photocatalyst for different environmental applications. The present work demonstrates various PMMA-based microreactors fabricated using the laser micromachining technique for inline photocatalytic reduction of Cr(VI) using TiO₂ as a photocatalyst upon light irradiation. Microfluidic platforms, such as flow rates and channel length, have been evaluated for the reduction of Cr(VI) to Cr(III). We have also explored various reactor designs, such as serpentine, branched, and micropillars to realize an effective photocatalytic reduction process. A comparative study has also been made to analyze the reduction efficiency of both inline and conventional batch photocatalysis. Wherein, the reduction efficiency using inline microfluidic reactors is way superior when compared to the batch synthesis platform.

B21. Comparative study on the mechanical behavior of microwave-assisted compression-molded and conventionally compression-molded nano-hydroxyapatite-reinforced UHMWPE composite

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The nano-hydroxyapatite (nano-HA)-reinforced ultra-high-molecular-weight polyethylene (UHMWPE) composite is a popular biomaterial due to its excellent biocompatibility. Better mechanical performance of the UHMWPE/nano-HA composite is required to sustain various static and dynamic loads caused by the normal kinematics of patients after implantation. The value of the mechanical performance may be less than the actual performance due to defects caused during molding and heating of UHMWPE/nano-HA. Uniformity in the heating during molding depends on the manufacturing technique. Microwaves are known for their uniform and rapid heating. Therefore, this manuscript compares the manufacturing time and mechanical performance of microwave-assisted compression (MAC)-molded and conventional compression (CC)-molded composite. The UHMWPE/nHA composite was molded slightly below its melting point, determined using a differential scanning calorimeter. A thermal imaging camera was used to observe the thermal profile of the molded material for uniform and non-uniform heating. The mechanical behavior of the molded composite was determined in terms of the Young's modulus, ultimate tensile strength, and Vicker's hardness. A lower molding time and better mechanical performance were observed in the MAC-molded UHMWPE/nano-HA composite.

B22. Study of Transition Areas in Press-hardened Steels in Combined Tool for Hot and Cold Forming

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Press-hardening, also called hot stamping, is a manufacturing process for producing parts of the car body that must meet high demands on their mechanical properties and safety parameters. Moreover, these components often have different requirements for mechanical properties in individual parts. This work presents the press-hardening process in a combined tool wherein one half of the tool is heated and the other half is cooled. The cooled part has been printed due to the complexity of the internal channels used for water cooling. The aim of this work is to investigate the variation of the sheet microstructures and their mechanical properties depending on the cooling process in the tool and to determine the transition area where these properties cross over. Modern high-strength steel with 0.2% C and alloyed with manganese and aluminium was chosen for the experiment. A temperature of 425 °C was set in the heated part of the tool, and different holding times in the tool were tested. In the heated part of the tool, a bainitic structure with a fraction of ferrite and retained austenite should be formed, while in the quenched part of the tool, a martensitic transformation is promoted due to rapid cooling. In addition to microscopic analyses, mechanical tests and hardness measurements were performed.

B23. Annealing Phenomena in Electroformed Invar

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Invar, whose coefficient of thermal expansion (CTE) approaches zero, is used as a material for the fine metal mask (FMM) in the evaporating process of producing red–green–blue (RGB)-type organic light-emitting diode (OLED) displays because the hole size of the FMM should not change during the process. The electroformation of Invar has recently been a hot topic in RGB-type OLED display industries. In the current work, Fe-33, 36, 42 wt.% Ni alloy foils were electroformed by employing batch-type electrodeposition simulating the drum-type cathode for a continuous electroforming equipment. In the as-deposited state, these Invar alloys revealed different distributions of phases depending on the alloy composition as follows. Fe-33 wt.% Ni consisted of the single α phase of BCC structure and Fe-42 wt.% Ni possessed the single γ phase of the FCC structure. In Fe-36wt.% Ni, the α and γ phases coexisted. These thin sheets were annealed under a mechanical load in the range of between 300 and 550 °C to investigate the microstructure evolution in terms of phase transformation and its possible effect on CTE values.

B24. Structure and Properties of γ -form Polypropylene Nanocomposites Crystallized under High-Pressure

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In this study, three kinds of nanofillers, namely carbon nanotubes (CNT), poly(tetrafluoroethylene) (PTFE), and an organo-montmorillonite (C15A) were used to fabricate isotactic polypropylene (iPP) based nanocomposites via a melt-mixing method. Neat iPP and the nanocomposites were crystallized in the orthorhombic gamma-form under elevated pressure, up to 200 and 300 MPa, in a custom-built pressure chamber under various thermal conditions. After releasing pressure, the crystallized materials were analyzed by wide-angle X-ray, differential scanning calorimetry, and polarized microscope techniques to have an insight into their structure, crystallinity, and the content of crystallographic forms. The materials are crystallized in the pure or almost pure crystallographic gamma-form. Plane-strain compression tests were performed in order to evaluate the mechanical properties of the crystallized samples. The mechanical properties mainly depended on the crystallization conditions, but they were also influenced by added nanofillers, especially CNT. We have also observed an important role of the expansion of specimens crystallized under high-pressure after pressure release.

B25. Development of newly polyester composites reinforced with waste marble and CdO particles for radiation shielding applications

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The use of radiation is mandatory for modern life, in the same manner, the outflow of radiation and harmful inhospitable byproducts from the nuclear plants is obvious which has created significant concern about radiation shielding materials because of the still occurring results of previous nuclear plant disasters. Generally, “shield” stands for a barrier, one of the major ways of defending any living being from high penetrating radiation. Considering this point, this study aims to manufacture marble samples as novel radiation shields. The physical and radiation shielding ability of the marbles was determined and analyzed. For this purpose, the HPGe detector was used to detect the incoming photons emitted from three-point sources (Am-241, Cs-137, and Co-60). The radiation attenuation factors for the new marbles will be measured for some energies ranging from 0.06 to 1.333 MeV. We examined the effect of increasing the PbCO₃ and CdO contents on the physical properties and radiation attenuation factors for the prepared polyester composites. We found that the density of the samples increases from 1.784 to 1.796 g/cm³ when the CdO changes from 0 to 12.5 w.t.%. The linear attenuation coefficient (LAC) for all marble compositions has the maximum value at 0.06 MeV, while the LAC decreases with increasing the energy. The highest LAC is found for the marble with 12.5 w.t.% of PbCO₃ and CdO. We studied the impact of the addition of CdO on the expense of PbCO₃ and we found that the HVL decreases with increasing the content of CdO. The radiation protection efficiency (RPE) of the new marbles was reported and we found that the RPE for the marble with the highest amount of CdO is higher than the other marbles, which confirms that the addition of CdO has a positive impact on the radiation shielding competence for these new marbles.

B26. Effect of forming and heat treatment parameters on the mechanical properties of medium manganese steel with 5% Mn

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Medium manganese steels fall into the category of modern third-generation high-strength steels. Thanks to their alloying, they use a number of strengthening mechanisms, such as the TRIP and TWIP effect, to achieve their mechanical properties. The excellent combination of strength and ductility also makes them suitable for safety components in car shells, such as B-pillars or floor side reinforcements. Press hardening technology is used for the production of these parts, which also enables the processing of metal parts from high-strength steels with a small springback effect.

Medium manganese steel with 0.2% C, 5% Mn, and 3% Al was used for the experimental program. Sheets with a thickness of 1.8 mm without surface treatment were formed in a press hardening tool. Since B columns require different mechanical properties in individual parts, the change of mechanical properties by local induction heating to the intercritical region was tested on the obtained omega profiles to increase the ductility. These results were compared with classically annealed specimens in an oven. In the case of tool hardening, strength limits of over 1400 MPa with ductility of about 15% were obtained. An excellent material for CO₂ capture capable of CO₂ absorption and fixation.

B27. Low-temperature structural, dielectric and ferroelectric properties of $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ ($x=0-0.45$)

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$\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ (BST) ($x = 0, 0.45$) ceramics were prepared by the solid-state reaction method. Their crystal structure, dielectric microstructure, and ferroelectric properties were studied. XRD data show that all of the ceramics possess a single perovskite phase. SEM results confirm that the ceramics are well sintered and exhibit relative densities higher than 97%. The results also reveal that the microstructures of the different compositions do not show a significant variation. The increasing concentration of Sr^{2+} ions leads to the shifting of T_c toward lower temperatures.

The temperature evolution of the electric permittivity and dielectric loss of $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ ceramics ($x = 0 - 0.45$) with increasing Sr content were observed. The permittivity maximum broadens and shifts towards a lower temperature. In addition, for a higher Sr content, the relaxor-like character of the phase transition seems to exist. The dielectric loss maximum broadens and shifts towards lower temperatures as a result of Sr doping. E-poling leads to a decrease in electric permittivity and dielectric loss due to increasing domain/polar region ordering.

The temperature evolution of Raman and IR spectroscopy along with X-ray diffraction (XRD) data was adopted to investigate the composition/E-poling-induced changes in the properties under investigation. The results obtained are discussed in terms of the microstructural/structural effects of Sr^{2+} incorporation into BaTiO_3 . It is shown that E-poling influences the properties under investigation. This includes modification of the local structure, dielectric response, and temperature of phase transformations. This could result from improvement by the electric field of the polarization ordering, previously disordered by introducing Sr^{2+} to BaTiO_3 .

B28. Exciton to Dopant Energy Transfer in Mn Doped (BA)₄AgBiBr₈ Layered Double Perovskite

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Metal halide layered double perovskites (LDPs) have emerged as a new class of semiconductor materials that can be the suitable green alternatives of their toxic Pb-based counterparts. By doping the semiconductor materials by suitable metal ion, their optical and electronic properties can be enhanced. We show here the Mn doping in hybrid inorganic–organic two dimensional halide layered double perovskite (BA)₄AgBiBr₈ (BA = n-butyl amine) via a simple solid-state mechanochemical grinding. The large band gap and high stability of these materials encourage us for doping of Mn ions in 2D LDP to improve their optical and magnetic properties. In our methodical strategy, we ground the as-synthesized perovskite crystals with Mn precursors and then annealed it for 2 hours. The successful incorporation of Mn ions inside (BA)₄AgBiBr₈ lattice was proved by XRD analysis and EPR spectra. The Mn-doped 2D LDP shows the energy transfer from the host excitons to the d-electrons of Mn²⁺ ions which results in red shifted broad Mn emission band centered at 625 nm, which is due to spin-forbidden ⁴T₁ to ⁶A₁ internal transition. The doping of magnetic Mn²⁺ ions in (BA)₄AgBiBr₈ make it promising candidate for spin-electronics and spin-photonics.

B29. Charge Transfer Dynamics in CsPbBr₃-CdSe/CdS/ZnS Nanohybrids Coupled with Bifunctional Ligands

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Mixed-dimensional nanohybrids (MDNHs) between zero-dimensional (0D) perovskites and two-dimensional (2D) II-VI semiconductors hold great potential for photonic device applications. However, a deep understanding of the charge transfer mechanism in these systems is essential to improving the performance of photovoltaic devices. Herein, we demonstrate a route for the synthesis of 0D-2D CsPbBr₃-CdSe/CdS/ZnS core/shell/shell (CSS) MDNHs using three bifunctional ligands: 4-aminothiophenol (4-ATP), p-aminobenzoic acid, and 6-amino-2-naphthoic acid. We investigated the electronic interactions between CsPbBr₃ nanocrystals (NCs) and CSS nanoplatelets (NPLs) in nanohybrid systems in the presence of these bifunctional ligands. Though in all the systems, the charge transfer is observed between CsPbBr₃ and CSS, the rate of charge transfer is greatly influenced by the presence of ligands. We observed that when 4-ATP is present as a molecular linker between CsPbBr₃ and CSS, the rate of charge transfer is faster as compared to other ligands. The small size of 4-ATP and its strong binding affinity with both the materials brings these two different classes of materials into close proximity, enhancing the charge-transfer process. Furthermore, for the elucidation of the charge transfer kinetics between CsPbBr₃ and CSS, a Poisson binding model has been proposed which assumes a Poisson distribution of CSS NPLs around CsPbBr₃ NCs. In this fashion, an average number of CSS NPLs present on the surface of one CsPbBr₃ NCs is obtained, which is found to be highest in the case of 4-ATP-linked MDNHs. This study opens up possibilities for coupling perovskites with chalcogenide semiconductors by using bifunctional ligands, which could be used in photonic device applications.

B30. Thermoplastic starch modified with deep eutectic solvents as multifunctional biodegradable materials intended for plants cultivation

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The aim of the project is to develop polyfunctional materials based on abundant, environmentally friendly sources, mainly of natural origin. One of the basic materials is starch (corn, potato), consisting of two polysaccharide fractions: amylose and amylopectin. Starch is a promising source for natural-based, environmentally friendly bioplastic production. It undergoes thermoplasticization with the presence of polar plasticizers, higher temperature and shear forces via methods standardly used for conventional plastics, i.e., extrusion and/or thermocompression molding. Thermoplastic starch (TPS) can be applied, e.g., in food packaging or in agriculture as a fully biodegradable material. In the project, starch is modified with a novel group of media: deep eutectic solvents (DES).

The main goal of the work is to develop materials with fertilizing and moisturizing cultivated plants. A multifunctional pellet is obtained via a simple, solvent-free, one-step extrusion method. This process leads to thermoplasticization of the starch matrix with the presence of DES both as a modifier and nitrogen source for growing plants. Thermoformable pellets can be applied directly as new-generation fertilizers, but they can also be transformed into sheets that can be processed into containers for seedlings or into thinner films as, e.g., fertilizing seed tapes. Moreover, food-processing side products are used both as fillers and supportive agents.

The methods of TPS/DES and TPS/DES/filler include: mechanical and barrier properties, dynamical-mechanical analysis (DMTA), thermal characterization, and infrared spectroscopy (FTIR-ATR). The biodegradation of the TPS-based films obtained via thermocompression molding was studied and the influence of the final material on the model plant growth was investigated.

B31. Structuring of silk-fibroin surfaces by phase separation

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Silk protein (*Bombyx mori*) surfaces are characterized by poor cell adhesion, hence additional surface treatments are required in order to create structured surfaces to increase the adhesive capabilities of selected cell lines. To solve this problem, surface treatment procedures use either patterning templates [1] or preparation of polymer blends [2]. Phase separation procedures are rather rare. In this study, silk protein-based coatings were structured by a dropwise addition of solvent/non solvent mixtures. A special device was developed to create controlled physical conditions during the multi-step, time-sequenced surface treatment [3]. The process parameters for the surface modification were optimized to control the texture formation from nano- up to microporous structures. The interaction of different cell lines was studied on the textured surfaces to explore their application scope in biomedical applications.

Acknowledgment

This work was financially supported by the project funded by Czech Science Foundation (Project No. 22-33307S) and within the project OP RDE Junior Grants of TBU in Zlín, Reg. No. CZ.02.2.69/0.0/0.0/19_073/0016941. The authors thank Prof. Thomas Scheibel, Chairholder of Department Biomaterials, University Bayreuth and Assoc. Prof. Aleš Mráček head of Department of Physics and Materials Engineering, Tomas Bata University in Zlín for providing the facility to conduct this research.

References

- [1] L. W. Tien et al., *Macromol. Biosci.* 2012, 12, 1671-1679
- [2] J. Saremi et al., *J Biomed Mater Res A* 2021, 109, 1588-1599.
- [3] E. Wrzecionko et al., *ACS Appl. Mater. Interfaces* 2017, 9, 6472-6481.

B32. Biopolymer hydrogel compositions as a carrier of active plant extracts used in oncological treatment

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The occurrence of various types of damage to the body integuments, including the most serious ones in the form of wounds or bedsores, and the problem with their difficult healing, is associated with both the cancer itself and the side effects of oncological treatment. The process of wounds formation is complex, because they arise as a result of physical factors, such as surgery, radiotherapy, prolonged pressure on tissues (pressure ulcers), as well as chemical ones—as a result of the toxic effect of drugs used during chemotherapy causing damage. On the other hand, the use of chemotherapy and radiotherapy reduces the body's natural immunity, which adversely affects the wound healing process. Another reason for the formation of wounds and problems with their healing may be the patient's age, due to the natural lowering of the immune parameters and the greater likelihood of comorbidities. One should also pay attention to the problem of pain related to the wound itself, it may limit the patient's mobility and, thus, aggravate the problem of wound healing.

An innovative solution in the form of mats with specific properties was proposed, dedicated to immobilized people undergoing oncological treatment, who are at risk of developing pressure ulcer wounds. The use of the mat will increase the effectiveness of therapy and will have an impact on the psyche of the patient and people dealing with medical care, which will increase the effects and effectiveness of treatment. The developed product will be based on a unique biopolymer hydrogel composition containing antibacterial, nourishing, moisturizing substances, and substances improving microcirculation in the place exposed to pressure ulcer development. The product will ensure a friendly micro-environment at the point of contact. It will drain excess moisture from the skin's surface, and will keep a beneficial biofilm on its surface.

B33. Films of polysaccharides from spent coffee grounds with ions Ca^{2+} as crosslinking agents

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Polysaccharides are the most abundant natural biopolymers. They are biocompatible and biodegradable and are easy to process into different forms of biomaterials, such as capsules, films, and fibers. Spent coffee grounds (SCG) are rich in polysaccharides (~50%), mostly galactomannans, arabinogalactans, and cellulose, which can be used for the production of biomaterials. For this present work, SCG have been delignified and dissolved in a zinc chloride solution for the development of biopolymeric films. The produced film was immersed in a calcium chloride solution with different contact periods and concentrations to form the crosslinking of the polysaccharide chains: 17.5 min in 6 % CaCl_2 (w/v) (F111); 5 min in 10 % CaCl_2 (w/v) (F211); 30 min in 2 % CaCl_2 (w/v) (F311); 30 min in 10 % CaCl_2 (w/v) (F411); 5 min in 2 % CaCl_2 (w/v) (F511). The films were evaluated by FTIR and thermogravimetric analysis. FTIR spectra suggested that ions Ca^{2+} interacted with polysaccharide chains and this interaction was corroborated by the thermal analysis results. F311 and F511 were demonstrated to be more brittle than those films with higher concentrations of Ca^{2+} , with the increased brittleness of films produced with lower concentrations of calcium ions in comparison to those produced with higher concentrations of calcium ion is attributed to the fact that excess calcium ions, in relation to those promoting crosslinking, have been demonstrated to act as plasticizer in the film. F311 and F511 were, thus, more thermally stable than the other films. F411 presented the lowest thermal stability. Ca^{2+} ions improved film compatibility since they break intermolecular and intramolecular bonds between polymer chains and promoted crosslinking. However, further studies should be carried out to have a clear understanding of the role of Ca^{2+} in the crosslinking and consequent mechanical properties of the films produced thereof.

B34. Lung Tissue Surrogates: Fabrication and Mechanical Testing

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In the most recent pandemic situation, COVID-19, it was reported that the lung tissue is one of the primary targets of this deadly virus, affecting respiratory function. Respiratory disorders have of course been reported in the past, but the current pandemic has brought about the need for medical models to better understand the mechanics of the human lung tissue. To date, the experimental testing of cadaveric lung tissue is challenging in a clinical setting due to ethical and biosafety issues. To overcome this challenge, in the present work, lung tissue surrogates were developed using a two-part castable and low-cost material system to mimic the mechanical properties of the human lung tissue. The developed tissue surrogates were mechanically tested in tension under varying strain rates (low-to-high) to investigate their mechanical behavior. In addition, the non-linear behavior of the novel lung tissue surrogates was characterized using different hyperelastic models. Such precisely characterized tissue surrogates would be indispensable for studying a wide range of respiratory disorders and simulating the mechanical behavior of lung tissue for surgical training.

Abstracts

Pre-recorded Talks

Synthesis and Characterization of Ce-doped SrTiO₃ perovskite oxide

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With the growing population and industrialization, the demand for energy as well as energy-storage devices is increasing rapidly. To meet this demand for energy-storage devices, in the present investigation, the system of SrTi_{1-x}Ce_xO₃ ($x=0.00, 0.02, 0.04$) was prepared using the solid-state reaction route. Among all synthesis techniques, the solid-state reaction route was employed as this is the simplest, easiest and cheapest method to synthesize materials. The XRD depicts that samples were crystallized into the cubic crystal structure. All the diffraction peaks were found to be matched with COD file No 1512124. The crystallite size and micro-strain values are determined using W-H plots. To further verify the formation of samples, Raman spectroscopy was employed. The optical properties represent the semiconducting behaviour of the system of samples. The electrical properties of samples were investigated as a function of the frequency and temperature. Based on these studies, the present materials, both pure and doped, can be explored for semiconductor devices and mixed ionic and electronic conductor-based device applications.

Concrete–soil composites: from CT images to mesoscale numerical modelling

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Research on structural applications of cement-aggregate–soil composites has been ongoing; in the present contribution, the first results of the numerical modelling of mesoscale mechanical behaviour are reported. In order to highlight the variations in density inside the material and therefore return a three-dimensional graphic reconstruction in grayscale, digitally computed tomography [1, 2] was applied to two series of cubic specimens of different sizes (50 and 100 mm side). In particular, an estimate of the percentage of voids and the identification of the matrix and inclusions [3] were obtained by an appropriate image treatment. Moreover, a tetrahedral modelling for finite element analysis was obtained from the voxel logic grid. The FE modelling was checked by comparison among the results of compression tests and numerical simulations of cubic specimens. At first, the comparisons were conducted in the elastic field to estimate the mechanical characteristic of RVE, then in the plastic field to analyse the failure behaviour of the composite. Starting from the previous results, an analysis was performed to highlight the effects of the composite mixture on the mechanical behavior of the material.

References

- [1] Flannery, B.P., Deckman, H.W., Roberge, W.G., and D'Amico, K.L., "Three-Dimensional X-Ray Microtomography", New Series Vol 237, page 1439-1444 (1987).
- [2] Latief, F.D.E., Mohammad, I.H., and Rasati, A.D., "Digital 3D Microstructure Analysis of Concrete using X-Ray Micro Computed Tomography SkyScan 1173: A Preliminary Study", IOP Conference Series: Materials Science and Engineering Vol 267, nr 012020 (2017).
- [3] Mazzucco, G., Pomaro, B., Xotta, G., Salomoni, V.A., and Majorana, G.E. "An efficient geometric reconstruction of mesoscale concrete structures accounting for confinement

Studies on the structural, optical, and electrical properties of modified ZnFe₂O₄ nanopowder

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The system of ZnFe₂-xNi_xO₄ (where x=0, 0.05, 0.10) was synthesized by a sol-gel combustion technique at 80°C. The phase identification of all the samples was carried out using X-ray diffraction technique. The pattern obtained was of great match with COD-1010130 which showed that the samples crystallized into a cubic spinel group. Crystallite size and microstrain of the samples were calculated using W-H and SSP plots. The optical bandgap was found to be in the range of 2.50 to 2.95 eV that revealed semiconducting behavior of samples. The incorporation of Ni in the lattice was reconfirmed by Raman Spectroscopy. The dielectric properties of the samples were studied as a function of temperature and frequency. The electrical properties were studied using Arrhenius model. The conductivity of samples was found to be higher than conventional electrolytes for IT-SOFCs. On this basis, it was noticed that these samples could find its application in semiconductor devices and electrolytes in IT-SOFCs.

Design of Experiment on Recycled Aggregate Concrete using Fuzzy logic and Response Surface Methodology

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Recycled aggregate is one form of construction and demolition waste that has been investigated by researchers worldwide for the past few decades. This study presents the optimization of replacing the coarse and fine aggregate portion with recycled aggregate for predicting the concrete's strength properties. Simultaneous Fuzzy logic (FL) using MAT lab and the response surface methodology (RSM) using Minitab18 software were utilized for suitability analysis of recycled aggregate ranging from 0 to 100%. The statistical model was developed to analyse the compressive strength at 7, 28, 56, and 90 days; split tensile strength; and flexural strength with the recycled coarse and fine aggregates. The target compressive strength response of such replacements was carried out, in which we found 30% was 26.41, 39.93, 47.65, and 50.42 MPa for 7, 28, 56, and 90 days, respectively. Based on the predicted responses, the relationships were established, and final mathematical models were developed. The parameters influencing the properties are plotted in surface and contour plots. The experiments were validated with the analytical results, which closely agreed with one another. Such results helped us to identify the trend of strength parameters at various replacement percentages of coarse and fine aggregates in recycled aggregate concrete. The optimization output results indicate the potential for the reduction/minimization of waste construction materials being dumped into landfill and extraction of natural resources.

