2023
MATERIALS, METHODS & TECHNOLOGIES

25th International Conference

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BOOK OF ABSTRACTS

Materials, Methods & Technologies

25th International Conference

17-20 August 2023

Burgas, Bulgaria

In collaboration with

Union of Scientists in Bulgaria

Science & Education Foundation, Bulgaria

Al-Farabi Kazakh National University, Kazakhstan

Institute of Hydrometeorology, Georgian Technical University, Georgia

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Ni AND Ti NANOPARTICLES AT HIGH TEMPERATURES

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Abstract

Ni and Ti nanoparticles were prepared by gas aggregation source and annealed in-situ in the transmission electron microscope. Sintering and coagulation of Ni nanoparticles occur already at 100 °C, followed by their gradual growth at higher temperatures and loose of nanosize features. On the other hand, Ti nanoparticles are stable up to 950 °C, due to the formation of a protective TiO2 shell. Combined core-shell nanoparticles containing Ni core and thin TiO2 shell exhibit good thermal stability up to 700 °C. However, their degradation occur above this temperature, most probably due to different thermal expansion coefficients of Ni cores and TiO2 shells.

Keywords: *Metallic nanoparticles, in-situ TEM, coagulation*

THERMAL PROPERTIES OF SUPER INSULATIONS AND THEIR APPLICABILITY LIMIT

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Abstract

In the world, nearly 40% of all energy consumption comes from buildings, while another 20-40% comes from vehicles. Energy losses in these sectors must be reduced in the European Union. To achieve this, thermal insulation provides an opportunity to increase energy savings. Today, in many cases, it is no longer possible to use traditional insulation materials (polystyrene or wool sheets), but new solutions and new types of thermal insulation materials are needed, such as aerogel or vacuum thermal insulation panels as well as thermal insulation materials doped with graphite. The use of these insulations is especially recommended for vehicles. Nowadays, these materials are often referred to as "Super Insulation Materials" in foreign literature. The mentioned products have much better thermal insulation properties, but the results achieved with these materials must be compared with the results for the thermal insulation materials that are very often used on the market and already mentioned above, in terms of actual applicability. Super insulating materials, as a new class of these products, can play an important role in the future of insulation. It should be noted that there is no precise definition for "SIMs", but Annex 65 of the IEA EBC (International Energy Agency, Energy in Buildings and Communities Programme) defines the elements of this group. In the presentation i will investigate the thermal properties (thermal conductivity, specific heat capacity) and the possible applications for buildings.

Acknowledgements: *Supported by the ÚNKP-22-5-DE-405 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund. This presentation was supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences, grant number: Ákos Lakatos - BO/269/20.*

TEMPERATURE-DEPENDENT Fe2+→Fe3+ CHARGE TRANSFER VS. OPTICAL SPECTRA IN CO-DOPED ZnSe: Fe,Cr

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Abstract

A comprehensive experimental and theoretical approach was applied to study the optical properties of single crystals ZnSe:Fe and ZnSe:Cr as well as co-doped ZnSe:Fe,Cr. The singly doped samples with concentrations of NFe ~10-19 cm-3 and NCr ~ 10-18 cm-3 (ISC, Kharkiv, Ukraine) and co-doped ZnSe: Fe,Cr with NFe,Cr ~ 10-18 cm-3 (3photon, Lithuania) were grown by the Bridgman method and had a homogeneous structure of solid solutions. EPR and optical spectra for Fe and Cr ions of ZnSe single crystals have been examined in the temperature range from 5 K to 300 K. Temperature-induced charge transfer from Fe3+ into Fe2+ on cooling is detected in the sample of ZnSe:Fe. The mechanism of the EPR spectrum formation has been studied using a complex theoretical approach that combines the semi-empirical Modified Crystal Field Theory and structure optimizations using the DFT-based band-periodic plane-wave pseudopotential method. A theoretical model of the EPR spectrum formation based on the coexistence and interaction of two alternative paramagnetic subsystems related to Fe2+ and Fe3+ ions is developed for the singly doped ZnSe: Fe sample. EPR spectra from ZnSe samples co-doped with Fe and Cr were analysed, accounting for four paramagnetic subsystems related to Fe2+/3+ and Cr2+/3+ and two possibilities for embedding them into the ZnSe host matrix. Appearing of structural defects occurring in the doping process in the EPR spectrum formation is explored.

Keywords: *EPR spectroscopy, Modified Crystal Field Theory, ab initio calculations, charge transfer*

Acknowledgements: *This research was supported by the Deutsche Forschungsgemeinschaft (DFG), Project No 517713174.*

MoS_2 OXIDATION: FROM SINGLE $(MoO_3)_X$ CLUSTERS TO MoO_3 / MoO_X LAYERS

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Abstract

Layered semiconductor MoS2 is a representative of transition metal dichalcogenides (TMDs) family and has been used in (opto)electronic, catalytic and energy-harvesting devices due to its various desired properties. However, its surface oxidation is an important aspect for any application [1].

Herein, heating single, microscopic MoS2 flakes in their etching regime (around 370 °C) resulted in formation of sub-nm oxide clusters. Comparison between height profiles obtained by atomic force microscopy (AFM) imaging and density functional theory simulations of the sub-nm MoxOy fragments onto a MoS2 monolayer suggested that these clusters are mainly MoO3 monomers and dimers at the sulfur vacancies. Due to small sizes and low amounts, their local chemical detection became difficult, but a combination of several surface science methods such as Raman measurements, energy and wavelength dispersive X-ray spectroscopies as well as X-ray absorption near edge structure data confirmed the MoO3 nature of such clusters [2]. Moreover, Kelvin-probe force microscopy in air has been used for detection of sub-nm oxide clusters and extended towards Mo oxide layers atop MoS2 crystals and other substrates [3].

Acknowledgements: This research has been supported by the National Science Center, Poland, grant no.2017/27/B/ST4/00697.

APPLICATION OF FUNCTIONALIZED NANOPARTICLES IN THE SYNTHESIS OF ION-IMPRINTED POLYMERS

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Abstract

There is a growing interest for synthesis of ion-imprinted polymers (IIPs) under different architectures, such as microspheres, membranes, blocks, etc., to address the needs for wastewater treatment and regeneration. In this work we present a facile method for obtaining ion-imprinted polymers from Pickering emulsions stabilized by functionalized silica nanoparticles. The key element for obtaining Pickering emulsions are the nanoparticle stabilizers, whose surface properties must be perfectly tuned to adsorb at the oil/water interfaces. For this reason, we have synthesized silica nanoparticles that carry glycidyl functional groups and are pseudo-amphiphilic making them ideal for stabilizing oil-in-water (o/w) Pickering emulsions. The ion-imprinted polymers were obtained by first generating a Pickering emulsion from a vinyl bearing monomer that is immiscible with water, a complex of a Schiff-base ligand with either Cu(II), Co(II) or Ni(II) and glycidyl functionalized silica nanoparticles as emulsion stabilizers. Through polymerization of these emulsions IIPs in the form of microspheres that exhibit good absorption capacities for the mentioned ions. We believe that in the future this method could be established as a platform for facile synthesis of IIPs under different architectures. Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).

Keywords: *ion-imprinted polymers, wastewater treatment, Pickering emulsions*

Acknowledgements: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization of Romania, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).*

HYDROXYPROPYL CELLULOSE OXIDATION BY MEANS OF SELECTIVE REAGENTS

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Abstract

Hydroxypropyl cellulose (HPC) is a widely used cellulosic ether in both industry and research. HPC is a thermoplastic cellulose derivative, soluble in water as well as in a range of organic solvents, allowing for a wide variety of processing possibilities. HPC has multiple pharmaceutical applications, including as an artificial tear lubricant and as a tablet binder. In addition, HPC has exceptional biodegradability and biocompatibility, which makes it advantageous in several industries, including the medical and eco-friendly electronic industries.

The chemical functionalization of HPC, such as through oxidation reactions, can introduce additional chemical groups into the macromolecular structure of the polymer, leading to new properties and potential practical uses. For example, the introduction of aldehyde and/or carboxylic groups into the HPC structure can provide additional sites for chemical reactions and enable the attachment of other functional groups or molecules. Therefore, our work focuses on the HPC oxidation following two of the most selective routes: i) TEMPO-mediated oxidation in the presence of NaClO/NaBr, and ii) sodium periodate. Supplementary, a combined one-shot process was further developed. The amount of aldehyde and carboxyl groups introduced and the changes in the morphological features of oxidized samples were deeply studied in correlation with each type of oxidant. The chemical structure, crystallinity, and thermal stability of oxidized HPC samples were investigated by Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron spectroscopy (SEM) and thermogravimetric studies (TG).

Acknowledgements: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-PD-2021-0462, within PNCDI III.*

ELECTRICAL PROPERTIES OF POLY(3,4-ETHYLENEDIOXYTHIOPHENE)/PERMODIFIED CYCLODEXTRINS POLYROTAXANES END-CAPPED BY PYRENE

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Abstract

The interest in the area of conjugated polymers (CPs) has intensified during the past two decades, owing to their numerous advantages over conventional inorganic materials [1]. Among the various CPs, poly(3,4-ethylenedioxythiophene) (PEDOT) polymer is widely recognized as an interesting material whose electrical properties are of great interest for optoelectronic applications [2]. However, several properties of the PEDOT need further improvements, such as the rigidity of chain structure and tight packing that affect its solubility and processability. Although tremendous effort has been devoted to tune PEDOT's charge-transport properties through molecular design, the final results are questionable and intensive research efforts have to pursue for the adjustment of its performances in terms of processability and transport properties. The construction of polyrotaxane architectures offers a new way to obtain PEDOT materials with particular challenges [3].

Acknowledgements: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-III-P4-PCE-2021-0906.*

SYNTHESIS OF POLYSTYRENE-BASED NANOPARTICLES AS A PLATFORM FOR JANUS NANO-COUPLES

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Abstract

Multifunctional nanoparticles are gaining popularity due to their uniqueness and remarkable ability to combine multiple properties, like electric, magnetic, optical, and amphiphilic properties. We present the synthesis and characterization of polystyrene-based nanoparticles with high potential for use as a support for multifunctional hydrophilic-hydrophobic as well as insulating-semiconductive nanomaterials (Janus-type nano-couples). In the first stage, we prepared non-polar polystyrene nanoparticles via emulsion polymerization of styrene using different amounts of divinylbenzene (DVB) and sodium dodecylbenzene sulfonate (NaVBS). The relative size of the nanoparticles may be changed by varying the amounts of styrene, DVB and/or NaVBS components.

In a second stage, we investigated the non-polar polystyrene-based nanoparticles with respect to structural (scanning electron microscopy – SEM), thermal (differential scanning calorimetry – DSC), and dielectric (broadband dielectric spectroscopy – BDS) properties. The SEM images demonstrate the preparation of perfect spherical and free of defects polystyrene-based nanostructures. The evaluation of permittivity and conductivity of nanostructures demonstrate that our nanoparticles are non-polar and insulating nanostructures.

The successful preparation of polystyrene-based nanoparticles has an important impact in the cost-effective fabrication of organic multifunctional nanoparticles that could improve the design of more efficient semiconducting nanocomposites.

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI–UEFISCDI, project number TE 94/17.05.2022, PN-III-P1-1.1-TE-2021-1332*

FLUORESCENCE QUENCHING SPECTRAL STUDY OF PYRENE-BASED CHEMOSENSOR FOR THE DETECTION OF Fe^{3+} IONS

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Abstract

Along with the urbanization process and rapid industrial development, the environmental pollution has become a severe humanity problem, heavy metal ions being the main pollutants with harmful effects on the human bodies through the food chain. These contaminants are difficult to be degraded and therefore, the methods for metal ions detection have aroused widespread attention. Among optical methods, fluorescent methods for the heavy metals determination are of great interest due to their high sensitivity, selectivity, low cost and easy operational procedure. To date, a variety of fluorophore molecules (pyrene, stilbene, anthracene, dansyl, fluorescein) with different sensing abilities have been used for various sensors expansion.

In recent years, much effort has been put into developing fluorescent probes for the detection of trivalent metal ions such as Al3+, Fe3+ or Cr3+ with vital role in various environmental and biological processes but with harmful effects when exceed certain quantity.

Pyrene-poly(methyl methacrylate-co-vinylbenzyl chloride) copolymer (Py-MMA-co-VBC) was prepared in order to be developed as a new fluorescent material for the detection of various metal ions (Cu2+, Fe3+, Ni2+, Zn2+, Co2+, Al3+, Pb2+, Mn2+, K+, [UO2]2+). Comparative quenching experiments evidenced higher detection sensitivity and selective response of the Py-MMA-co-VBC sensor for trivalent iron ions compared to the other metal ions, with detection limit around 4 × 10−7 M. Also, the quenching mechanism analyzed through Stern-Volmer and Lehrer equations evidenced a combination of static and dynamic processes assumed for the Fe3+ metal ions.

Keywords: *fluorescence, sensors, metal ion detection, photochemistry, Stern-Volmer*

Acknowledgements: *This paper was financially supported by the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-III-P4-PCE-2021-0933 (Nr. 33/2022), within PNCDI III.*

PHOTOCATALYTIC PERFORMANCE TOWARD VISIBLE RANGE OF TiO_2 NANOPARTICLES PREPARED VIA SOFT CHEMISTRY PROTOCOLS

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Abstract

Titania nanomaterials (TiO2 NPs) have attainted lot of attention as they have found numerous applications in the field of solar cells manufacturing, sensors, photocatalysis, or in the biomedical field. A trendy exploitation of TiO2 NPs consists in the photocatalytic degradation of organic environmental pollutants but the process suffer from a serious drawback related to the wide band gap energy (3.2 eV for anatase) of TiO2 NPs that limits the absorption of photons with wavelengths higher than 400 nm from the solar spectrum (visible spectrum). Consequently, the employment of the sunlight as radiation source is somehow restricted, given that a maximum of only 4% of sunlight energy can be used in the visible light phototriggered processes. Accordingly, various strategies directed toward the increase of TiO2 photocatalysts efficiency under visible-light illumination are highly welcome.

In this present study, TiO2 nanoparticles with enhanced photocatalytic performance toward visible range via "soft chemistry" protocols were successfully prepared. Structural, morphological, optical and catalytic properties of the final products were also examined. Our intention was to shed light on the reaction parameters that directly affect the structural and morphological properties of the nanoparticles with subsequent hints on the final electrochemical properties.

Keywords: *TiO2 NPs, photocatalysis, anatase, sensors*

Acknowledgements: *The authors acknowledge financial support to the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-III-P4-PCE-2021-0933 (Nr. 33/2022), within PNCDI III.*

CHITOSAN SPONGES WITH ANTIBACTERIAL ACTIVITY, ANTIOXIDANT PROPERTIES AND CONTROLLED DELIVERY OF CURCUMIN

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Abstract

New chitosan (CS) sponges with characteristics modulated by preparation conditions and feed mixture composition were prepared by cryogelation or by room-temperature gelation, through glutaraldehyde cross-linking. The sponges exhibited honeycomb morphology, excellent mechanical properties, and water-triggered shape recovery. They were investigated for antibacterial activity, antioxidant properties, and controlled delivery of a plant-derived polyphenol, namely curcumin (CCM). The CS sponges demonstrated remarkable antibacterial properties against Gram-positive (Staphylococcus aureus, Listeria monocytogenes) and Gram-negative (Escherichia coli, Salmonella typhimurium) bacterial pathogens. The investigation of the release properties of CCM, a valuable plant-derived polyphenol, indicated that release behavior was influenced by the sponges composition and preparation strategy. The release mechanism of CCM was estimated by linearly fitting the Higuchi, Korsmeyer–Peppas, and the first-order kinetic models onto the experimental data. The antioxidant performance of CCM was slightly reduced by incorporation into the network of developed CS sponges.

Acknowledgments: *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-TE-2021-1683 (TE6/2022).*

EXTRACTION AND CHARACTERIZATION OF NANOCELLULOSE FROM COMMERCIAL CELLULOSE SAMPLES

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Abstract

Cellulose, the most abundant biopolymer on earth, has attracted much attention as a cheap, renewable, and biodegradable material. Chemically, it is composed of repeating β-D-glucose monomers linked by a β-(1,4) glycoside linkage. The morphology of natural cellulose is usually fibrous, with intermittent crystalline and amorphous sections. Separation of the fibers results in nanoscale cellulose substances, known as nanocellulose, which exist in different morphologies such as cellulose nanocrystals (CNCs) and cellulose nanofibers (CNFs). In this study, we propose a chemical, low energy process for the direct extraction of cellulose nanofibers (CNFs) from four types of cellulose by oxidation. Oxidation is the most commonly used method to prepare carboxylated CNFs because the C6-OH on the cellulose surface can be easily oxidized to a carboxyl group. The physical and chemical properties of the prepared CNFs were investigated, such as by morphological (TEM, AFM), structural (FTIR), thermal (TGA), and rheological analysis.

Acknowledgments: *This work was supported by grants of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, project number PN-III-P1-1.1.-TE-2021-0597, within PNCDI III.*

DEVELOPMENT OF MIXED OXIDES WITH SPINEL STRUCTURE VIA THE SOL-GEL AUTO-COMBUSTION TECHNIQUE

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Abstract

Spinel-nanostructured ferrites, due to their remarkable magnetic properties and electric properties, have acquired significant attention in recent years. Many fields, including high-frequency devices, microwave and electronic devices, hyperthermia, contrast agents for MRI applications, drug delivery systems, catalysis, adsorption and photocatalytic applications for wastewater treatment, succesfully incorporate these materials. Spinel ferrites properties are significantly influenced by their chemical composition, phase purity, grain and/or crystallite size, or specific surface area. Several methods have been used to alter these properties for a specific purpose, including: thorough method selection in consideration of the targeted application, varying the time or the calcination temperature, the substitution of divalent or trivalent ions, doping, etc [1, 2].

Co-precipitation, microemulsion, hydrothermal and sol-gel methods are the most popular tehniques used of the bottom-up synthesis strategies. These wet-chemical procedures often encounter challenges regarding complex schedules and slow production rates. One of the finest methods to obtain spinel ferrites has indeed been the sol-gel auto-combustion approach, since it is effective at embedding the cations into the ferrite structure. This synthesis route is simple, versatile and fast.The fuel agent plays an key role in this process, bounding stable complexes with the metal cations, preventing the selective precipitation of the metal ions during water evaporation and providing enough heat for the spinel ferrite formation [1].

Rare earth (RE) cations insertion procedure was observed to enhance the characteristics and performances of ferrites, by altering crystallite and grain sizes and/or producing crystal defects in the spinel structure. High temperature thermal treatments are applied to promote the integration of rare earth ions into the spinel matrix [3]. The manganese ferrite is one particular case, which is unstable at high temperatures, because manganese ions have a susceptibility to oxidize. Therefore, doping $MnFe_2O_4$ with lanthanides cations by increasing temperature is detrimental for the phase purity.

In this study, nanosized spinel manganese ferrites, with the general formula $MnFe_{1.96}RE_{0.04}O_4$ (RE = La, Gd, Er, Ce) were succesfully prepared by sol-gel auto-combustion procedure at low temperature, using citric acid as a combustion agent. The materials were characterized by XRD, FTIR, TEM and VSM.

Acknowledgement: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS–UEFISCDI, project number PN-III-P1-1.1-TE-2021-0030, within PNCDI III.*

ELECTROCATALYTIC PROPERTIES OF NICKEL OXIDE FILMS DEPOSITED ON A NON-METALLIC SUBSTRATE

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Abstract

Chemical metallization of dielectrics is an important technological process in the production of many technical devices because it insures improvement of their properties. One of the most commonly metallized polymers in practice is acrylonitrile butadiene styrene (ABS). To start the metallization process, the surface of the polymer must be pre-activated.

In previous studies, the possibility of surface modification of ABS polymer by deposition of thin nickel film from a solution without reducing agent was shown. In the present research an attempt is made to evaluate the catalytic activity of ABS samples modified by this method in terms of hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline medium (1M KOH). The results from the electrochemical investigations show that the modified samples are catalytically active. The rate of HER or OER depends on the composition of the solution from which the nickel films are deposited. After staying of the samples in an alkaline environment, the open circuit potential becomes more positive, and the rate of HER or OER increases.

The modified polymer surface is characterized using SEM, EDS and XPS analyses.

Acknowledgement: *The research was carried out within the National Science Program "Young Scientists and Postdoctoral Fellows" Bulgarian Academy of Sciences.*

SPONTANEOUS SILVER DEPOSITION ON CARBON SCREEN PRINTED ELECTRODES

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Abstract

In the present study, the process of spontaneous deposition of silver on different types of carbon screen-printed electrodes in the absence of a reducing agent in the solution is examined. These electrodes consist of mesoporous carbon (MC), carbon nanofibers (CNF), and single-walled carbon nanotubes (SWCNT). Before being immersed in the metal deposition solution, the carbon electrodes were reduced at constant potential in supporting electrolyte. The metal deposition process was monitored by measuring the open circuit potential. The amount of the deposited metal phase was evaluated by anodic stripping voltammetry. The size and type of the silver particles was determined by scanning electron microscopy.

The process of spontaneous deposition of silver resulted in the formation of homogeneously distributed metal nanoparticles with different sizes and surface distribution on the three carbon substrates. The type and amount of deposited metal depended significantly on the potential used in the preliminary electrochemical reduction step. Using a more negative reduction potential produced silver particles with smaller sizes and higher number densities.

Studies of double and triple depositions of silver were also carried out. It was found that the amount of metal increased with each subsequent cycle, with differences observed depending on the type of carbon substrate. These studies reveal the important role of the type of nanostructuring of the carbon supports for the spontaneous metal deposition process.

Acknowledgements: *The authors are grateful to the financial support of INFRAMAT (National Roadmap for Research Infrastructure) funded by Bulgarian Ministry of Education and Science*

IMPROVEMENT OF THE CORROSION PROTECTION ABILITY OF CERIA-BASED CONVERSION LAYERS FORMED ON AL 1050 BY CHEMICAL POST-TREATMENT IN PHOSPHATE-NITRATE SOLUTION

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Abstract

Mixed ceria (Ce_2O_3+CeO_2) conversion layers were deposited on Al-1050 substrates (before or after their anodizing (in H_2SO_4)) by electroless treatment in solution based on $CeCl_3.7H_2O$ (Stoyanova and Stoychev, 1997; Andreeva, Stoyanova and Stoychev, 2014; Andreeva et al., 2016, 2018, 2021). Then, the so coated samples were post-treated in mixed phosphate-nitrate solution containing NaH_2PO_4 + $Ca(NO_3)_2$. The task of the so formed coatings was to increase the corrosion resistance of Al 1050 in the Cl^--containing model corrosion media (0.1 M NaCl). Scanning electron microscopy (SEM) and characteristic energy dispersive X-rays analysis (EDS); X-ray (XRD); X-ray photoelectron spectroscopy (XPS) and a complex of electrochemical, experimental methods (based on potentiodynamic polarization measurements, chronoamperometry, Open circuit potential (OCP) transients, Rp method, etc.) were used to analyze the basic properties (morphology, structure, chemical composition and chemical state of the elements, phases deposited on coating(s) surface, cathodic and anodic behavior, corrosion resistance, etc) of the consecutively formed conversion layers - protective systems, respectively. The electrochemical tests indicate that the deposited conversion layers strongly: decrease corrosion current; broaden area of passivity and increase polarization resistance of studied systems. The other analytical investigations illustrate that the coatings are made up of Al, O, Ce^{3+}, Ce^{4+}, Ca, P, Na. According to the high-resolution XPS spectral and XRD analysis, the elements detected in the coating are in the form of Al_2O_3, Ce_2O_3+CeO_2, AlOOH, $AlPO_4$, $CePO_4$, $Ca_5(PO_4)_3(OH)$. Based on the all obtained results, the corrosion-protective influence of the formed conversion coatings under studied conditions was discussed.

Acknowledgments: *The authors are grateful to the financial support of INFRAMAT (National Roadmap for Research Infrastructure) funded by Bulgarian Ministry of Education and Science.*

THE CORROSION BEHAVIOUR OF NICKEL-BASED ALLOYS AND COMPOSITES IN ACIDIC AND ALKALINE ENVIRONMENTS

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Abstract

Nickel-based alloys are characterized by good catalytic activity for the hydrogen evolution reaction. They are a good alternative of noble electrode materials. For practice application, it is necessary to study their corrosion resistance in the environment in which they will work.

In the present work, the corrosion behaviour of electrodeposited alloy and composite coatings of Ni was investigated by the electrochemical impedance spectroscopy (EIS) method. The experiments were carried out in two model environments: acidic (0.5 M H2SO4) and alkaline (6 M KOH). The morphology, electronic structure, the content of the components in the coating and thickness were studied by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray fluorescence analysis (XRF).

ADAPTIVE BIOMASS OBSERVER IN FED-BATCH CULTIVATION OF ESCHERICHIA COLI ON THE BASIS OF ON-LINE MEASUREMENTS OF OXYGEN

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Abstract

A new adaptive asymptotic biomass observer for fed-batch E. coli growth on glucose is proposed. The observer works on the basis of on-line measurements of oxygen and stirrer speed only. The observation algorithm includes an on-line estimation procedure of yield coefficients on the basis of off-line measurements of biomass concentration.The preliminary investigations of the observer are realiased by simulations. The on-line measured experimental data is used as input information. The observation algorithm is verified by laboratory experiments of a recombinant E. coli strain.

Acknowledgments: *This research was funded by the National Scientific Fund of Bulgaria, Grant КП-06-Н32/3 "Interactive System for Education in Modelling and Control of Bioprocesses (InSEMCoBio)".*

MULTISTEP MODELING OF A CLASS BIOPROCESSES

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Abstract

A new approach is proposed for modelling the dynamics of biomass growth of a bioprocess characterized by different metabolic states. According to preliminary research, process dynamics cannot be described by a single model. For this reason, three phases of the bioprocess are defined – periodic, exponential and stationary. During each of the phases, the process passes through one or more physiological states. Each physiological state is represented by a sub-model with a different structure and parameter values. The transition of the process from one physiological state to another is carried out by switching the sub-models based on a predefined key parameter. The proposed approach was tested by deriving a process model for obtaining the phytase enzyme with E. coli.

Acknowledgments: *This research was funded by the National Scientific Fund of Bulgaria, Grant КП-06-H32/3 "Interactive System for Education in Modelling and Control of Bioprocesses (InSEMCoBio)".*

ADAPTIVE CONTROL OF PROTEIN PRODUCTION BIOPROCESS WITH THREE PHYSIOLOGICAL STATES

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Abstract

A new adaptive linearizing control algorithm is proposed that stabilizes the carbon source concentration to a preset value. This algorithm is applied on recombinant protein production by Escherichia coli. A model for control of the investigated process is derived. The operating model includes three sub-models. Each of them describes a physiological state through which the process passes. Switching from one model to another depends on the sign of a key parameter obtained from the acetate measurements. A cascade scheme is derived from software sensors for the estimation of three biomass growth rates included in the structure of the proposed control algorithm. Simulation studies of the developed closed system have been carried out. The results with the impact of an open loop control system on the same object are compared.

Acknowledgments: *This research was funded by the National Scientific Fund of Bulgaria, Grant КП-06-Н32/3 "Interactive System for Education in Modelling and Control of Bioprocesses (InSEMCoBio)".*

A NEW ELECTRODE BASED ON ZEOLIT/CoNPs FOR FUNGICIDE DETECTION

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Abstract

This work presents a composite material based on zeolite and cobalt nanoparticles (Z/Co-NPs), used for the electrochemical investigation of Cymoxanil. Zeolite sample was prepared by solvothermal method at a temperature of 90°C for 24 h. The zeolite/Co-NPs was obtained using ion-exchange capacity of synthesized Na zeolite with 5% $CoCl_2$. The Brunauer, Emmett and Teller (BET) technique was used for determining the surface area and porosity of obtained porous materials. The morphological and structural characterization of the powder deposited onto a solid substrate was investigated by SEM, EDS. The zeolite/Co-NPs screen printed modified electrode was tested for fungicide Cymoxanil detection and showed an adsorbtion effect for this fungicide.

Keywords: *composite material, zeolite, Cobalt nanoparticles, fungicide, electrochemical sensor*

Acknowledgment: *This work was supported by grants from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, project number PN-III-P1-1.1-TE-2021-0358.*

GRAPHENE/CoNPs MODIFIED SCREEN-PRINTED ELECTRODES FOR CYMOXANIL DETECTION

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Abstract

This work presents a composite material based on graphene/Co-NPs, used for the electrochemical investigation of Cymoxanil. Graphene/CoNPs sample was prepared by exfoliation of graphite rods in solution containing 5% CoCl2, by plasma method. The morphologycal and structural characterization of the powder deposited onto a solid substrate was investigated by SEM, XRD, and FTIR . The graphene screen printed modified electrode was succesfully tested for Cymoxanil detection.

Keywords: *Graphene/CoNPs, Modified Screen-Printed Electrodes, Cymoxanil, Electrochemical Detection*

Acknowledgment: *This work was supported by grants from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, project number PN-III-P1-1.1-TE-2021-0358*

ANALYTICAL APPLICABILITY OF GRAPHENE MODIFIED ELECTRODE IN SUNSET YELLOW ELECTROCHEMICAL ASSAY

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Abstract

Due to the recent increase in average living standards, food safety has caught public attention. It is necessary to conduct a qualitative and quantitative rapid test of prohibited food additives since the inclusion of food additives or the improper usage of synthetic dyes can negatively impact on the human health. Herein, a highly sensitive method for Sunset Yellow detection based on a glassy carbon electrode modified with few-layer graphenes was proposed. The electrochemical behaviour of SY at the GR-exf/GCE modified surface was investigated by Cyclic Voltammetry, Square Wave Voltammetry, Electrochemical Impedance Spectroscopy and Amperometry. The influences of pH, scan rate, and interfering species were studied. Under optimized conditions, the developed sensor shows good linearity over a broad SY concentration range, e.g., 0.028–30 μM, with a low limit of detection (LOD = 0.0085 μM) and quantification (LOQ = 0.028 μM) (data obtained by amperometric technique). Furthermore, the modified electrode shows good selectivity, precision and sensitivity and has been successfully applied for SY quantification from commercially available pharmaceutical formulation as well as from candy bars and orange juice.

Keywords: *Sunset Yellow, graphene-modified electrode, electrochemical detection*

Acknowledgment: *This work was supported by grants from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, project number PN-III-P2-2.1-PED-2019-2410 (500PED/2021) and "Nucleu" Programe within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 03 01.*

APPLICATION OF MACHINE LEARNING TECHNIQUES FOR ASSESSING THE ORIGIN OF WINE BASED ON ^{1}H-NMR SPECTROSCOPY

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Abstract

The application of different types of spectroscopies in association with advanced supervised statistical methods represents nowadays an important topic of research and control groups for the development of suitable models for wine differentiation. Recently, alongside metabolomic approaches, a new tendency of establishing AI-based omics strategies is increasingly recorded. This is because Artificial Intelligence tends to extend its capability in all domains from day-to-day life to high science. Against this background, the present study aimed to develop new wine recognition models through the corroboration of Artificial Intelligence and ^{1}H-NMR spectroscopy in order to develop robust and feasible tools. In this regard, three distinct Machine Learning (ML) methods, namely Support Vector Machines (SVM), K-Nearest Neighbors (KNN), and Logistic Regression were applied for classifying wine samples with respect to the grape variety, vintage and geographical origin. The proposed data processing workflow for developing reliable ML-based classifiers involved using a feature selection technique for reducing the dimensionality of the input space and tuning the hyperparameters specific to each learning method. Based on this approach, highly accurate wine differentiation models were built.

Keywords: *^{1}H-NMR, machine learning, wine, recognition models, SVM*

Acknowledgements: *This work was supported by the Ministry of Research, Innovation and Digitization CNCS/CCCDI – UEFISCDI through project number PN-III-P2-2.1-PED-2021-1095 (Contract No. 651PED/ 2022) within PNCDI III and through Programme 1 - Development of the National Research and Development System, Subprogramme 1.2 - Institutional Performance - Funding Projects for Excellence in RDI, Contract No. 37PFE/30.12.2021.*

NEW NANOCRYSTALLINE Nb DOPED TiO_2 MATERIALS

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Abstract

Titania-based materials have various applications in catalysis due to their outstanding properties such as low cost, low toxicity, availability, and good biocompatibility. TiO_2 is usually obtained using several methods, including sol-gel, hydrothermal/solvothermal, sonochemical, or aerosol synthesis. This study used the solution combustion method (SCS) to obtain Nb-doped TiO_2 with Nb concentrations of 5%, 10%, and 15%. The obtained materials were characterized by N2 adsorption/desorption, XRD, DR/UV-Vis. The catalytic activity of the obtained materials was also investigated. XRD analysis demonstrated the formation of a crystalline structure. The presence of only the anatase phase and the absence of diffraction lines corresponding to Nb compounds suggest the incorporation of Nb into the TiO_2 lattice. The UV-Vis analysis revealed that all the samples absorb at a wavelength lower than 400 nm. A shift to a higher wavelength was observed for the Nb (5%)-doped TiO_2 and Nb (10%)-doped TiO_2 samples. The surface area increases from 91 m^2/g for pure TiO_2 to 160 m2/g for 15% Nb-TiO_2. The highest catalytic activity was obtained for TiO_2 doped Nb 15% sample after 1 hour of irradiation.

Keywords: *Nb doping TiO_2, TiO_2 materials, combustion method, TiO_2 materials*

MODULATING THE TRAMETES VERSICOLOR LACCASE ACTIVITY WITH GOLD NANOPARTICLES

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Abstract

It is not clearly understood what are the effects of gold nanoparticles (AuNPs) on enzymes structure, if it is possible to control them and how the interfacial chemistry impacts the enzyme activity in various applications. As a result, research on the interaction of laccase from Trametes versicolor (Lc) with AuNPs was designed. We aimed to characterize the interaction between laccase and AuNPs by spectroscopic (UV-Vis, Fluorescence, CD) methods. Moreover, the spectroscopy results were correlated with calorimetric data and new insights on noncovalent forces and desolvation/solvation phenomenology that governs the interactions were gathered. Furthermore, the decomposition naphthol green B, a real pollutant found in wastewaters, was performed using Lc in presence of AuNPs. The thermodynamic parameters of the interaction were investigated by isothermal titration calorimetry and finally, molecular docking was performed to analyze the binding site position and interaction types of dye with Lc. The findings of this work provide important knowledge for laccase-based bio-nanoconjugates and their use in the field of environmental remediation.

INVESTIGATION OF HOST-GUEST INTERACTIONS MEDIATED BY THE APPENDED UNITS ON POLYMERS

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Abstract

Advanced supramolecular materials have been developed and investigated during the past few decades, due to their potential applications in a variety of fields, including catalysis, nanomedicine, electronic devices, sensors, etc. In this study, functionalized polyacrylic acid (PAA) with alkyl chains and functionalized alginate (Alg) with cyclodextrin (CD) units were used to create host-guest supramolecular complexes. Methods used to study the synthesized polymers and their mixtures were surface tension, dynamic light scattering, fluorescence spectroscopy, FTIR spectroscopy, and electron paramagnetic resonance (EPR) spectroscopy. Surface tension results for systems containing hydrophobically modified polyacrylates showed typical behavior of a tensioactive agent, while the fluorescence study revealed that that pyrene probe is solubilized closer to the nonpolar core when hydrophobically modified polyacrylates are added. Moreover, the local changes in the EPR spectra of the mixtures of spin-labelled Alg-CD and polyacrylates are small and can be explained by the fact that the main components involved in Ca2+ complexation and host-guest interactions are diamagnetic. In conclusion, the study showed that the mixture between Alg-CD units and PAA-alkyl chains develop supramolecular host-guest assemblies which are strongly dependent on the alkyl chain length attached to polyacrylate.

REAL-TIME STUDY OF THE POLARIZATION PROPERTIES OF POLARIZATION HOLOGRAPHIC GRATINGS WITH AND WITHOUT SURFACE RELIEF AT THE RECORDING BEAM WAVELENGTH

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Abstract

It is well known that during polarization holographic recording in azopolymers usually surface relief grating (SRG) is formed together with the volume anisotropic grating. Here, we present a study of the polarization of the recording beams transmitted through the grating. This is done in real time during the recording process using a novel optical setup including two polarimeters and two power meters. This allows us to obtain detail information about the influence of the SRG on the polarization properties of the recorded holograms. A simple and yet efficient method is proposed to suppress the SRG formation and thus to improve the polarization properties of the polarization holographic gratings. The feasibility of the method is demonstrated by our experimental results.

Acknowledgements: *This study is funded by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT". Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.*

PHOTOANISOTROPIC NANOCOMPOSITE MATERIALS FOR POLARIZATION HOLOGRAPHY

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Abstract

Thin film samples of photoanisotropic nanocomposite materials with different compositions have been prepared and studied. Azo-containing polymers were used as a matrix and doped with nanoparticles of different shape, size and composition. Polarization holographic recording was performed in the nanocomposite thin film samples. The influence of the nanoparticles on the photoinduced birefringence, diffraction efficiency and relief height of the recorded polarization diffraction gratings was investigated.

Acknowledgements: *This study is funded by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT".*

2D POLARIZATION HOLOGRAPHIC GRATINGS IN AZOPOLYMER THIN FILMS AND THEIR POLARIZATION PROPERTIES

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Abstract

Azopolymer materials are very efficient for inscription of polarization holographic gratings. However, mostly 1D gratings have been studied by now. Additionally, during the holographic recording, mass transfer is observed which leads to formation of surface relief structures. We examine different ways of recording of these gratings which result in presence or absence of relief structures. The polarization properties of 2D holographic gratings inscribed in azopolymer PAZO are investigated in both cases.

Acknowledgements: *This work was supported by the Bulgarian Ministry of Education and Science under the National Research Programme "Young scientists and postdoctoral students-2" approved by DCM 206/07.04.2022 and through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT".*

BIOSORBENTS IMPREGNATED WITH DEEP EUTECTIC SOLVENTS AS EFFICIENT MEDIA FOR REMOVAL OF VOLATILE ORGANIC COMPOUNDS FROM GASEOUS FUELS

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Abstract

Biogas and natural gas are the so-called green alternatives to the currently used non-ecological fossil fuels. Both types of gaseous fuel consist mainly of methane and carbon dioxide, as well as a wide range of organic and inorganic impurities. Unfavorable impurities include volatile organosulfur compounds (VSCs), such as sulfides, disulfides, and mercaptans. During the combustion of fuel-containing VSCs, highly corrosive sulfuric acid (H2SO4) is formed in reaction with water and oxygen, which destroys plant components. In addition, toxic sulfur dioxide is formed, which is released into the atmosphere. Therefore, it is extremely important to remove VSCs from gaseous fuels prior to their use.

Among the well-known purification technologies, adsorption and absorption are the most commonly used because of their relatively high efficiencies. To increase the efficiency of VSCs removal from gaseous fuels, it is possible to combine the benefits of both methods by impregnating adsorbents with absorbents. However, to meet green engineering criteria, it is necessary to use biodegradable and non-toxic components. Therefore, in this study, various lignocellulosic biosorbents were impregnated with a new generation of green solvents called Deep Eutectic Solvents (DES). The research focused on the removal of carbon disulfide, dimethyl disulfide, 1-propanethiol, 2-propanethiol, and carbon dioxide from model gaseous fuels. DES characterized by the highest absorption capacity was impregnated on biosorbents including energetic poplar wood (Populus L), Antipka tree (Cerasus mahaleb), Corn cobs (Zea mays), and Beechwood, (Fagus L). Characterization of new soption materials before and after impregnation was performed using thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and X-ray diffraction (XRD) analysis. Subsequently, the adsorption of VSCs from biogas was performed. This study demonstrated the high competitiveness of the new sorbents compared to that of commercially available sorbents. The coexistence of the two processes, absorption and adsorption, is attributed to the high removal efficiency of VSCs.

Acknowledgements: *This work was supported the National Science Centre, Poland within the grant project (No. UMO-2021/43/D/ST8/01791).*

APPLICATION OF DEEP EUTECTIC SOLVENTS FOR THE REMOVAL OF ORGANOSULPHUR COMPOUNDS FROM BIOGAS

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Abstract

The key to environmental sustainability of the energy sector is the proper extraction and exploitation of renewable energy from biowaste. The main barrier to the efficient and commercial use of biogas is contaminants, which should be removed before further use. Many biogas purification technologies have been described in literature. However, they are mainly dedicated to the removal of inorganic compounds such as H2O, CO2, SO2, H2S, and NH3. New solutions are still being sought to enable effective purification of biogas from volatile organic compounds.

In these studies, special attention was paid to obtain new biosorbents for the treatment of biogas from organosulfur compounds. The biosorbents were obtained by a simple and inexpensive method of impregnating coffee residues (CR) using a deep eutectic solvent (DES) based on quaternary ammonium salts (such as choline chloride (ChCl), tetraethylammonium chloride (TEACl), tetrabutylammonium chloride (TBACl), tetramethylammonium bromide (TMABr), and glycols (such as 1,2-Ethanediol (EG), ethylene dimethacrylate (EGDMA), 1,5-Pentanediol (PG), 1,2-Propanediol (HG), DL-1,2-Hexanediol (PrG) in the appropriate molar ratio. The surface morphology and structure of the new biosorbents modified with the selected DESs were characterized using Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and X-ray Diffraction (XRD). The biosorbents prepared in this manner were used for desulfurization of the biogas stream from carbon disulfide (11.6 ppm), dimethyl disulfide (11.8 ppm), isopropyl mercaptan (11.5 ppm), and propyl mercaptan (11.3 ppm). These studies show that the newly developed biosorbents based on coffee residue-modified DESs have a high sorption capacity, which provides a promising alternative method for the removal of volatile organosulfur compounds from real biogas streams. In addition, the new biosorbents showed good thermal stability, making it possible to regenerate the adsorbents by heating at 100°C. This makes biosorbents a new class of functional material that can be used in practical applications.

Acknowledgements: *This work was the National Science Centre, Poland within the grant projects No. UMO-2021/43/D/ST8/01791 and No. UMO- 2020/37/N/ST4/02924.*

INFLUENCE OF TOOL GEOMETRY ON THE PROPERTIES OF FRICTION STIR WELDED ALUMINIUM ALLOY JOINTS

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Abstract

The Friction Stir Welding (FSW) process was simulated for joining AA6082 aluminium alloy using two different tool geometries – with a tapered cylindrical pin (simple pin) and with a hexagonal pin with grooves (complex pin). The analysis of the simulations performed was discussed in terms of temperature evolution during the process, total heat input, residual stresses and material flow. Simulations revealed that a 5% higher temperature, equal to maximum 406 ºC, was provided when using the complex pin than with the simple pin. Higher temperature and higher shear stresses during the welding with the complex pin caused the introduction of higher residual stresses in the weld. Experimental results on the produced welds allowed observation of the microstructure of the joints, hardness tests in cross sections and tensile strength tests. Due to the higher temperature during the process with the complex pin and the more efficient recrystallization process, grain refinement in the SZ was more pronounced. The average grain size in the stir zone for the weld produced with the complex pin was equal to 10.770 ± 1.386 µm, and in the case of the simple pin 14.321 ± 1.319 µm. The presented hardness profiles showed that the weld produced with a complex pin had higher hardness in the stir zone, which is consistent with the Hall-Petch relationship. The obtained UTS values corresponded to the joint efficiency of 72.5 ± 4.9 % and 55.8 ± 8.6 % for the weld produced with the complex pin and the simple pin, respectively.

Keywords: *Friction Stir Welding, Aluminum Alloys; Computational Fluid Dynamics; Mechanical Properties; Microstructure; COMSOL*

COMPARATIVE MEASUREMENTS AND ANALYSIS OF ELECTRICAL PROPERTIES OF MOIST COMPOSITE OF CELLULOSE–BIO-INSULATING OIL–LIQUID WATER TO DETERMINE STATE OF WATER CONTAINED IN COMPOSITE

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Abstract

This paper presents the measurement results of the direct current (DC) and alternating current (AC) electrical properties (conductivity and permittivity) of an electrical pressboard–Nynas NYTRO BIO 300X bio-insulating oil–water composite over a wide temperature range. To analyse the experimental results, a model of the DC and AC conductivities of nanocomposites that considers the quantum mechanical phenomenon of electron tunnelling was applied shows that in a low-frequency region, the conductivities of AC and DC are equal. Moreover, the activation energy and relaxation times of AC conductivity and permittivity were established. The dependence of distance among water molecules on DC conductivity was found to be an exponential function. The average number of water molecules in a nanodrop located in the composite of moist electrical pressboard–NYTRO BIO 300X bio-insulating oil was determined to be (125 ± 20), according to the conductivity model using electron tunnelling among potential wells.

The DC and AC conductivities, permittivities, and dielectric relaxations were found to be in good agreement with the results of computer simulations performed on the model. Accordingly, the real conductivity and dielectric relaxation mechanisms are applied to improve the accuracy of moisture estimation in the solid component of power transformer insulation based on the measurements of DC and AC properties.

THE REACTOR FOR CAPTURING CARBON DIOXIDE IN MOLTEN SALTS

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Abstract

Carbon Capture in Molten Salts (CCMS) a new method of capturing CO_2 was developed on a sorption and desorption principle similar to that used in the calcium loop, but proceeding in the molten salt environment (alkali metal chlorides and fluorides):

$$MeO_{(s,\ diss\ in\ MS)} + CO_{2\,(g)} \leftrightarrow MeCO_{3\ (s,\ diss\ in\ MS)} \quad (1)$$

The idea of the CCMS reactor presented in the only patent assumes its operation in a two-chamber system, allowing to separate the stages of CO_2 sorption and desorption.

The paper presents the development of a reactor prototype consisting of three basic elements, i.e. a sorption, desorption an intermediate chamber.

The transport/pumping of salt between the reactor elements will take place on the principle of a gas lift, i.e., the transport will be forced by the pressure of inert gas. It was necessary to determine what the gas pressure in the gas lift should be to effectively pump molten salts.

The reactor chambers will be located inside the heating modules however, some elements for transporting molten salts will protrude above the heating zones and they must be thermally insulated. And here another problem arose, whether the insulation of the pipelines for the transport of molten salts is sufficient to protect them from freezing during contact with colder elements, and if not, then how to prevent it.

The scope of the research included performing numerical simulations in order to:

• determination of the gas pressure needed to pump the molten salt between the reactor chambers;

• determination of the temperature distribution as the molten salts flow through the conveying system to anticipate the possibility of loss of pumpability due to salt freezing.

The above-mentioned problems of the CCMS reactor prototype operation were solved by means of thermal-flow analysis, performed using computational fluid mechanics methods (AnsysFluent and SolidWorks programs).

Keywords: *carbon capture, molten salts, CCMS reactor*

NON-DESTRUCTIVE MONITORING OF DYNAMIC EVENTS BY SPECKLE PHOTOGRAPHY

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Abstract

Speckle photography is an intensity-based approach for non-destructive monitoring of processes that relies on acquisition of sequences of correlated in time speckle patterns formed on the surface of diffusely reflecting objects under laser illumination. Statistical pointwise processing of the captured patterns enables 2D visualization of the speed distribution of processes ongoing in the objects. Accurate monitoring of speed changes requires a considerable amount of raw data. In this work, we evaluate efficiency of compression of the acquired speckle patterns and check feasibility of outdoor application of speckle photography. Analysis is based on processing synthetic and experimental data.

ON THE OPTICAL AND ELECTRICAL PROPERTIES OF CHLORINATED POLYMER THIN FILM USED IN TERNARY ORGANIC SOLAR CELL APPLICATIONS

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Abstract

There are a multitude of external factors that influence the performance of solar cells: materials used, deposition conditions, storage conditions (environment: temperature, light, humidity, etc.). In this sense, the electrical properties in different situations and working conditions (illumination, temperature variation) are identified, for thin films based on polymer:non-fullerene:fullerene blends, prepared in several weight ratios, in order to highlight the differences in optical and electrical properties.

Moveover, this paper presents an in-depth surface analysis on optical parameters using spectroscopic ellipsometry and spectrophotometry and on morphological properties using atomic force microscopy of binary and ternary blends deposited as thin films. The used materials are of great interest in the photovoltaic field: a donor (PBDB-T-2Cl polymer) and two acceptors (ITIC-F non-fullerene and PCBM fullerene). Regarding the electrical properties, the temperature dependence of resistivity is highlighted in parallel and perpendicular measure configuration.

Keywords: *polymer thin film, ternary solar cell, electrical conductivity*

Acknowledgement: *This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0394, within PNCDI III.*

AN EXPERIMENTAL SETUP FOR INSOLATION FAULT DETECTION OF XLPE CABLES

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Abstract

Insulation coordination is one of the most critical issues in high-voltage electrical installations. The smallest defect in the insulation will cause major problems in the near future. Timely insulation failure diagnosis can prevent life-threatening occupational accidents. Insulation fault diagnostics create maintenance costs for the business but prevent much larger costs that are highly likely to occur in the long run. This paper presents an experimental setup to detect insulation problems of XLPE cables. The experimental setup is composed of a coupling capacitor, voltage divider circuit, High-Voltage transformer, coupling device, and coaxial cable. The specimen of XLPE cable is connected from the high-voltage side of the transformer and the data is collected from the measuring device connected at the end of the coupling device. The paper presents different test results for different XLPE cable specimens tested on the presented system. It is possible to test different medium or high-voltage cables using the presented experimental setup.

Keywords: *partial discharge, insolation fault detection, XLPE cable, high-voltage*

HIGH-TEMPERATURE MECHANICAL BEHAVIOURS OF IRON ALUMINIDES WITH YTTRIUM ADDITION

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Abstract

Intermetallic compounds have many desirable properties as matrix-compatible 2-phase structural materials with good mechanical properties, and low diffusion rates due to their ordered structure. However, these materials show low strength at high temperatures and low ductility due to hydrogen embrittlement at room temperature. High-temperature strength and creep resistance of Fe3Al alloys are tried to be improved by alloying processes. In the present study, the effect of Tungsten addition on room temperature and high-temperature strength properties was investigated by applying a compression test at room temperature and 600 °C to Fe-28Al and Fe-28Al-0.1Y alloys. With the increase in tungsten content, an increase in strength was achieved.

Keywords: *Intermetallics, Iron Aluminides, High temperature, Yttrium*

PROCESSES IN NANOSTRUCTURES SIMULATED BY MOLECULAR DYNAMICS

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Abstract

Molecular dynamics (MD) is a simulation method that integrates Newton's equation of motion to predict the time evolution of individual atoms. The method is suitable for investigating processes in nanoscale objects such as nanoparticles, thin layers, and multilayers. The main advantage of this approach is its ability to show ongoing mechanisms in atomistic detail.

Results of the MD simulations of nanoscale objects under deformation and at elevated temperatures will be presented.

Keywords: *molecular dynamics, nanoparticles, thin films*

INITIAL RESULTS OF 3D PRINTED Mg-Y ALLOY

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Abstract

This work is focused on investigating binary Mg-Y alloy manufactured by selective laser melting process (3D printing) as potentially new material for biodegradable applications, namely temporary bioresorbable devices or implants. In terms of bioresorbable devices, the mechanical properties and corrosion resistance of our 3D printed material were investigated, and the results were compared and discussed to those of the identical material prepared by another powder compactization method (Spark plasma sintering), as well as by hot extrusion. Moreover, the microstructure of the 3D printed samples was studied by scanning and transmission electron microscope, and the observations were related to the results of mechanical and corrosion properties. Compression deformation tests examined the mechanical properties of the 3D-printed samples. The linear polarization and electrochemical impedance spectroscopy methods tested the initial corrosion resistance in the salt solution.

INVESTIGATION OF THE CHANGE OF VIBRATION IN CARTESIAN 3D PRINTER SYSTEMS WITH MECHANICAL IMPROVEMENTS AND ITS EFFECTS ON SURFACE ROUGHNESS

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Abstract

3D printers are widely used in every industry these days. However, the features required from the products are becoming more and more important. Especially in the field of prototyping, 3D printers have become indispensable in design and manufacturing. One of the most important factors determining the product quality is the surface quality. Also, the most important factor determining the surface quality in production is the robustness of the production machine. Therefore, a 3D printer with a Cartesian system, which is the most widely used mechanical system, was chosen in this study. A production sample in the shape of a cube was preferred and a total of nine different parameters were used at three different printing speeds (40, 60, 80 mm/sec.) and three different filling forms (hilbert curve, octagram spiral, concentric). The standard system vibrations of this printer were recorded with the help of dataloggers that measure 3-axis acceleration during production. Afterwards, mechanical improvements were made in the system in all 3 axes. After these improvements, the same production process was carried out again and the difference in mechanical vibrations in the system was examined. In addition, in order to observe the change in the production quality, the surface roughness values in each production were examined in 3 axes and the changes in the production quality were examined. Mechanical improvements provide quality increase in every axis on the surface quality. However, when compared with the measured vibration values, there is no significant correlation between them. As a result, it can be said that the rigidity feature in 3D printer mechanical system has a great effect on the product properties and quality.

Keywords: *3D printing, Surface roughness, mechanical vibration*

THE EFFECT OF METAKAOLIN USED AS CEMENT REPLACEMENT ON THE PROPERTIES OF HARDENED CEMENT PASTE

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Abstract

The article analyses the effect of expanded glass production by-product rich in metakaolin on the properties of hardened cement paste. Portland cement CEM II/A-LL 42.5 N with the average particle size of 14.21 µm and metakaolin with the average particle size of 22.34 µm were used for the tests. Six cement paste compositions were formulated by replacing 0 %, 2 %, 4 %, 6 %, 8 %, 10 % of cement with metakaolin. Ultrasonic pulse velocity, compressive strength, flexural strength, water absorption and porosity of hardened cement paste specimens were measured at 28 days. The analysis of hardened cement paste microstructure (SEM) and physical and mechanical properties leads to the conclusion that the replacement of 8% of cement in the mix with metakaolin creates the densest microstructure that produces the highest values of compressive and flexural strengths and ultrasonic pulse velocity and the lowest values of closed porosity and water absorption rate. It was found that 8 % was the optimal ratio of cement replacement with metakaolin. Metakaolin can be added at 8 % by weight of cement in the production of modified high-performance concrete.

Keywords: *metakaolin, hardened cement paste, compressive strength, water absorption*

INFLUENCE OF MINERAL ADDITIVES ON BIO-BASED POLYMER COMPOSITES

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Abstract

Bio-based materials are becoming more and more popular, especially in applications where biodegradability provides an advantage for customers and environment. However, biodegradable materials are more expensive compared with durable plastic materials, so to reduce costs and in order to improve their mechanical properties, biocomposites are created by reinforcement with natural fibers: cellulose, hemp, jute, cotton, etc. This study is focused on the investigation of the selected group of biocomposites based on poly (3-hydroxybutyrate-co-3-hydroxyvalerate) with the addition of 15 wt% of various fillers (nanocellulose, walnut shell flour, eggshell flour, and tuff). Thus far, there is limited information concerning comparison of the different natural fillers introduced into the poly(3-hydroxybutyrate-co-3-hydroxyvalerate) matrix. Here, the following mechanical properties were evaluated: the tensile strength, modulus of elasticity, strain at break, flexural modulus, and flexural stress at 3.5% strain. The tensile test was performed at various temperatures (− 24, + 23, and + 60 °C), followed by samples conditioning in water and compost. Thermal behavior of the biocomposites was studied by means of differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The study showed that the value of the elasticity modulus of each composite was higher in comparison with neat poly (3-hydroxybutyrate-co-3-hydroxyvalerate), at each of the above temperatures.

EVALUATION OF ALNUS GLUTINOSA TIMBER STRENGTH PARAMETERS AND APPROBATION THE QUALITY REQUIREMENTS OF ROUNDWOOD ASSORTMENTS

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Abstract

When freshly cut, black alder (Alnus glutinosa (L.),Gaertn.) timber presents a light orange colour and during air exposure it changes to red – orange. European alder tends to be light tan to reddish brown; color darkens and reddens with age. Large aggregate rays appear as occasional small streaks on the face grain that can be mistaken for defects in the wood. The felling date, habit and drying affect the intensity of the colour that can be mistaken for defects in the wood. Heart colouring and heartwood hard rot are not clearly distinguishable from each other.

Although the tree has a wide distribution throughout Europe there are no unified quality requirements for roundwood assortments due to lack of scientifically approved information related to wood structure.

The main goal of study is to work out the Alnus glutinosa roundwood, harvested in final felling sites, guality requirements depending on timber quality characterized data based on the testing methods: density - according to ISO-13061-2-2014; Compression strength paralel to the grain- according to ISO 13061-17-2017; Three point bending strength and modulus of elasticity- according to ISO 13061-3(4)-2014. The results of study where the strength properties of Alnus glutinosa sound timber, timber coloured caused by fungi when strength parameters aren't significantly affected, early stage of rot, characterized by discoloured fibres and patches in the wood, where the general texture and strength properties only start being affected were investigated would help for practical applications so that this wood species can be processed more efficiently for value -added products.

Keywords: *Alnus glutinosa (L.),Gaertn, strength parameters, quality*

THE EFFECT OF CROWDING AND EXCLUDED VOLUME ON ACID-BASE EQUILIBRIA OF WEAK POLYELECTROLYTES

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Abstract

Weak polyelectrolytes (WPE) are responsive materials used as active charge regulators in a variety of applications including controlled release and drug delivery in crowded bio-related and synthetic environments. These environments are rich in solvated molecules, ions, nanostructures and mesostructures. Often shifts the equilibrium constant and pKa of WPE, as compared to single-component solutions, is observed. Here we present experimental investigation of the effect of high concentrations of non-adsorbing, short chains of poly (vinyl alcohol), PVA, non-ionic micelles and colloids on charge regulation (CR) of poly (acrylic acid), PAA. Titration experiments of PAA (mainly 100 kDa in dilute solutions, no added salt) carried out in high concentrations of PVA (13-23 kDa, 5-13 wt%) and dispersions of carbon black (CB) decorated by the same PVA (CB-PVA, 0.2-1 wt%). Titration experiments show up-shifts of about ~0.9 pH units in the pKa and down shifts in CB-PVA dispersions (of ~0.4 pH unit). Thus, while the presence of solvated PVA increases the charging of the PAA chains, as compared to PAA in water, that of CB-PVA particles reduces PAA charging. In addition, coupling between weak intermolecular interactions and steric effects are observed in micellar solutions of Pluronic block copolymers. Detailed analysis of the nano-structure of the mixtures using Small-Angle X-ray Scattering (SAXS) and transmission electron microscopy at cryogenic temperatures (cryo-TEM) indicate local re-organization of the different components. The observations clearly indicate that while steric (entropic) effects shift the acid-base equilibrium of WPE and affect their degree of ionization in crowded liquid environments, the direction of the shift depends on the size and geometry of the seemingly the additives, probably due to depletion and excluded volume interactions. Thus, entropic effects should be taken into consideration when designing functional materials in complex fluids environment.

SIMULATED RADIONUCLIDES INCORPORATION IN LEAD BASED GLASS STRUCTURE

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Abstract

Copper-lead base glass formulations were studied under simulated conditions and showed good potential as a waste form for radioactive waste management. Radiation shielding properties, thermal stability, glass forming ability and solubility of different simulated radioactive waste compounds of copper-lead glass were evaluated. Amorphous materials containing high amount of both MoO_3, and Cs_2O were obtained. The structural modifications induced by the incorporation of simulated radioactive waste in copper-lead host matrix were investigated by X-ray diffraction analysis, Fourier Transform Infrared and Electron paramagnetic resonance. The analyses of the results obtained indicate a high potential for the glassy composition as a waste form to improve the solubility of molybdenum and immobilization of cesium ions in glass.

Keywords: *copper-lead glass, solubility of molybdenum, immobilization of cesium, radioactive waste managemen*t

ACKNOWLEDGMENTS

This work is funded by the Ministry of Research, Innovation and Digitalization through: CNCS–UEFISCDI, project No: PN-III-P1-1.1-PD-2021-0721, within PNCDI III and Programme 1 - Development of the National Research and Development System, Subprogramme 1.2 - Institutional Performance - Funding Projects for Excellence in RDI, Contract No.37PFE/30.12.2021.

TWO-PHASE FLOW: SOLID-LIQUID

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Abstract

Liquid is the aggregate state of matter. Liquids differ significantly from solids and gases due to the different nature of the thermal motion of molecules. The molecular pressure in liquids is very high, millions of times greater than in gases. Molecular pressure is a conventional designation of a quantity that takes into account the action of molecular forces. Molecular pressure is calculated from the work done by molecules passing through the surface layer of a liquid.

Liquids, unlike solids, have a short-range order in the arrangement of particles of matter. If the particles of solids in liquids are tightly arranged then they oscillate around the equilibrium position. Liquids are practically incompressible.

Despite the fact that the molecules of a liquid are arranged in much the same way as in a solid, the liquid has fluidity. This is explained by the fact that, unlike a solid, the oscillation of molecules around an equilibrium position in a liquid is not eternal, at some point in time the molecule makes a "jump", moving to another position. As a result, the liquid retains its volume but does not retain its shape.

Keywords: *Liquid, solid, molecular pressure, oscillation*

ECO-FRIENDLY DESIGN OF A COMMERCIAL REFRIGERATOR FOR ENERGY EFFICIENCY LABEL

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Abstract

Adopting hydrocarbon-based refrigerants (R290) and environmentally friendly designs can significantly positively impact energy consumption reduction and sustainability within the food service sector. In commercial kitchens, energy-intensive appliances like refrigerators, ovens, and dishwashers are prevalent, consuming more energy than their household counterparts. These products come in various models and sizes based on enterprise needs. Energy efficiency labels are mandatory for many household products, such as white goods (e.g., refrigerators, washing machines) and electronic devices (e.g., screens), reflecting their energy performance. However, the energy efficiency label is currently limited to commercial coolers (refrigerators and freezers) in the commercial kitchen realm, following EU regulations 2015/1094 and 2015/1095. Ozti manufactures cooler products of diverse models and capacities, emphasizing the importance of energy consumption performance. The study evaluated the energy consumption performance of an innovative commercial refrigerator prototype. This evaluation included using M packages (Tylose test packages) during the test phase, adhering to the EN16825 standard. Apart from eco-friendly design considerations, the appropriate selection and placement of equipment like compressors and evaporators played a crucial role. As a result of employing hydrocarbon-containing refrigerant gas, the commercial refrigerator prototype demonstrated an impressive reduction of approximately 30% in energy consumption.

Keywords: *Commercial refrigerator, energy efficiency label, eco-friendly design, energy consumption*

Acknowledgments: *This study was prepared within the scope of TÜBİTAK-TEYDEB 1501 coded Industrial Research Technology Development and Innovation Projects Support Program project numbered 3151264. We would like to thank TÜBİTAK-TEYDEB Transport, Defense, Energy and Textile Technologies Group (USETEG) for their contribution to the project.*

CLOUD TYPE CLASSIFICATION IN GROUND-BASED SKY IMAGES WITH DEEP LEARNING

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Abstract

Clouds cover more than half of the Earth's surface and are the subject of intense research in climate modeling, weather forecasting, meteorology, solar energy research, and satellite communications. Determination of cloud types and characteristics is of great importance in developing and applying solar radiation forecasting models. Therefore, classifying clouds into different categories according to their optical properties is essential for developing solar radiation forecasting algorithms. In this study, we have tried to develop a more efficient, reliable, and cost-effective solution for cloud classification. In this context, a deep-learning CNN model that can classify six different cloud types is developed, and its performance and applicability are examined. The SWIMCAT-EXT dataset, available for research activities, is used for training and testing the model. The experimental results show that the proposed CNN model can successfully classify cloud types and can be integrated into the solar radiation forecasting process.

Keywords: *Cloud classification, convolutional neural network (cnn), deep learning, solar irradiance prediction*

NEW OPTICAL METHOD IN LASER PHOTOTHERAPY

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Abstract

In this study we investigate the kinetics of oxygen tension (pO2) in skin tissue under the influence of the transcutaneous laser irradiation. The results of in vivo experimental measurements of pO2 by a method of transcutaneous oxygen monitoring (TcOM) are presented. The results show that under laser irradiation the value of tissue oxygenation increases and after approximately 10 minutes of exposure exceeds its initial level up to 1.6 times. The observed increase in pO2 indicates the process of photodissociation of oxyhemoglobin (HbO2) in skin blood vessels, which results in local O2 increase in the tissue. Such laser-induced enrichment of tissue oxygenation can be used in phototherapy of pathologies, where the elimination of local tissue hypoxia is critical.

Keywords: *Hemoglobin, oxyhemoglobin, tissue oxygenation, phototherapy, photodissociation*

IMPACT OF 222 NM UV-C RADIATION ON COLOR ACCURACY OF VIDEO DISPLAYS IN PUBLIC BUSES

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Abstract

The purpose of this study is to investigate the effects of 222 nm UV-C radiation on the color accuracy of bus interior materials, specifically video displays. The research examines the effects of exposing bus interior displays to UV-C radiation and measuring the resulting changes in monitor color accuracy over time. This wavelength of UV-C radiation is commonly used for disinfection purposes and can be used against COVID-19. The results show that UV-C radiation has a significant negative effect on display color and other parameters. The results may be useful in ensuring optimal color accuracy and durability under UV-C exposure, while providing a safe and effective method of disinfection against COVID-19.

Keywords: *UV-C radiation, video display, public bus, color difference, correlated color temperature, gamma*

POLARIZATION DIFFRACTION GRATINGS IN PAZO POLYMER FILMS RECORDED BY DIGITAL POLARIZATION HOLOGRAPHY USING SPATIAL LIGHT MODULATOR (SLM)

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Abstract

Diffraction gratings with various profiles were programmed in order to be used with reflective phase spatial light modulator (SLM). Using digital polarization holographic setup including the SLM and two quarter-wave plates, the spatial modulation of polarization was recorded on azopolymer PAZO thin films. Gratings with different profiles and parameters were recorded and the kinetics during recording in ±1 diffraction orders were obtained in real time. Diffraction efficiencies were calculated for each grating and the polarization characteristics (azimuth, ellipticity, degree of polarization) of the diffracted waves were determined.

Acknowledgements: *This work is financially supported by contract КП-06-Н38/15 with the National Science Fund of Bulgaria. Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.*

MACHINE LEARNING BASED DAMAGE IDENTIFICATION IN COMPOSITE STRUCTURES

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Abstract

Due to significant advances in computational techniques and artificial intelligence methods, a data-driven structural health monitoring (SHM) approaches have become very attractive for detection of faults and prognosis of the remaining useful life of composite structures. The present study focuses on development and implementation of data-driven structural health evaluation method for damage identification in carbon fibre reinforced plastic plates. Five machine learning algorithms, namely, k-NN, discriminant analysis, decision trees, Naïve Bayes and Support Vector within two supervised learning schemes are used to create classification models by learning from simulated response data. The predictive performance of the developed classification models is evaluated by performing experimental identification of delamination damage in composite plates.

EVOLUTIONARY ALGORITHM IMPLEMENTED IN THE INTERACTIVE SYSTEM FOR EDUCATION IN MODELLING OF BIOPROCESSES

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Abstract

The Interactive System for Education in Modelling and Control of Bioprocesses (InSEMCoBio) has been developed as a dynamic system flexible enough to allow new features to be easily integrated, specifically, additional experimental data for different biotechnological processes, various appropriate kinetic models and optimization algorithms.

The presented research is related to the implementation of a new optimization algorithm in InSEMCoBio. The system has been upgraded with an Evolutionary Algorithm (EA) for parametric identification of available kinetic models based on already integrated experimental data of the E. coli MC4110 fed-batch cultivation process. The existing set of operational features and options for graphical visualization of the results has also been updated. The obtained results confirm the workability of the developed software system.

InSEMCoBio allows access to contemporary high-level fundamental knowledge for bioprocesses modelling that can assist teaching programmes in biotechnology and bioengineering. The system could be considered a tool for enhancing education quality by transferring innovative scientific knowledge and technologies to students.

Acknowledgements: *This research was funded by the National Scientific Fund of Bulgaria, Grant КП-06-Н32/3 "Interactive System for Education in Modelling and Control of Bioprocesses (InSEMCoBio)".*

MODELLING AND SIMULATION OF A SUBSTRATE THERMOMECHANICAL BEHAVIOR DURING THE PLASMA SPRAYING

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Abstract

In our study, a 3D thermal plasma jet was simulated using the ANSYS-CFX code with two turbulence models and for different cases of effective powers. The analysis of the turbulent flow during the thermal jet using the RNG k-ε and SST k-ω models was also presented. The velocity and temperature profiles at the nozzle outlet were deduced from the literature and used as inlet boundary conditions. The results obtained from the two turbulence models show that the RNG k-ε model with different effective powers (790 W; 1050 W; 1350 W and 1780 W) is in good agreement with the experimental results. The RNG k-ε model gave results closer to the experiment than the results obtained from the SST k-ω model. It can also be concluded that when increasing the power supplied to the gas used, the temperature increases and it is maximum in the central axis. In the second step, the flow analyzed by the RNG k-ε model generated the initial conditions for the unsteady flow. Transient simulations for the 2D plasma jet are performed to obtain the velocity and temperature fields and also to obtain the temperature distribution in the substrate for the different time values. The transient simulations in the substrate for the different time values have also been studied. The results showed that the variation of the temperature of the plasma jet is always insignificant near the substrate for any value of time (flat curves) this says that the maximum of the temperatures obtained at the level of the substrate in the axial direction (Z axis) are maximum at the interface between the flow and the substrate (i.e. the contact surface at the centerline), and the maximum of the temperatures obtained at the substrate in the radial direction (y-axis) are maximum at the center of the substrate (i.e. x=0 and y= 0).

Keywords: *thermal plasma jet, turbulent flow, transient simulations, Substrate, ANSYS-CFX*

BINOMIAL HYPERFILTERS. THE APPLICATION OF THE SPECTRAL METHOD IN THE NEURAL STRUCTURES

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Abstract

The given paper describes the design and the method of hyperlinear filter's synthesis. On its basis the scheme of the binomial filter is offered that will provide the increase in the efficiency of the neural structures. Methods of calculations using the spectral representations of Walsh are given. The estimates of the synthesized structures efficiency are indicated.

Keywords: *hyperlinear and binomial filters, a neural structure, a tangent bundle*

FLUORENE DERIVATIVES AS BIPOLAR CHARGE TRANSPORTING MATERIALS

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Abstract

Holes transporting material (HTM) is one of the main constituents of organic photovoltaic devices (OPV), determining the cost, energy conversion efficiency and longevity of the device. The main disadvantage of majority of organic HTMs is the low mobility of the holes. To overcome this shortcoming, HTM additives, which reduce the stability of the OPV, are often used. Therefore, organic semiconductors that do not require additives have been receiving increasing attention. One of such organic semiconductors is bipolar organic semiconductors [1].

The aim of this work was to synthesize fluorene derivatives with hole- and electron-transporting ability and to investigate the properties of new compounds V1374, V1383, V1384 and V1416.

INFLUENCE OF POSITION OF METHYL SUBSTITUENT ON THE LIQUID CRYSTALLINE AND PHOTOSWITCHING BEHAVIOUR IN BENT-CORE COMPOUND

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Abstract

Due to their multiple properties induced by azo linkage group, the bent-core molecules present importance in the field of material science. These are characterized by reversible conversions from trans form to cis form during UV or visible light irradiation, therefore existing a dependent relation in photochemical composition with wavelength and temperature. Such materials have been directed towards display applications, or semiconductors and optical devices. Also, it is known that behaviour mesomorphic of compounds with liquid crystalline properties is influenced by linking groups and side chains from structure. [1-4]

Here, we present a study of 1,3-disubstituted benzene derivatives, with asymmetric structure, which differ by the length of terminal flexible chain. In order to obtain thermally stable bent-core mesogens, we synthesized new azo-substituted compounds, with and without Schiff's base unit, with potential for applications in electrooptic devices. We investigated the effect of methyl substituent at two different positions, in one of the arms and on the central core, on the mesogenic properties. We observed that such a change in molecular structure influence not only liquid crystalline properties, but also the transition temperatures. The liquid crystalline behavior was confirmed by differential scanning calorimetry (DSC) and optical polarizing microscopy (POM). Also, the thermogravimetric analysis showed that the presented azo derivatives have a good thermal stability in the mesophase behavior, since the degradation of the compounds begins over the isotropization temperature. Modeling studies were made for the theoretical characterisation of molecules and were consistent with the experimental data. The investigations have been carried out to reach a better understanding of the structure-properties relation in bent-shape compounds.

Keywords: *bent-core molecules, optical properties, mesophase, liquid crystals*

Acknowledgments: *Catalina I. Ciobanu is thankful to Romanian Ministry of Research, Innovation and Digitization, within Program 1 – Development of the national RD system, Subprogram 1.2 – Institutional Performance – RDI excellence funding projects, Contract no.11PFE/30.12.2021, for financial support.*

PHOTOCATALYTIC PROPERTIES OF N-DOPED ZrO_2 THIN FILMS

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Abstract

Undoped and nitrogen-doped ZrO_2 thin films were deposited by HiPIMS sputtering method, on unheated Indium Tin Oxide substrates. The structure was investigated by X- Ray Diffraction method and the films surface elemental composition was obtained by X-ray photoelectron spectroscopy.

ZrO_2 is a direct wide optical band-gap material, being absorbent in UV. The purpose of N-doping was to shift the fundamental absorption edge toward the visible range, in order to efficiently use the solar radiation. The optical bandgap width was obtained from optical absorption measurements, by diffuse reflection spectroscopy. The hydrophilic properties of the films were determined by contact angle measurements during UV irradiation. The photocatlytic performance of the films was obtained by studying the decomposition of Rhodamine B under UV irradiation.

EVALUATION OF THE THERMAL DECOMPOSITION MECHANISM FOR A SERIES OF FERROCENE DERIVATIVES

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Abstract

Ferrocene derivatives are precursor organometallic compounds for chemical vapor deposition (CVD). The optimization of the experimental conditions of the deposition processes involves both the knowledge of the vapor pressure and the thermodynamics of the sublimation of the precursors as well as the mechanisms of their thermal decomposition. In this work, the complex thermal analysis technique was applied: thermogravimetric analysis (TGA) coupled with mass spectroscopy (MS) and Fourier transform infrared spectroscopy (FTIR) to elucidate the thermal decomposition mechanism of some ferrocene derivatives. A STA 449F1 Jupiter type equipment (Netzsch –Germany) coupled with a mass spectrometer model QMS 403C Aëolos (Netzsch-Germany) and a FTIR spectrophotometer model Vertex-70 (Bruker-Germany) was used. Work was done in an inert atmosphere (nitrogen), in the temperature range 25-700 □C, with a rate of 10 □C/min. The mass of the analyzed samples was between 9.5 and 15.2 mg.

The recorded MS curves allowed the identification of the ionic fragments in the temperature range 25-700 □C in which the recordings were made. It was found that the initiation of thermal degradation occurs at the pentadienyl groups from ferrocene. In the first stage of degradation, a maximum of the ionic current was highlighted for the ionic fragments m/z=65 and m/z=66. The results are also confirmed by the FTIR spectra which indicate a peak at 622 cm-1 which corresponds to the vibration of the cyclopentadienyl ion.

MICROSTRUCTURAL CHARACTERIZATION AND PROPERTIES OF COLD SPRAYED NICKEL COATING

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Abstract

Dendritic nickel (Ni) particles were deposited onto aluminium alloy (Al 7075) substrates in order to investigate the deformation and bonding mechanisms of particles. The coatings were sprayed by means of an Impact Innovations 5/8 system. To evaluate influence of substrate topography on adhesion of Ni coatings surface of 7075 Al alloy was prepared by sand blasting. The Ni coatings showed negligible porosity, and the grain structure of the feedstock powder was retained after the cold spray process. The high modulus and microhardness values exhibited by the cold sprayed Ni coatings are comparable to the results obtained by electrodeposition of Ni material and are superior to the hardness values reported for polycrystalline cold-worked coarse grained Ni.

OPTIMIZATION THE PHASE COMPOSITION OF ALUMINUM ALLOYS FOR MOTOR PARTS OPERATING AT ELEVATED TEMPERATURES

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Abstract

The revolutionary transition from internal combustion engines to electric motors did not significantly change the exploitation conditions of aluminum castings in cars. High strength and dimensional stability at elevated operating temperatures of around 200 - 300 °C remain the main ones, regardless of the type of applied propulsion energy.

The common in both cases is that to avoid overheating inside the engines, different cooling systems are used wherever it is possible at stable operation.

As more the electricity advances in providing comfort and power, so more the complexity of aluminum body parts in electric motors increases.

A method for optimizing the phase composition of aluminum alloys operating at elevated temperatures is presented in this work.

The use of no more than one percent of a suitable alloying material can produce the desired effects and achievement of the set goals. The example refers to the widely used aluminum alloy of the Al-Si-Cu group.

Keywords: *Aluminium alloys, phase composition, carters, electric motors, elevated temperature*

POSSIBILITIES FOR IMPROVING SURFACE DEFECTS OF 3D PRINTED TITANIUM PRODUCTS THROUGH REACTIVE ELECTRO-SPARK PROCESSING

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Abstract

There are two main reasons why researchers are looking for solutions to improve the surface characteristics of products produced by 3D printing (most often by SLM, DMLS technologies):low hardness and the low tribological characteristics of titanium alloys, which limit their application in friction assemblies in many industrial branches; high roughness and defects such as irregularities, micropores, and cracks on the surface of 3D titanium products, which require complex labor-intensive and energy-intensive finishing operations.

In the present work, an analysis of literary sources was carried out on ways to improve the surface characteristics and properties of titanium surfaces produced by selective laser melting (SLM). The technological characteristics of the electrospark deposition method as the lightest, most accessible and inexpensive way to improve the surface qualities of 3D products are indicated. The authors' results are presented, where reactive electrospark treatment based on the ESD method has been used based on the ESD method. A simultaneous multidirectional effect is achieved, which is expressed in: up to a fivefold reduction in the roughness of 3D titanium surfaces; filling of the surface pores, cavities and voids; a double increase of microhardness of the modified surfaces; ecological replacement of finishing treatments and economy of labor, equipment, consumables, and energy.

Appropriate process and electrical parameters and materials are indicated to realize the above effects.

Keywords: *3D printing, selective laser melting (SLM), Direct metal laser sintering DMLS, electrospark deposition (ESD), titanium alloys, roughness, microhardness*

ADSORPTION OF Zn(II), Cu(II), Cd(II) AND Co(II) FROM AQUEOUS SOLUTION ONTO HALLOYSITE

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Abstract

Halloysite nanotubes are naturally occurring aluminosilicate clay minerals with a framework composed of numerous rods with nano straight holes. This rare mineral is found in Polish deposit, located in the Lower Silesia near Legnica town, which is owned by the Intermark Company. The aim of this study was to investigate Zn(II), Cu(II), Cd(II) and Co(II) adsorption onto halloysite coming from the Dumino deposit in Poland. The surface morphologies of halloysite samples were examined by a scanning electron microscope (SEM) before and after sorption of metals. Two techniques, ED-XRF and ICP-OES were employed to investigate the chemical compositions of halloysite. Batch experiments were carried out to determine adsorption isotherm of Zn(II), Cu(II), Cd(II) and Co(II). The data obtained allow to identified that the metal ions uptake is significantly dependent on pH. The one-component system equilibrium data is well represented by empirical adsorption models. The isotherm parameters reveal the heterogeneous nature of the halloysite surface and nonideal behavior of the adsorption system. Thought the modelling of two-component system equilibrium requires estimating all equilibrium parameters.

IMPORTANCE OF SIZE AND "NAKED" STRUCTURE OF GOLD NANOPARTICLES FOR THE FORMATION OF SPECIFIC CATALYTIC PROCESSES

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Abstract

After the discovery of catalytic activity of metal nanoparticles (NPs), unique properties of gold nanoparticles (Au NPs) in heterogenous processes have been emerged. In this paper, our research activities were focused on determination of size-depent catalytic activity of synthesized Au NPs in the model reaction of 4-nitrophenol reduction with sodium borohydride. The Au NPs were synthesized by the reduction method of tetrachloroauric acid using sodium borohydride and hydrazine in presence of polymer polyvinylpyrrolidon (PVP) at various concentrations to control the size and distribution of gold nanoparticles. The average particle size has been tuned in the range of 1 to 15 nm. Interestingly, the catalytic activity depends on the size becoming highest when the average size was 8 nm. Variation in the size and determination of the most convenient size of gold nanoparticles for catalytic activity were discovered here. The Langmuir-Hinshelwood reaction mechanism is accounted for evaluation of kapp values with comparison to Eley-Rideal mechanism. The above results reveal that Au NPs catalyst demonstrates excellent catalytic performance for nitro-compound reductions at room temperature.

NANOPOROUS POLYMERS WITH IMMOBILIZED SILVER NANOPARTICLES

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Abstract

Polymeric membranes with etched ion tracks have been investigated for decades and are still being studied today for their wide range of applications in applied and basic sciences. A unique property of ion track membranes is that both the pore density and the pore diameter can be varied independently, which makes such polymeric membranes particularly interesting. Additional important properties that characterise the membrane include the transport properties and functionalisation of pores by appropriate modification. In this work we introduce a simple and versatile technique for incorporation of silver nanoparticles (AgNPs) into a different structural forms of PET by the action of excimer laser light. This technology, known as Laser Induced Forward Transfer (LIFT), is capable of firm anchoring of silver nanoparticles to pristine PET foil, as well as to nanostructured PET with laser-induced periodic surface structures (LIPSS) or ion-tracked porous PET, creating the reactive seeds for further modification with stimuli-responsive molecules. Such a concept enables the control of PET-based membrane permeability with respect to a specific stimuli-responsive agent bonded to AgNPs, e.g. in a temperature, pH, or electrical field-directed manner. We demonstrated that LIFT technology is a suitable tool, which, under specific conditions, enables uniform decoration of the PET surface with AgNPs, regardless of whether the surface is in the form of a planar foil or an ion-tracked membrane. Nanostructured PET with embedded AgNPs may open up new possibilities in the production of templates for replication processes in the construction of functional bactericidal biopolymers or may be directly used in separation processes as permeability-controlled membranes.

Keywords: *Polyethyleneterephthalate, ion-tracked membrane, excimer laser, silver nanoparticle, immobilization*

Acknowledgments: *This research was funded by the Czech Science Foundation, grant number 22-17346S.*

THERMAL AND SURFACE CHARACTERISTIC OF CHEMICALLY CROSSLINKED COPOLYMERS BASED ON 1-ETHENYLPYRROLIDIN-2-ONE AND ETHENYL ACETATE

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Abstract

Copolymers based on 1-ethenylpyrrolidin-2-one and ethenyl acetate are usually produced as linear polymers in the form of colorless liquid or in the form of yellowish-white powder. The aim of this study was production of the chemically crosslinked copolymers poly(1-ethenylpyrrolidin-2-one-co-ethenyl acetate), p(EP-EA) using the free radical polymerization method. Comonomers, 1-ethenylpyrrolidin-2-one and ethenyl acetate, with different amount of ethylene glycol dimethacrylate, as crosslinker, were thermally initiated in the presence of a chemical initiator. Surface characterization of the obtained p(EP-EA) copolymers was performed using scanning electron microscopy method. Fourier transform infrared spectroscopy analysis indicates that the structure of the new molecule, different from the reactants, was formed. The absence of characteristic absorption bands from the vibrations of the vinyl group confirmed successful chemical crosslinking of polymer chains, occurred by breaking double bonds from the comonomers and crosslinker. SEM micrographs exhibit crosslinked, macroporous topology of p(EP-EA) copolymers surfaces. Differential scanning calorimetry (DSC) method was applied to detect their thermal characteristic. The glass transition and melting temperatures of the p(EP-EA) copolymers indicate good miscibility of the comonomers in the homogenous polymer network. The obtained synthesized cross-linked p(EP-EA) copolymers could be potential candidates for different application, i.e. as active substance carrier.

Acknowledgments: *Republic of Serbia - Ministry of Education, Science and Technological Development, Program for financing scientific research work, 451-03-47/2023-01/200133.*

APPLICATION OF EGGSHELLS AS HETEROGENEOUS CATALYSTS FOR BIODIESEL FUEL PRODUCTION

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Abstract

In biodiesel synthesis, the process of transesterification of vegetable oil is applied, in which heterogeneous catalysts can be used. Among them, one of the most effective is calcium oxide. Chicken eggshells heated at 850 oC for 4 hours and crushed to a fraction of 0.315-0.1 mm contain about 89% calcium oxide; therefore they can be used as a heterogeneous catalyst in the synthesis of biodiesel fuel by applying process of rapeseed oil transesterification with methanol. The yield of rapeseed oil methyl esters depends on four independent variables. By applying the surface response methodology, the influence of the following variables on biodiesel yield and optimal process conditions were determined: 6.8% calcium oxide (from oil mass), methanol to oil molar ratio 10.9:1, temperature 64 oC and process duration 9.5 h. Under such conditions, a 97.8% yield of rapeseed oil methyl esters is obtained. The physical and chemical parameters of produced biodiesel meet the requirements of the standard EN 14214 for biodiesel fuel.

CREATING NANOFIBERS BASED ON PROTEIN HYDROLYSATES EXTRACTED FROM HIDE AND HAIR DONKEY BY-PRODUCTS

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Abstract

Animal by-products are organic substances that can be rich sources of various proteins, including collagen and keratin. Collagen is a biopolymer with regenerative and tissue reconstruction properties that has been extensively studied for its potential in wound healing. Keratins are a group of fibrous structural proteins that have several advantageous properties, such as strength, durability, resilience, thermal stability, and biocompatibility.

The focus of this paper is to obtain nanofibers through the electrospinning process, using collagen and keratin hydrolysates extracted from donkey (Equus asinus L.) by-products, hides and hair, respectively. Electrospinning is a technique used to produce nanofibers by applying an electric field to a polymer solution, creating thin fibers with diameters in the nanometer range. Collagen and collagen-keratin solid mixture, each constituting 12%, were dissolved in a solution of acetic acid in water at a volume ratio of 9:1. The resulting nanofibers showed variable diameters ranging from 73 to 133 nm. The protein-based nanofibers were tested for microbial contamination, and the levels of aerobic microorganisms, yeasts, and filamentous fungi (including Staphylococcus aureus, Escherichia coli, and Candida albicans) fell within the acceptable limits required for pharmaceutical and topical formulations.

The valorization of low-cost substrates like donkey hides and hair by-products reduces the environmental impact and allows for the production of nanofibers for potential non-active wound dressings in a cost-effective and eco-friendly process.

Keywords: *nanofibers; collagen; keratin; donkey by-products; antimicrobial activity; wound dressing*

Acknowledgements: *This research was funded by a grant of the Romanian Ministry of Research, Innovation and Digitalization, CCCDI - UEFISCDI, project number PN-III-P3-3.5-EUK-2019-0237 within PNCDI III (NonActivPans), Contract 219/23.12.2020.*

DEVELOPMENT OF AN ECOLOGICAL PROCESS FOR THE PRESERVATION OF WET BLUE AND CRUST LEATHER USING GAMMA IRRADIATION

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Abstract

Semi-finished leathers, wet-blue / wet-white or crust, are very susceptible to mold and yeast attack due to their high-water content and pH value. If long-term storage, at room temperature is required, molds can grow on the surface of the leather, causing it to stain. To prevent the attack of molds, isothiazolinones are used, but these products can cause contact dermatitis and polluted waste waters. Finding a new method of preserving wet-blue or crust leather is necessary both to reduce pollution and to eliminate the negative effects of biocides on health. The experiments were performed on goatskin tanned with basic chromium salts (wet-blue) and sheepskin crust leather. Samples were irradiated at 5, 10 and 15 kGy to establish the required dose for long-term preservation of leather, at room temperature and atmospheric pressure. Irradiated and non-irradiated leather were physico-chemical and physico-mechanical analysed according to the standards in force for the determination of shrinkage temperature, volatile matter, total nitrogen, total ash, chromium oxide content, elongation at break, tear strength and tear resistance. The antimicrobial tests were performed according to standard SR EN ISO 11137/2015. The results of physico-chemical analyses on the wet-blue and crust leather showed that there were small differences between the non-irradiated and the irradiated leathers, which mean that gamma irradiation didn't affect the collagen macro structure. Physico-mechanical test have shown that elongation at break and tear resistance values have grown suggesting that the collagen fibres, after irradiation, were able to line up in the direction of the force and some hydrogen bonds were broken. Antimicrobial analyses showed that after 14 days of incubation, microorganisms and fungi on irradiated wet-blue and crust leathers are under 100 UFC/g compared to 10.000 UFC/g for control, gamma irradiation being a suitable method for long-term preservation of wet-blue and crust leather.

Keywords: *wet-blue leather, gamma irradiation, long-term preservation, physico-mechanical properties*

AN OVERVIEW OF THE AVAILABLE WATER TEXTILE EFFLUENT TREATMENTS

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Abstract

The textile industry is one of the most significant contributors to water pollution, with the dyeing and finishing processes being major culprits. The effluent generated from these processes contains various chemicals and dyes that can harm aquatic life and pose a significant threat to human health. Several effluent treatments have been developed to minimise the impact of these effluents on the environment. Fashion is vital to the textile industry supply chain, which determines consumer demand and industrial production. Sustainability requires action from all parts of the chain. Communication and understanding, however, are not always possible due to the different fields of knowledge involved. This overview discloses the available solutions for liquid effluent treatment from textile dyeing and finishing providing a fast, precise and deep understanding of methods such as the Physicochemical and Biological treatments and the recent Advanced Oxidation Processes.

Keywords: *textile wastewater, water pollution, effluent treatment, sustainable fashion*

GEOPOLYMERS WITH GRAPHENE USED FOR BUILDING MATERIALS

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Abstract

The geopolymers are inorganic aluminosilicate binders, considered an ecological and cheap alternative for materials used in construction, having a good resistance against corrosion and a good durability. The addition of graphene oxide or of other metal oxides in the composition of geopolymers can give them a photocatalytic effect. GO ensures a dense structure in the cement matrix leading to strong adhesion.

A batch of experimental hydraulic mortar (HM) was made, obtained in accordance with the standards in force, to which were then added different concentrations of graphene oxide (GO) powders, in order to improve some properties, for its use in the rehabilitation of heritage buildings. Combinations of GO were used with silver nanoparticles (GO-Ag,) with ZnO (GO-ZnO), with TiO2 (GO-TiO2) and with fly ash, noted as GO-Fly ash. The characterization of the hardened mortars was performed by: Fourier transforms infrared spectroscopy, the mechanical properties (compressive strength, bending strength and adhesion to the substrate) and the morphological analysis of the surface by SEM were determined.

The results revealed that the resistance to compression and bending in the presence of additives and GO is reduced compared to the control samples, the adhesion of the mortar to the brick substrate increases. So, increasing the workability of the combine's proportions and fineness also affects the strength of the mortar.

Regarding the microstructure and mechanical properties obtained depending on the composition of the mortars, the optimal proportion of the mixture studied was appropriate by 5% HM with GO-ZnO and GO-TiO2 by weight.

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number COFUND-M-ERANET-3-GEOSUMAT, no. 314/2022. and by the Polish National Centre for Research and Development, grant number M-ERA.NET3/2021/70/GEOSUMAT/2022.*

THE FLY-ASH BASED GEOPOLYMER COMPOSITES FOR CIRCULAR ECONOMY

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Abstract

Fly ash-based geopolymers can be considered as a greener alternative to ordinary Portland cement, featuring comparable properties and cost yet with lower CO2 emissions. New wood fiber reinforced geopolymer composites with glass fiber and hemp fiber addition have been synthesized at room temperature by mixing powder (fly ash, glass fiber and randomly reinforced hemp fiber) with sodium silicate and sodium hydroxide as alkaline activators. The applications of geopolymers have been identified and future perspectives for supporting a circular economy by reusing waste for obtaining of new ecological materials. The design and investigation new materials were based

by varying the fiber percentages (2.5-10 wt. %) and hemp fiber (2.5-7.5 wt. %). New materials were cured at 90°C for 24 h. The flexural strength increased with addition of glass fiber more than addition of hemp fiber. The flexural modulus was influenced of quantity of fiber added it. Fractured surface of geopolymers with glass fiber and hemp fiber addition was evaluated by SEM. New materials developed could could be the limit for a promising green material for construction.

Keywords: *fly-ash, geopolymer composites, cement, glass fibers, hemp fiber, circular economy, SEM morphology*

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number COFUND-M-ERANET-3-GEOSUMAT, no. 314/2022. and by the Polish National Centre for Research and Development, grant number M-ERA.NET3/2021/70/GEOSUMAT/2022. The authors thank COST Action CA21103 and CA21121 for COST meeting.*

APPLICATION OF LOW-COST FLY ASH-BASED ADSORBENT FOR REMOVAL OF ACETOCHLOR HERBICIDE FROM WATER

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Abstract

In order to satisfy man's existential needs for food and energy, two major problems arise in the environment. Excessive use of herbicides based on acetochlor (ACT) in order to maximize food production causes surface water contamination. Its effect on endocrine disorders in humans and animals has been proven. By burning coal in thermal power plants, in addition to electricity, we also get huge amounts of by-products in the form of fly ash and boiler ash, the disposal of which requires large areas of land, a huge amount of water and energy.

These problems represent a major health, environmental and economic problem. In this work, the feasibility of using adsorbent based on fly ash as a cheap adsorbent for the removal of herbicide acetochlor from water was investigated instead of using commercial activated carbon. This study recognizes that fly ash (FA) is a promising adsorbent for the removal of various pollutants. Fly ash from the Morava thermal power plant was simply chemically treated with CaO and water to give modified fly ash (MFA), which proved to be an effective adsorbent for the removal of acetochlor (ACT) from water. The content of lime (CaO and water) in the fly ash was optimized in relation to the adsorption capacity of acetochlor using the D-Optimal Design method of response surfaces (RSM). For this purpose, the commercial software "Design expert 9" was used. The results showed that the pseudo-second-order rate equation effectively describes the adsorption kinetics and that the adsorption equilibrium is established after 60 minutes. The Freundlich model showed a better fit to the adsorption isotherm than the Langmuir model. The maximum Langmuir capacity of the adsorbent for ACT was 102.6mg g-1 at 25 °C at a solution pH of 8.

Key words: *fly ash, adsorbent, acetochlor, water, adsorption capacity*

TESTING OF FILTRATING PROTECTIVE CLOTHING ON THE BURNING NAPALM MIXTURE

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Abstract

The great technological revolution in filtrating protective materials and clothing intended for body protection was the implementation of flame-retardant polymer fibers like aromatic polyamides - aramids) and polybenzimidazole. Meta-aramids are known for their good thermal tolerance and long-time stability at high temperatures, and are therefore broadly applied in thermal protective clothing. Meta-aramids (the main representative is Nomex, produced by DuPont) and para-aramids (Technora and Twaron from Teijin and Kevlar from DuPont) are widely used fibers. Para-aramids have good thermal stability at high temperatures. In this paper, we will describe bench-scale testing, such as the vertical flame test, which is an excellent screening tool for evaluations of materials and fabrics, instrumented manikin test, according to the ASTM F1930, and specific instrumentation for testing and evaluation of filtrating protective clothing on the burning napalm mixture in the laboratory conditions.

CLOSED VESSEL TESTING OF A PCL-RDX ENERGETIC COMPOSITE MATERIAL

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Abstract

This research presents preliminary work done in order to analyze a PCL-RDX energetic composite material intended to be used for fabrication by FFF additive manufacturing technology (3D printing) of propellants. To obtain solid grains of this new energetic material a solution of liquid PCL and RDX crystals was precipitated in a warm polar solvent. The ballistic tests were done in a 40 cm3 closed vessel equipped with a PCB piezoelectric pressure sensor. Several loading densities were used in order to calculate impetus, covolume and the burning rate law. The calculated high burning rate can be explained by the porous structure of the grains observed during the SEM analysis.

NOVEL POLYURETHANE FORMULATIONS DESIGNED FOR COMPOSITE ROCKET PROPELLANTS APPLICATIONS

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Abstract

Composite rocket propellants are heterogeneous energetic mixtures based on crystalline compounds as oxidizer, fine metallic powders as fuel, and polyurethane matrix as organic fuel and binder.

It is essential to include a binder in the developing process since the oxidizer and metallic fuel must physically combine with one other and are both solid particles.

Nowadays, composite rocket propellants use hydroxyl-terminated polybutadiene (HTPB), an oligomer of butadiene terminated class, to provide the optimal thermal and mechanical behavior to the propellant grain. Novel polyurethane binder formulations comprising commercial polyols, an aliphatic isocyanate as crosslinking agent, an organic catalyst, and an inert plasticizer, are herein reported.

The developed polyurethanes were investigated by specific analytical techniques: Fourier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA) and dynamic mechanical analysis (DMA).

Moreover, to demonstrate the applicability, the formulations were employed in the development of composite mixtures for rocket propellant applications.

STATIC CHARACTERISTICS INCLUDING INFLUENCE OF SUBSTITUTE INHIBITION OF THE ANAEROBIC DIGESTION OF ORGANIC WASTES WITH PRODUCTION OF HYDROGEN AND METHANE

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Abstract

Anaerobic digestion (AD) is a multi-step biotechnological process with H2 as a non-accumulating intermediate product. The interest in H2 production through AD has increased last years. The main limitation of dark fermentative H2 production is the rather low energy recovery. In order to completely utilize the organic acids produced during dark fermentation and improve the overall energy conversion efficiency, a two-stage AD concept consisting of hydrogenic process followed by methanogenic process has been proposed. Performance of any system is the ultimate decider for its application and utility. The two basic characteristics of performance are static characteristics and dynamic characteristics. The process characteristics that do not vary with respect to time are called static characteristics [1]. The aim of this study is to develop and to analyse some static characteristics of a continuous process of AD with production of hydrogen and methane in a cascade of two bioreactors.

Acknowledgements: *This study is funded by the Bulgarian National Science Fund under contract KP-06-H46/4 "Experimental studies, modeling and optimal technologies for biodegradation of agricultural waste with hydrogen and methane production".*

EFFECT OF MINT ESSENTIAL OIL ADDITION ON LACTIC ACID FERMENTATION IN STIRRED TANK BIOREACTOR

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Abstract

The increasing consumer's demand for healthy beverages lead to the production of lactic acid fermented wort-based beverages. They can be classified as functional because of wort vitamins, antioxidants and fibres content and probiotic properties of used lactic acid bacteria strain. However, lactic acid wort-based beverages are not well accepted by consumers because of their poor sensory characteristics. The aim of this study was to investigate the effect of the addition of 0.025 and 0.05 % (v/v) mint (Mentha piperita) essential oil on probiotic, antioxidant, and sensorial properties on lactic acid wort-based beverages. Lactic acid fermentation was carried out at 25°C in a stirred bioreactor without aeration. The addition of mint essential oil inhibited lactic acid fermentation but all the beverages produced can be classified as functional. Although the beverage with 0.05% mint essential oil showed the highest total phenolic compounds and antioxidant activity, measured by cupric reducing antioxidant power (CUPRAC), ferric reducing antioxidant power (FRAP) and ABTS radical scavenging assay, it received the lowest score by tasting panel because its strong taste and aroma. The results obtained will be used for modeling of lactic acids fermentation with addition of mint essential oil for the production of beverage with high biological value and acceptable sensory profile.

Keywords: *lactic acid fermentation, wort, mint essential oil, phenolic compounds, antioxidant activity*

POSSIBILITIES FOR THE UTILIZATION OF BREWERS' SPENT GRAINS IN BIOTECHNOLOGICAL INDUSTRY

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Abstract

The brewing industry is a major branch of the food industry in the Republic of Bulgaria. Like any industry, the brewery generates waste products, the disposal of which is a top priority. About 85% of the waste products in the brewing industry are taken up by brewer's spent grain (BSG). They are obtained at the end of the mashing process, and their qualitative and quantitative composition depends on the selected technological scheme for wort production, malt technological parameters and the selected operational regimes for mashing and lautering BSG are lignocellulosic material that contains certain amounts of cellulose, non-cellulosic polysaccharides and lignin. Currently, BSG is used as an animal feed. In the present work, the possibilities for the use of BSG as a raw material in the biotechnological industry are considered. Data are presented on the application of BSG in various branches of biotechnology, as well as the necessary steps for their processing in order to extract valuable biological components and nutrients.

A NEW CROSS-LINKED COMPOUND WITH THERMO REMENDABLE PROPERTIES

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Abstract

A new cross-linked macromolecular compound was obtained by the Diels-Alder reaction of castor oil modified with maleimide groups and furan-functionalized chitosan. The molecular weight of chitosan was determined by the viscosimetric method, while the degree of acetylation was established from the 1H-NMR spectrum. Chitosan was modified by its reaction with furfural, followed by the reduction of the Schiff base formed intermediary. Castor oil was functionalized with 4-maleimido-benzoil-azide in order to obtain the dienophile component from the Diels-Alder reaction. The structure of the compounds was confirmed by the spectral techniques (ATR-FTIR and 1H-NMR) and their properties were investigated by different methods, such as thermogravimetric analyses and differential scanning calorimetry.

Key words: *thermoreversible, chitosan, Diels-Alder*

Acknowledgments: *This work was supported by a grant of Ministry of Research, Innovation and Digitization, CNCS/CCCDI - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0513, acronym "ReMendBioCoat", within PNCDI III.*

UTILIZATION OF POLYMERIZED PICKERING EMULSIONS IN EXTRACTION AND RECOVERY OF METAL IONS FROM WATERS

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Abstract

Extraction and recovery of metal ions from wastewaters for the purpose of decontamination or hydrological mining has become of great importance in the current eco challenges. In this work we propose a novel technology for metal ion extraction and recovery, which utilizes nano- and micromaterials obtained via Pickering emulsion polymerization. Pickering emulsion polymerization technology enables facile synthesis of the nano-, micromaterials in different shapes and forms, from particles, to low dimensional films to nanoporous monoliths. The target metal ions are the transitional metal ions that present a high level of toxicological risk for the living organisms or metal ions that have economical importance. The nano- and micromaterials we obtained are polymeric and are nanostructured. These carry ligands, or chelates, capable of binding specific metal ions and have good ion absorption capacity and selectivity. Furthermore, these materials can float on the surface of water, which means that they can be deployed under a variety of environmental circumstances with minimal energy input and can be easily collected after the extraction cycle and sent to recovery or regeneration. These materials can be deployed for a significant number of extraction-recovery duty cycles and represent a promising platform for future generation of materials employed in water purification and mining.

Keywords: *Pickering emulsions, nanoparticles, water treatment, metal ion recovery*

Acknowledgements: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization of Romania, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).*

CATALYTIC BEHAVIOUR OF DOPED MANGANESE FERRITE WITH SPINEL STRUCTURE

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Abstract

Spinel ferrites are a special class of mixed iron oxide-based compounds with the general chemical formula MFe2O4 where M is a divalent metal e.g., cobalt, manganese, nickel, zinc, etc., or a mixture of them, which are often proposed as strong candidates for various catalytic applications in organic processes [1]. Besides their catalytic performance, chemical stability, high specific surface area, small bandgap, controllable size and shape, and relative ease of modification, low production cost and low toxicity, perhaps the main advantage for catalytic purposes is that these compounds present unique magnetic properties. Therefore, these materials can be easily recovered after completion of catalytic processes by applying an external magnetic field [1-3].

Among ferrites, the manganese-based one have become the most promising candidates for catalysis. On the other hand, recent studies have shown that small amounts of rare earth cations can improve the properties and performances of ferrites by altering the crystallite and grain size and/or creating crystal defects in the spinel lattice. To facilitate the insertion of rare earth ions into the spinel matrix, the materials are frequently subjected to a series of thermal treatments at high temperatures [3]. Manganese ferrite is one particular example, which is unstable at high temperatures, because Mn2+ ions have a tendency to oxidize to Mn3+. Therefore, doping MnFe2O4 with lanthanides cations, using elevated temperature, is detrimental for the phase purity.

In this study, we focused on the synthesis and exploration of the catalytic performance of manganese ferrite doped with various rare-earths such as: La, Ce, Gd, Er.

Details on the preparation method and the catalytic behaviour of the resulted materials will be given.

Acknowledgements: *This work was supported by a grant from the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-III-P1-1.1-TE-2021-0030, within PNCDI III.*

FLEXIBLE NETWORK FORMATION BY PULLULAN FUNCTIONALIZATION WITH VERSATILE CHROMOPHORES

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Abstract

Photoreactive polysaccharide-based networks are among the most disputable materials lately due to the remarkable and unique properties that put them higher on the list of desired materials syntheses in research experiments. Pullulan is a biocompatible, environmentally friendly polysaccharide whose structure consists of maltotriose chains. Having multiple hydroxyl groups in the repeating units, pullulan is not only eye-catching because of its increased hydrophilic behavior in the most common solvent, water, but also because it can participate in many functionalization reactions to form derivatives that may play a role in designing photopolymerizable materials with innovative uses.

This work describes and investigates the synthesis and chemical structure characterization of oxidized pullulan derivatives via NaIO4 and TEMPO radical system-oxidation, as well as their involvement in coupling processes with aromatic amines containing chromophore groups, which resulted in the development of their corresponding crosslinked networks via photopolymerization when exposed to UV light. The appeal of these light-sensitive linked compounds is that no photoinitiator is required for photopolymerization because they already contain comparable moieties that may initiate the process. Finally, the effect of light irradiation on their unique characteristics is investigated briefly.

Keywords: *pullulan, oxidation, chromophores, photopolymerization, crosslinked networks*

Acknowledgements: *This work was supported by a grant of Executive Agency for Higher Education, Research and Innovation Funding, UEFISCDI, project code PN-III-P4-PCE-2021-0933, acronym "PHYCOMAT", within PNCDI III.*

PHOTOTHERMAL ANTIBACTERIAL ACTIVITY OF PLASMONIC BLACKBODY AGAINST PATHOGEN BACTERIA

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Abstract

Broadband light absorbers are attracting increasing attention due to their remarkable physical and chemical properties, with potential applications in various fields, including biotechnology. Black gold nanoparticles (BGN) are a prime example of such absorbers in the visible and near-infrared ranges. Our study presents compact supramolecular BGN aggregates with dimensions of 50 nm, self-assembled from individual gold nanoparticles at temperatures below 100°C, exhibiting intense and uniform absorption across a wide spectral range from 400 nm to 1100 nm. We evaluated the thermal photoconversion performance and stability of the obtained supramolecular BGN, revealing a 40°C increase in temperature compared to ambient for an incident laser radiation power density of just 1.5 W/cm2. The supramolecular BGN also exhibited a stable, reversible temperature response for 7 heating/cooling cycles without significant loss of heating capacity. We investigated the photothermal antibacterial activity of BGN against reference bacterial strains, by exposing it to NIR light irradiation. Our results showed that the higher photothermal conversion efficiency of supramolecular gold assemblies under NIR light irradiation led to strong antibacterial activity against all tested strains. This offers a new possibility to design efficient light-absorbing materials that can be used as effective platforms to fight against bacterial infections.

Keywords: *black gold, nanoparticles, photothermal; antibacterial activity*

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0739, within PNCDI III.*

IRON AND CERIUM OXIDE NANOCONJUGATES WITH BIOMEDICAL APPLICATIONS

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Abstract

Cerium oxide nanoparticles present the mimetic activity of superoxide dismutase, being able to inactivate the excess of reactive oxygen species correlated with a large number of pathologies, such as stents restenosis, cancer proliferation and cardiovascular diseases, accelerate aging. This study presents the synthesis, physico-chemical and biological characterization of nanoantioxidants based on of iron oxide nanoparticles interconnected with cerium oxide nanoparticles via a polyethyleneimine shell. The synthetized nanoparticles were characterized by several techniques, such as EDX, XPS, Raman, DLS, TEM, in order to confirm their chemical structure and to investigate their properties. In vitro and in vivo analysis of antioxidant properties highlights the synergistic interaction regarding the free radical scavenging properties of iron oxide - polyethyleneimine - cerium oxide components, a phenomenon that correlates with XPS analysis of cerium nanoparticles. The synthetized inorganic conjugate have radical scavenging properties, offering simultaneous the possibility of guidance in magnetic field and therapeutic action.

Keywords: *magnetic nanoparticles, ceria nanoparticles, antioxidant activity.*

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0739, within PNCDI III.*

INORGANIC NANOPARTICLES FOR DUODENOSCOPE REPROCESSING

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Abstract

One of the most concerning issues of recent years has been the multiple outbreaks of nosocomial infections caused by multidrug-resistant organisms (MDRO) in digestive endoscopy. In this regard, the microbiological safety of duodenoscopes has become a hot problem, frequently appearing on the agenda of professional discussions and debates on a global scale. The influence of routine procedure use and reprocessing cycles on the duodenoscope is described in this study. Surface roughness and morphological modifications were observed, indicating that both coating and working channel polymers were altered. Because of all of this damage, the dudodenoscope is vulnerable to bacterial contamination and biofilm formation. Metal oxide nanoparticles were investigated within this context to overcome the reprocessing failure of routinely used disinfectants. Metal oxide nanoparticles had notable antibacterial action against the reference strains represented by Enterococcus faecalis, Escherichia coli, Klebsiella pneumoniae, Pseudomonas aeruginosa, Salmonella typhimurium, and Staphylococcus aureus. The nanoparticles were also compatible with the duodenoscope polymer coatings.

Keywords: *inorganic nanoparticles, duodenoscope reprocessing, antibacterial activity*

Acknowledgments: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-0739, within PNCDI III.*

NOVEL NANOTHERAPEUTIC SYSTEMS BASED ON PEGYLATED SQUALENE FOR IMPROVING THE IN VITRO ACTIVITY OF COMMONLY USED ANTITUMOR DRUGS

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Abstract

Nanomedicine is a broad scientific research field that includes numerous studies involving various types of nanotherapeutics, which has received great attention since nanotherapeutics could provide a better treatment for many severe diseases such as cancer, neurological disorders, or cardiovascular pathologies, with benefits for related applications such as diagnostics, contrast reagents, and medical devices.

Even recently discovered drugs, such as peptides, siRNA, therapeutic nucleic acids, or proteins, are frequently requiring a delivery system due to their poor bioavailability in conventional formulations and extreme instability in biological environments. The superior characteristics of nanotherapeutics' (including minimal toxicity, better bioavailability, and enhanced therapeutic impact) make them suitable candidates for clinical trials or clinical application.

As a result of our previous studies, PEGylated squalene (SQ-PEG) is a biocompatible amphiphilic compound that can self-assemble into micellar structures in an aqueous environment and encapsulate various drugs for safe delivery to different targeted regions. To illustrate our contribution in this field, SQ-PEG was used as an amphiphilic carrier for encapsulating antitumor drugs to enhance their biological characteristics. The stability and release kinetics of the developed nanotherapeutics in saline PBS were investigated using UV-Vis and DLS techniques, and the results showed better stability and drug release profiles. STEM images showed spherical morphology with nanometric dimensions. The effectiveness of their anticancer activity and cell viability were tested in vitro, and the results indicated enhanced biological behavior.

Keywords: *PEGylated Squalene, Drug Delivery, Antitumor, Controlled Release, Micelles, MCF-7, HeLa, Nanotherapeutic*

Acknowledgements: *This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0606, within PNCDI III.*

MODEL TESTS AND NUMERICAL SIMULATIONS ON THE BEHAVIOUR OF UNSATURATED SAND UNDER IMPACT LOADING DURING DEEP DYNAMIC COMPACTION

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Abstract

Deep Dynamic Compaction (DDC) is an ecological soil improvement method for increasing bearing capacity in large areas. The conversion process of kinetic energy during pounder impact into the soil is not well understood to date. Accelerometers mounted on the pounder can be used to measure the momentum transfer from the pounder to the ground. The article shows a possibility to use the motion quantities measured at a pounder to describe soil intrinsic phenomena. 1g model experiments of deep dynamic compaction were performed to study the ground motion during the impact. Several impact series were recorded using optical surface measurements as well as a high-speed camera along with digital image correlation. Accompanying numerical FEM simulations using the hypoplastic constitutive law were performed in ABAQUS to validate the phenomena observed in the model. The model and FEM investigations show that the energy conversion process in the soil is affected by the impact velocity, as well as the mass and geometry of the pounder. In the case of rigid body impact on granular surfaces, these influencing variables must be taken into account when describing the kinetics of DDC.

THE INFLUENCE OF ALGINIC ACID WITH THE ADDITION OF NON-IONIC SURFACTANTS ON STABILITY OF AQUEOUS SUSPENSIONS OF HALLOYSITE

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Abstract

*The influence of alginic acid (AA) with the addition of non-ionic surfactants on stability of aqueous suspensions of halloysite (N-H) was studied. Alginic acid belongs to the group of marine bipolisaccharides because it is obtained from the cell walls of some marine algae (brown algae). From a chemical point of view, it is a copolymer of mannuronic acid and guluronic acid linked by a β-1,4-glycosidic bond. It has many uses, among others in the food industry as an emulsifier and thickener, in cosmetology as an ingredient of shower gels, shampoos, toothpastes and soaps. Due to its healing properties, AA is also used in medicine in the production of dressings and hydrogels. Halloysite is a hydrated aluminum silicate with the chemical formula Al4[Si4O10](OH)8*4H2O. Halloysite clay is rich in easily digestible micro and macro elements, i.e. silicon, aluminum, iron, potassium, magnesium, calcium, sodium, manganese, phosphorus, zinc, selenium and copper. This clay mineral has antibacterial properties and the ability to absorb impurities from the skin surface, which is why it is very often used in the cosmetic industry for the production of masks, gels, creams for acne skin and seborrheic lesions. Refreshes and smoothes, nourishes, absorbs impurities and toxins from the skin, gently tightens pores. Accordingly, the colloidal system containing AA and N-H has a high application potential.*

In the experimental part, the influence of alginic acid and non-ionic surfactants (TX-100, TX-165, TX-405) on stability of aqueous suspensions of halloysite was investigated. Based on the adsorption measurements, the most likely stabilization mechanism was determined. Additionally, surface tension measurements were performed to confirm the formation of the polymer-surfactant complexes. It can be concluded that alginic acid adsorbs well on the halloysite surface, while the addition of TX-100 and TX-405 surfactants causes a decrease of the adsorption amount, which is caused by the formation of the polymer-surfactant complexes. The interaction between this two adsorbates is stronger than between the adsorbate and adsorbent, therefore the complexes are reluctant to adsorb on the clay mineral surface. In the case of TX-165, no change in the adsorption amount is observed, because the surface tension measurements show that no complexes are formed. On the other hand, the stability measurements show that stability of the tested systems increases with the increase of the AA concentration.

INFLUENCE OF HEAVY METAL IONS ON THE STRUCTURE OF THE ELECTRICAL DOUBLE LAYER OF SILICA-CARBON COMPOSITES

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Abstract

Adsorption occurring at the solid-solution interface is a process commonly used in various industries. This type of adsorption occurs, among other things, during the purification of liquids from undesirable and toxic components. In a system consisting of a solid, adsorbate and solvent, various types of interactions can occur - such as electrostatic interactions, the formation of chemical bonds and hydrogen bridges, as well as hydrophobic and van der Waals interactions. Practical applications of the adsorption process require knowledge of its mechanism, in which electrokinetic measurements are highly necessary.

For this purpose, measurements of the surface charge density and the zeta potential of solid particles dispersed in a liquid medium as a function of the pH of the solution were made. Two heavy metals, Pb(II) and Zn(II), were used as adsorbates, while three silica-carbon composites (C/SiO_2, C/Fe/SiO_2, C/Mn/SiO_2) were used as adsorbents. Then, the obtained curves made possible to determine the point of zero charge (pzc - point of zero charge) and isoelectric point (iep - isoelectric point) of the adsorbent. All these parameters characterize the electrical double layer formed at the solid-solution interface. In addition, the stability of the examined suspensions was also measured. The results obtained confirm the effectiveness of the electrical double layer examination towards better optimization of adsorption processes.

DEVELOPMENT AND CHARACTERIZATION OF CHITOSAN HYBRID COATINGS BY SOL-GEL METHOD

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Abstract

This paper describes the preparation and characterization of hybrid coatings constituted by SiO2, TiO2 and chitosan in varying compositions on aluminium, and glass substrates by sol–gel method. The optimized sol-gel solutions were deposited using by dip-coating and spray coating and the thermal treatment conditions (temperature) were optimized. In particular, condensation reactions necessary to allow the formation of the metal oxide networks were performed by storing the films in an open-air oven at 100°C and 80 °C for 30 minutes. Moreover, the functionalization of hybrid has been carried out with vinyltrimethoxysilane (VTMS).

The films were investigated by scanning electron microscopy (SEM), Fourier transformed infrared (FTIR) spectroscopy, hydrolytic degradation, corrosion resistance and adhesion test.

The process yields transparent chitosan hybrid coatings with good adhesion on glass substrates.

The obtained results suggest that the functionalization of the hybrid coatings was affected through in situ hydrolysis–condensation reaction of vinyltrimethoxysilane (VTMS) in the reaction medium. The best surface properties are found after thermal treatment at 100°C and after the addition of VTMS.

A potential shift towards more positive values was recorded by potentiodynamic polarization measurements, showing an enhanced corrosion resistance provided by the 50C50S hybrid coating.*

Thus, the composition of the coatings as well as their chitosan content affect the final chemical-physical properties. On the basis of the obtained preliminary results, chitosan-silica coating, seems to be highly promising as a novel sustainable film maker for packaging industry

Keywords: *sol-gel process, chitosan, hybrid, corrosion*

THE SYNTHESIS AND RADICAL SCAVENGING ACTIVITY OF NEW BENZAZOLE-RESORCINOL HYBRIDS

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Abstract

Accessible approach for amidoalkylation of various phenols was successfully developed. New quercetin and benzazole-resorcinol hybrids with high radical scavenging activity were synthesized and spectrally characterized. The in vitro radical scavenging activity of four newly obtained benzothiazolines and benzimidazolines containing a resorcinol fragment in the structure was investigated by ABTS-method. The results showed more active profile of benzothiazole derivatives than benzimidazole ones. The radical scavenging activity of 2-(2,4-dihydroxyphenyl)-N-carboxymethyl-benzothiazoline is comparable to resorcinol and quercetin with IC50 - 46.3µM. The established results give good lead for further biological activity testing.

STRAIN RATE DEPENDENT MECHANICAL BEHAVIOR OF NANOSTRUCTURED MG-3%AL ALLOYS

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Abstract

This work focused on the strain rate-dependent mechanical behavior of Mg-3%Al alloy fabricated via powder metallurgy. The effects of ball milling for different durations are also discussed in this study. Powder metallurgy approach integrating sintering at inert atmosphere followed by hot extrusion was used to fabricate Mg-3%Al alloys. Microstructural analysis and X-ray diffraction (XRD) studies demonstrated that the alloy of the solid solution of Mg and 3%Al were successfully fabricated using the powder metallurgy route. Both the milled powder and their extruded bulk samples revealed evidence of the formation of second-phase particles. Tensile tests were carried out at different strain rates, and the yield strength, tensile strength, and elongation to failure of samples made from milled and un-milled powders were measured and compared. The findings demonstrated that the strain rate and the grain sizes of the extruded samples have a significant impact on the strength and ductility of the bulk samples. The possible deformation mechanisms for each sample are discussed. It is hypothesized that the grain boundary movement mechanism and the geometrically necessary dislocations primarily governs the deformation process. The possible fracture mechanisms were predicted from the microstructural study of the fracture behaviors of the deformed samples. The micro-mechanical properties of each sample were analyzed using the loading-unloading curves of the micro-indentation test.

Keywords: *Mg alloy, powder metallurgy, strain rate, mechanical alloying, mechanical properties*

A CRITICAL EVALUATION OF THE USE OF HEMP AS A SUSTAINABLE SOLUTION IN GARMENT MAKING

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Abstract

The fashion industry is one of the world's largest and most polluting industries, significantly impacting the environment and human health. The production of conventional textiles involves toxic chemicals, excessive water consumption, and significant amounts of energy, contributing to greenhouse gas emissions and other environmental problems. Recently, there has been a growing interest in more sustainable and eco-friendly alternatives to conventional textiles. A promising solution is using hemp fabrics in the textile fashion industry. Hemp is a versatile and sustainable material used to make various textile products, from clothing and accessories to upholstery and home decor. Hemp requires less water and fewer pesticides than cotton and can be grown without herbicides or fungicides. This work discusses the sustainability of hemp while exploring the use of hemp fabric in the textile garment fashion industry as part of cotton substitution. A woven hemp fabric is used to create a casual final garment to prove that it can be quickly processed using the same design patterns, cutting and sewing procedure, offering the same comfort and aesthetic result. The fabric is tested and compared to a cotton woven fabric of similar characteristics for its drape, tensile and tear strength, resistance to wear, breathability, and sewability through needle penetration force. Finally, the dyeability of hemp is tested using natural dyes.

Keywords: *hemp, sustainability, eco-friendly fashion, sustainable farming, cannabis sativa*

INFLUENTIAL CONTROL CHARTS FOR PROCESS MONITORING IN ADDITIVE MANUFACTURING

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Abstract

Additive Manufacturing enables the production of complex parts layer by layer by using a 3D nominal model. It brings significant freedom in design, yet it can be difficult to obtain repeatable quality properties of build part. These systems show high variation in product features which could lead to poor quality of printed parts. Obviously, reducing assignable variation in both key product features and AM processes is a fundamental way of decreasing product defects and improve product quality. In the present work we propose methods for statistical process monitoring and control of key AM product features and process variables. Cumulative sums of influence functions are proposed to monitor the evolution of the process, its stability along the vertical growth direction and to show up the presence of assignable causes that affect variability, orientation, or the structure of relationships between variables.The proposed technique is general, and influential measures may be used for offline data or in-situ data generated during the printing process.

AUTOMATED MULTI-SPECIES CLASSIFICATION USING WILDLIFE DATASETS BASED ON DEEP LEARNING ALGORITHMS

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Abstract

The classification and identification of wildlife for monitoring and conservation purposes have become increasingly important, particularly as environmental degradation becomes a growing concern. Several studies have employed manual methods that are time-consuming, erroneous, and laborious for classification on wildlife datasets. A fully automated classification system is required to address this issue. The use of deep learning for the automatic identification of wildlife has been suggested. However, studies that compare and validate the use of different models in real-world monitoring scenarios are lacking. In this study, we collected wildlife image datasets from the Animals with Attributes repository, and we evaluated the performance of two mainstream Convolutional Neural Network (CNN) architectures, EfficientNetB0 and VGG16, in multi-species classification and identification. We deployed a multi-species classification model, based on deep-learning techniques, that could effectively recognize 37 distinct species categories. Our analysis showed that the EfficientNetB0 model outperformed the VGG16 model overall. The model was trained on a diverse dataset of 185,111 images and tested on 3,131 images, achieving over 80% accuracy and a top-5 accuracy of more than 90%. The F1-score, precision, and recall values for each species category exceeded 0.90, indicating high accuracy in identifying individual species. The model's prediction performance was validated through experimentation and through the Gradio and Tkinter interfaces, which showed the model to be highly accurate and reliable in image classification. This model could be used in various wildlife monitoring and conservation applications and could make a significant contribution to the field of computer vision. The high accuracy of the model in identifying individual species categories and its reliability in managing a large number of species categorizations make it a valuable tool for conservationists and researchers who seek to monitor and protect wildlife species.

Keywords: *Wildlife monitoring, computer vision, transfer learning, accuracy, top-5 accuracy, Gradio interface, Tkinter interface*

AUTOMATED IDENTIFICATION OF NON-INFORMATIVE IMAGES IN CAMERA TRAP DATA USING DEEP LEARNING APPROACHES

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Abstract

Camera traps are used primarily for the monitoring, conservation, and habitat management of wildlife, especially rare and endangered species. They are preferred among ecological community members who are engaged in protecting and studying the animal ecosystem. Camera traps generate a vast number of images over a given period; however, the majority of these images do not contain any animal sightings. These non-informative images, which are referred to as "garbage images" or "empty images," are irrelevant and should be eliminated during the research process. The manual process of separating these non-relevant images from those containing the desired animal sightings consumes a significant amount of time and resources, which hinders the efficiency of the research process. To address this challenge, we compiled a diverse collection of camera trap images from various locations and created a dataset consisting of 38,669 empty and 35,083 non-empty images. Additionally, we developed dataset filtering software that sorts the images into folders designated for empty and non-empty images. This software enabled the manual selection and classification of images and facilitated the creation of a large, labeled dataset. Evaluating various state-of-the-art deep learning algorithms using our custom dataset revealed that transfer learning with EfficientNet_B2 resulted in greater than 98% accuracy in distinguishing between empty and non-empty images. With these results, we have been developing an automated filtering program that utilizes deep learning models to effectively discard empty images from camera trap datasets.

Keywords: *Camera Traps, Deep Learning, Transfer Learning, Image Classification, Automated Filtering, Dataset Filtering Software, Image Processing*

REVIEW OF FIREWALL APPLICATIONS IN MULTI-CONTROLLER-BASED SOFTWARE-DEFINED NETWORKS

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Abstract

A firewall is the defensive guard of a network. It is an application that has sets of rules configured on it to prevent the network from unwanted viruses and attacks. Multi-controller techniques ensure that the firewall applications in a network function consistently. The working mechanism of a software-defined network (SDN) is based on the control and data planes. The data plane forwards packets to the targeted destinations. The control plane is the brain of an SDN. It plays a vital role in policy creation and its implementation according to defined rules or by creating new rules. Researchers around the world are working on the development of firewall applications to mitigate attacks and critical data losses (data theft and data loss) in SDNs. During this review study, we discovered that almost every research on SDN firewall applications has used a threshold limit for the number and size of packets. Conversely, very little research has been conducted on the multi-controller approach. However, there are the disadvantages of identifying packet information on a layer basis and a lack of network availability. Without packet-type information, it is difficult to identify an attacker. We compared and analyzed different methods of firewalls for securing SDNs by studying approximately 75 different studies related to SDN security. Furthermore, we provided a detailed overview and techniques for SDN protection.

Keywords: *Software-Defined Network, Multi-Controller, Firewall Application, Packet, Attack, Data plane, Control plane*

A SHORT ANALYSIS OF THE APPLICATION(S) OF INTELLIGENT AGENTS IN COMPUTER GAMES

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Abstract

The study of artificial intelligence techniques quickly moved to computer games, a sector in which they are of enormous practical utility. Artificial intelligence has advanced significantly in the last five decades. The concept of intelligent agents provides a crucial theoretical framework to compare numerous diverse methods to the smart, logical conduct of computer-controlled characters in games. Computer games represent one of the best environments for artificial intelligence research as they are typically designed to be played multiple times by many players and can thus be studied. Furthermore, advances in computer hardware have allowed game developers to create increasingly complex and engaging games that have forced computer scientists to produce even more creative solutions to complex problems.

Artificial intelligence techniques are often used to make computer games more exciting and entertaining by providing the designers with the tools they need to create interactive characters capable of responding to the player's actions. We can achieve behavior that resembles that of a human player, which is also preferred in games, by combining rationality with some restrictions on our agents' skills. In addition, we can simulate behaviors observed in humans during social interaction between individuals or groups. In this paper we interpret, analyze, and bring a simple case study for using intelligent agents for computer games. From an interpretative literature review and a case study approach, we concluded that intelligent agents could improve the gameplay experience, gain insight into Artificial Intelligence behavior, and increase game difficulty.

Keywords: *Artificial Intelligence, Intelligent Agent, Computer Games, Behavior, Social, Complexity*

STUDY OF LIGHT ANTIMATTER PRODUCTION MECHANISMS IN THE MILKY WAY GALAXY WITH AMS DETECTOR

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Abstract

The main topics of the AMS-02 physics program are the precise measurement of the cosmic rays fluxes and the search for indirect signatures of dark matter and other phenomena. Experimental data indicate that dark, non-baryonic matter of unknown composition is much more abundant than baryonic matter, accounting for a large fraction of the energy content of the Universe. Apart from antiparticles produced in the interactions of the primary cosmic rays with the interstellar medium, the annihilation of dark matter could produce additional antiproton and antideuteron fluxes. Detailed Monte Carlo simulations of AMS-02 detector response have been performed to evaluate the possibility for identification of light antimatter. Results of these studies are presented.