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Optoelectronic studies on hybrid perovskites films for solar cells applications

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Novel materials have been developed for overcoming the challenge of solar cells with low cost and high efficiency. Recently hybrid perovskites ABX₃ [A=CH₃NH₃⁺, CH=CHNH₃⁺; B= Pb⁺², Sn⁺²; X=I⁻²] solar cells have reached high power conversion efficiencies i.e. above 20% using simple manufacture methods and low temperature deposition, which have generated great interest in scientific-technological areas for the commercialization. Perovskites solar cells (PSCs) could compete respect to silicon technologies however present critical issues in thermal stability under external factors (moisture, light-oxygen, heat) as well as lack of reproducibility in fabrication methods. This work is focused on structural- optoelectronic studies on CH₃NH₃PbI₃ to understand the interface influence on the degradation process. The CH₃NH₃PbI₃ films were realized by one-step spin coating and characterized by X-ray diffraction and photoluminescence PL. The films showed a smooth surface with excellent cover on glass and high PL like have been reported in previous works. We prepared solar cells (ITO/PEDOT:SS/CH₃NH₃PbI₃/PCBM/Al) and measured current-voltage (J-V) and electrochemical impedance spectroscopy (EIS). Important differences were observed in rapid and low process (frequency) when the devices were put under illumination before IS measurements. Significant structural changes were observed by XRD. Optical studies reveal degradation mechanisms, which they are going to discuss.

Biography

M Solis de la Fuente has done his PhD from UNAM Mexico. He is currently a Post-doctoral student at LBNL, California, United States. His areas of interest are renewable energy, solar cells, light emitting diodes (LEDs), metallic oxide and semiconductor quantum dot synthesis, optoelectronic characterization hybrid perovskites, and thin films growth.

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Valorization of feather wastes as useful and environmental friendly materials

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Statement of the Problem: Poultry industry produces worldwide around 80,000,000 ton of chicken meat per year. Since feathers represent about 7-10% of the meat production, a huge amount of such waste is generated annually. Nowadays, the treatment of this left-over is associated to high environmental and economic impacts since chicken feathers are a truly waste that requires management and treatment (incineration, compost, etc.) which have a high cost compared with the near zero value of the feathers. For this reason, the proposal of commercial alternatives to valorize this waste is important to reduce the environmental impacts, increase the efficiency of using natural resources, and provide economic benefits. Our project has tackled different routes for reusing chicken feathers wastes with the aim of obtaining materials with industrial application and involving environmental benefits. The proposed solutions include the manufacture and characterization of two types of materials using or incorporating chicken feather waste in the process formulations for different final applications. Thermoplastic biocomposites including feathers could be used for manufacturing structural elements while non-woven materials could find an application niche either as bio-sorbent or as insulating barriers.

Methodology & Theoretical Orientation: Chicken feathers were stabilized by an oxidative cleaning with aqueous hydrogen peroxide and processed as filler in composite materials by using a Brabender mixer. Alternatively, the cleansed feathers were treated in a Shirley analyzer machine to remove the central quill and the resulting fibers were mixed with wool long fibers (50/50 %wt) in a card machine to obtain a non-woven material. Regarding the characterization of samples, on the one hand, tensile tests were carried out to determine mechanical properties of composites and, on the other hand, the biosorption of heavy metals and the acoustic absorption coefficient were determined.

Finding: It was possible to include up to 30% v/v of the residue in the composite and some formulations yield composites with enhanced properties. Moreover, the non-woven proved an efficient retention of metal ions such Cu²⁺.

Conclusion & Significance: Research shows that the strategies used reduce the consumption of raw materials by incorporating the properly treated waste.

Biography

Macanás J is an Associate Professor in the Department of Chemical Engineering at Universitat Politècnica de Catalunya. His present research is mainly focused on Materials Science and Nanotechnology. He has developed some metal-polymer nanocomposites with different configurations for environmental and catalytic applications. He is currently working on the valorization of several industrial residues as materials with approaches such as the reported here.

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Manufacturing of gasket sheet using paper manufacturing process without organic solvent

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This paper is about ceramic gasket manufacturing technology that can be used in extreme temperatures. This gasket is manufactured using ceramic fiber and talc as main raw materials, and inorganic content is about more than 95 percent. Therefore, gasket has thermal stability, chemical and corrosion resistance and superior properties. So the chemical plant, high pressure thermal processing, streamlines and can be used. In this study, paper manufacturing method applied for preparation of the ceramic gasket sheet and its new economic process will be discussed. Inorganic fiber, talc and binders evenly distributed in the water for manufacture the gasket. Then dehydration on the wire mesh by supplying the slurry, and compression, through drying process completed the gasket for extreme temperature. The characteristics of manufactured product during the experiment like tare density was 1.88g/cm³, tensile strength was 0.15 kg/mm², compressibility 39%, recovery 17% and ignition loss 6.55% at 1,000°C. And there was no pressure drop when subjected to 150 LB (two inch) 10 kgf/cm² nitrogen for 10 minutes. All the additives are being evenly distributed to the surface of the gasket, and each other's bonds have been completed successfully, and the applicability by paper manufacturing process.

Solvent free gasket manufacturing process

1) All gasket materials such as water-based latex, mineral fiber and fillers are easily in water and evenly distributed.

2) Was dehydration a lot of influence on the size of the cohesion within the slurry in forming process.

3) An example a continuous process for a product is as follows: Mixture of raw materials \rightarrow forming and dehydration \rightarrow third stage compression \rightarrow two stage drying \rightarrow third stage calendering \rightarrow rolling

4) New process is no odor is a clean work environment.

Acknowledgment

This subject is supported by Korea of Environmental Industry& Technology Institute(KEITI), Korea Ministry of Environment (MOE) as "Advancement of Environmental IndustryTechnology DevelopmentProgram" (PN :1485013985)

Biography

Yoonjong Yoo's Major Research Fieldare Honeycomb adsorbents for VOC, CO₂, humidity adsorption, Ceramic paper, Zeolite paper, Active carbon paper for adsorption materials, Carbon (chopped)fiber paper and mat for GDL and plane heater and Solvent free gasket manufacturing process for high temperature using. And working at Korea Institute of Energy Research(KIER).

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Visible light driven photo-active nano Ag-TiO, for coating applications

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In recent times, the use of TiO_2 for photo catalytic purposes has attracted much attention. This is mainly due to TiO_2 having many advantages over other photo catalysts. It has been proven to be nontoxic, biologically inert, physically and chemically stable against corrosion. Nevertheless, some characteristics limit the practical application of TiO_2 . TiO_2 is known to exhibit photocatalytic properties only in the presence of UV light radiation. These limit the applications of TiO_2 as coating materials since the sunlight only consists of 3% to 5% UV light. Visible light driven photo catalytic nano Ag- TiO_2 was successfully synthesized using a low temperature, facile electro less deposition technique. Various wt% of nano Ag was deposited onto commercial Degussa P25 TiO_2 nanopowders. The photo catalytic effect of the synthesized powders was studied using the UV-Vis spectrometer on the degradation profile of methylene blue (MB). Contact angle measurement was also done on Ag- TiO_2 coated steel plate to evaluate its hydrophilicity/self-cleaning effect. The results showed significant improvements in MB degradation under visible light compared to commercial TiO_2 nano powders. The amount of deposited Ag on TiO_2 (1-10wt %) was also found to have negligible effects on its degradation profile. Super hydrophilicity (self- cleaning) effects were also observed for the coated surface compared to non- coated surface.

Biography

J L Cheng completed his PhD in Materials Science and Engineering from Nanyang Technological University, Singapore and was awarded with the Ian Fergusson Fellowship at the Georgia Institute of Technology, USA. His expertise includes synthesis and characterization of nano materials for coating, thermal insulation and grease absorption applications. He is currently a Lecturer and Principal Investigator of several government agencies funded projects at the Temasek Polytechnic, Singapore.

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Preparation of leucite from analcime by ion exchange process: An experimental study

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The preparation of leucite from K⁺/Na⁺ ions exchange process of analcime in K₂CO₃ solution was studied. Abundant K⁺ in leucite after exchange is beneficial for the application in agriculture as slow release fertilizers. This is a good method to translate non water-soluble potassium resources into water-soluble potassium resources. It can solve the problem of the shortage of water-soluble potassium resources. It is also a new and popular way for the preparation of slow release fertilizers. In this study, X-ray diffraction (XRD), Fourier transformation infrared spectrometry (FTIR) and scanning electron microscopy (SEM) were utilized to characterize the as-exchanged samples. Flame photometry was applied to determine the concentrations of potassium oxide. XRD data and FTIR results determined that leucite was prepared from K⁺/Na⁺ ions exchange process of analcime in K₂CO₃ solution at 60°C, 90°C and 120°C for 1 h, 2 h, 4 h, 6 h and 10 h. The crystal structure of analcime and leucite show that potassium atoms surrounded by six oxygen atoms in leucite are located in the sites of water molecule in analcime. The preparation of leucite from analcime in K₂CO₃ solution is a reversible chemical reaction. The K⁺/Na⁺ ions exchange was stabilization at higher temperatures (90°C and 120°C) and longer time according to the K₂O contents in samples. It turned out that the reaction rate was controlled by product layer diffusion from the experiments and analysis of kinetics according to shrinking core model. It shows that the potassium oxide of samples maximum is 17.10% (in theory is 21.58%) obtained from analcime reacted with 4 mol/L K₂CO₃ solution (KAlSi₂O₆/K₂CO₃ mole ratio=1:10) at 120°C for 4 h.

Biography

Qianqian Chang is a Post-graduate student at the China University of Geosciences (Beijing) in Material Science and Engineering. Currently, she is working on the preparation of leucite from analcime by ion exchange. Leucite processed in this method is used as a slow release potassium fertilizer. Preparation of leucite from analcime by ion exchange of K⁺/Na⁺ is significant for the application of analcime in fertilizers, which can not only supply the necessary potassium element to plants and enhance dissolution of the rock phosphate, but also can reduce the loss of nutrients and water as well as the environmental pollutions compared to traditional chemical fertilizers.

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Preparation and luminescent properties of orange reddish emitting phosphor KCaBi(PO₄),:Sm³⁺

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A novel orange reddish light emitting phosphor KCaBi(PO4)₂:Sm³⁺ for UV excitations has been synthesized by the solid state reaction technique. The powder X-ray diffraction patterns and XPS were utilized to confirm the phase composite and crystal structure. The excitation and emission spectra, decay curves and chromaticity coordinates of the as-prepared phosphors were characterized to investigate the photoluminescence properties for application in white light-emitting diodes. The results revealed that the KCaBi(PO4)₂:Sm³⁺ phosphors can be effectively assimilated with near ultraviolet excitation at 405 nm, and exhibit four emission bands originating from the ${}^{4}G_{2}{}^{-6}H_{J}(J=5/2, 7/2, 9/2 \text{ and } 11/2)$ transitions of Sm³⁺ ions. The concentration quenching mechanism was verified as dipole-dipole interaction. Additional, KCaBi(PO₄)₂:0.04Sm³⁺ has a better thermal stability and the prepared samples have a potential application in w-LEDs.

Biography

Mi R Y is a PhD student studying at the School of Materials Science and Technology, China University of Geosciences Beijing. She has her expertise in design and structural analysis of the novel rare earth doped phosphors, controllable preparation and luminescence properties of phosphate materials applied for the w-LED and solar cells.

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Synthesis of nano-analcime with potassic hornblende syenite by direct alkali-hydrothermal treatment

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Synthesis analcime with natural minerals and rocks has the characteristics of low raw material price and short synthesis time. The synthesic analcime was considered as promising materials for in situ recovery of contaminated soils. Analcime zeolite in nanometer scale was synthesized using alkali-hydrothermal treatment with potassic hornblende syenite as source of silica and alumina. Both the raw materials and the final products were characterized using X-ray diffraction (XRD), scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR). XRD results of the hornblende syenite exhibited microcline and plagioclase as main mineral components. Nano-analcime (nano-ANA) was obtained after 4 h hydrothermal-treatment at temperature of 240°C in 3.5 M NaOH solution. Higher NaOH concentration and longer reaction time led to decrease in the amount of analcime phase with corresponding increase in hydroxycancrinite. SEM images of the analcime crystals showed the formation of trapezohedral morphology with the size ranging from 300 nm to 600 nm. The dynamic light scattering (DLS) analysis demonstrated the average crystal size of the synthesized analcime was 410 nm. The results showed that the readily available potassic syenite could be used to prepare nano-ANA with good crystallinity in a short reaction time as well as leaching potassium to solve the problem of potassium resources deficiency in China. The results also indicate that the crystalline analcime can be prepared using natural quartz syenite as an economic raw material.

Biography

Qi Yuxiang is pursuing his Master's degree from the China University of Geoscience. His research focuses on comprehensive utilization of mineral resources, such as hydrothermal synthesis of zeolite, stabilization of heavy metals in soils or waste water using synthetic zeolite.

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Angle-insensitive multicolor display device based on phase change materials

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Reflective type display device based on phase change materials is attractive because of the ultrafast response time and high resolution compared to conventional display device. We demonstrate a unique device in that tunable three colors can be obtained on a single device by the sequential crystallization of double phase change materials. Without the need for RGB (red, green and blue) color filter or spatially modulated color scheme, the color can be clearly and continuously modulated optically. The optical contrast is optimized by calculation. The device has a low sensitivity to the angle of incidence and requires ultrathin phase change materials for visible light. The structure has the potential for a variety of applications, such us wearable devices, ultrafast solid-state displays and implantable displays in human bodies.

Biography

Hongkai Ji has his expertise in phase change memory and phase change materials-based displays. He has constructed a model to evaluate the color performance and improved the color depth modulation capability of phase change materials-based displays. In phase change memory field, he has employed the Hydrogen Silsesquioxane (HSQ) electron resist as insulating material to reduce the preparation process.

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Gate-tunable Schottky junction solar cells with light transparent and electric-field permeable graphene mesh on n-Si

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Schottky junction solar cells (SJSCs) that utilize a built-in potential across metal-semiconductors or metal-insulator-semiconductors have an advantage over standard p-n junction solar cells in that complementary doping is not indispensable for a Schottky junction. Recently, the SJSCs made with graphene electrodes, intended to replace vacuum-evaporated metal grids, have attracted interest due to their high power conversion efficiency (PCE), simple structure and easy fabrication process. Graphene is advantageous over normal metal grids, in that the optically active built-in potential can be developed over regions just beneath the graphene. Despite of the rapid enhancement in power conversion efficiency (PCE) of graphene-on-silicon Schottky junction solar cells (Gr-Si SJSCs), it is still lower than the best record for Au/Si Schottky junction solar cells, indicating that there remains lots of room for improvement. Herein, we introduce a new approach for modulating the interface potential of the SJSCs by applying an external gate voltage (Vg) to the Gr-Si SJSCs for improving the efficiency. Specially, by replacing the graphene with graphene mesh, we have demonstrated: (1) higher PCE values at Vg in the range of 0V to -1V; and (2) more rapid enhancement of PCE values with varied Vg (from 7.9% to 11.2%). We further found that the PEC values were hardly saturated and increased continuously until Vg=-1 V. This result illustrates that the PCE can be further improved by introducing dielectric materials with higher dielectric strength. This approach, which exploits the light transparent and electric-field permeable electrodes, would be applicable to many types of energy-conversion devices. Moreover, this work provides new opportunities to reach the maximum theoretical efficiency limits, such as the Shockley-Queisser limit of solar cells.

Biography

Won II Park is an Associate Professor in Material Science and Engineering, Hanyang University. He received his PhD degree in Material Sciences and Engineering from POSTECH in 2005, and joined Liber group of Harvard University as a Post-doctoral Fellow from 2005 to 2007. His present research interests are synthesis and characterization of semiconductor nanostructures such as nanowires, nanorods and 2D materials, and development of nanoscale photonic and electronic devices.

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Characterization and stability of TiO, nanoparticles in industrial dye stuff effluent

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S tability studies were conducted in different solutions (deionized water (DI), NaCl, CaCl₂ and MgCl₂) at different pH. Agglomeration and zeta potential was influenced by ionic strength, type of electrolyte and the presence of dye stuff. The DLVO theory was used to analyze the stability and/or agglomeration of the nanoparticles in the different solutions. Repulsive or attractive forces stipulated by the DLVO theory were used to quantitatively discuss the results. The increase in ionic strength increased agglomeration which was linked to pHPzc, as there were minimal electrostatic repulsions at the pzc, yet the attractive van der Waals forces were dominant. Addition of the dye stuff significantly decreased the agglomeration as the dye stuff changed the overall zeta potential of TiO₂ nanoparticles to negative across the entire pH which improved stability as there were particle-particle repulsions. Monovalent and divalent cations were compared and Ca²⁺ increased the mean diameter of nanoparticles as it effectively decreased the EDL of the nanoparticles, thus enhancing agglomeration. The DLVO theory was successful at explaining, in terms of the interaction energies between nanoparticles, the phenomena that caused either agglomeration or stability of the as-synthesized TiO₂ nanoparticles in the different solutions.

Biography

L N Dlamini has his expertise in synthesis and application of nanomaterials used as photocatalyst in the remediation of pollutants in water. His research also focuses on the understating the fate and behavior of nanomaterials in surface water and also in waste water treatment plant. He, not only conducts research, but also lectures to undergraduates and postgraduate students at the University of Johannesburg. He lectures general chemistry, organic chemistry and materials. He is also involved in high school science, where he teaches lower grades and upper classes.

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Effect of binder on adsorption of cesium on silica gel containing embedded phosphotungstic acid

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Statement of the Problem: Radioactive isotopes ¹³⁴Cs and ¹³⁷Cs are among the most hazardous contaminants that can be released into the environment byaccidents at nuclear power plants (e.g. the Fukushima accident) or small incidents, which may occur during fissile materials processing. Currently, the development of materials that can adsorb Cs⁺ selectively in the presence of Na⁺ and K⁺ is a challenging problem. While other hazardous isotopes, e.g., ⁶⁰Co or ⁹⁰Sr, can be separated easily due to the insolubility of many of their salts, most compounds of cesium are soluble and highly mobile in aqueous media. The objective of this work is the synthesis and study of superacidic adsorbents for removal of Cs⁺ ions from contaminated waters.

Method: The active ingredient of the adsorbents was synthesized by co-condensation of tetraethoxysilane with phosphotungstic acid by the sol-gel method. Its formulations with γ -Al₂O₃, kaolin and charcoal were prepared with 10-50 wt% of the binders. Their granulating was conducted by tableting at the pressure of 7 metric tons and the separation of 1-2 mm fraction. All adsorbents were characterized by FT-IR spectroscopy, porosimetry, SEM, DLS and thermoanalysis.

Results: The obtained silica gel with embedded phosphotungstic acid had a mesoporous structure with a significant fraction of micropores. The adsorbent was present mostly in the form of nanoparticles, however, part of the material agglomerated. It demonstrated a high adsorption capacity towards cesium. Comparison of its formulations with different binders demonstrated their effectiveness in adsorption at much higher mechanical strength. Kinetics of the adsorption was studied. A significant advantage of H-PTA/SiO₂ is its stability against leaching.

Conclusion & Significance: A hybrid functionalized material containing phosphotungstic acid embedded into a silica network was successfully synthesized and studied. The obtained data could be used in the development of an adsorbent for the removal of radioactive cesium from nuclear wastes or contaminated water.

Biography

Aleksey Vasiliev has completed his PhD from the Institute of Bioorganic Chemistry and Petrochemistry in Ukraine. His main field of expertise is materials chemistry, in particular, chemistry of mesoporous and microporous materials. He continued his professional career in the National Technological University in Argentina, and further moved to Rutgers University. Currently, he is working as an Associate Professor in East Tennessee State University.

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A highly efficient photoanode for enhancing degradation of the azo dye and electricity generation of dualphotoelectrode photocatalytic fuel cell

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ischarging organic matters into water bodies directly not only causes serious environment pollution but also wastes energy source. A visible light driven photocatalytic fuel cell (PFC) system comprised of photoanode and photocathode/cathode was established for organic matters decomposition and electricity generation. Under visible illumination, the PFC system is driven by mismatch Fermi levels between photoelectrodes with an interior bias can be produced. The photogenerated electrons of photoanode were excited and transferred to combine with photogenerated holes of photocathode through the external circuit. Meanwhile, the photoanode provides a negative bias for photocathode; in contrast, the photocathode provides a positive bias for photoanode then generates electricity. At the same time, the organic matters decomposed by photogenerated holes stay in photoanode. In this study, we investigated the photoanode modification by Ni-Fe layered double hydroxide (NiFe-LDH) for enhancing the photocatalytic fuel cell (PFC) using Cu₂O/Cu photocathode. The experimental results show that the NiFe-LDH/BiVO4 photoanode obtains a photocurrent density of 0.620 mA/cm² at 1 V vs. SCE in 0.5 M sodium sulfate (Na SO4) as the electrolyte exposed under AM 1.5 solar light. The highest short-circuit current, open-circuit voltage and maximum power density of the NiFe-LDH/BiVO4-Cu_O/CuPFC are 0.251 mA/cm², 0.742 V, 0.186 mW/cm², respectively. For tests using methylene blue and Na SO4 as the model organic substrate and supporting electrolyte, respectively, NiFe-LDH/BiVO4-Cu_O/CuPFC achieves a degradation efficiency of 81%. The NiFe-LDH/BiVO4 photoanode effectively improves the performance of the PFC in terms of wastewater degradation rate and electricity generation. The experimental results show that the proposed heterojunction photoanode can decrease the interface recombination at the NiFe-LDH/ BiVO4 junction and extend the spectrum of visible light absorption. It is attributed to enhanced connectivity of BiVO4 particles by the NiFe-LDH layer to avoid loss of the photoexcited electrons.

Biography

He Yun is a final year PhD student from Professor Michael Leung's group, City University of Hong Kong. She is doing her research on photoelectrochemical system and photocatalytic fuel cell.

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MATERIALS SCIENCE AND ENGINEERING

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Preparation of zeolite for slow-release fertilizer using K-feldspar powder

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The 30-50% of crop yields is attributed to the commercial chemical fertilizers according to conservative estimation. Abuse of L chemical fertilizers causes serious contamination and environmental hazards, and very low amount of nutrition is absorbed by the plants. The utilization of slow release fertilizer can slow down the migration rate of nutritional elements, which is beneficial to the improvement of fertilizer use efficiency and production, as well as the decrease of soil contamination. The global demand of potash has exceeded 32 million metric tons of K.O in current time and will have a continuous increase in the coming decade potassium-bearing framework aluminosilicate minerals have been proposed as a substitute source of potassium. As a kind of K-zeolite, zeolite F still provide K element necessary to the growth of plants and amend soil besides the function of retaining water and nutrition. Synthesis of F zeolites from K-feldspar is one of the promising applications of K elements in soil. The X-ray diffraction (XRD) patterns of zeolite F(KALSiO4.1.5 H₀O) obtained by the hydrothermal method after the fusing of K-feldspar. All of the diffraction peaks can be basically indexed to the tetragonal phases of zeolite F (JCPDS file 38-0216) as shown in Figure 1a. The strongest peak of zeolite F at 30.17° is assigned to its (114) crystal plane. We can see the morphology of zeolite F from Figure 1b that presents tetragonal cross-shaped composed of rectangular sheet. According to the test of water solubility, accumulative release of K₂O can be fitted by the equation as follows: y=0.6349-0.0157ln(x-0.994), where y is accumulative release of K O (%) and x is test time (days); and the correlation coefficient R²=0.991. which indicates the release of zeolite F belongs to Elovich equation. By the observation and prediction of Figure 1a, the accumulative release of K₀O reaches 68.97% after water solubility testing for 42 days, 72.09% for 240 days, and 72.75% for 365 days, respectively, indicating the sample could be used as a long-term slow-release potassium fertilizer with nutrient K₂O release.

Biography

Jiangyan Yuan has her expertise in Material Science and Engineering. Her research interests consist of comprehensive utilization and green processing of mineral resources, such as hydrothermal leaching of valuable elements, hydrothermal synthesis of zeolite; crystal structure transformation; and preparation and characterization of nano-materials as well as their application.

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Raman microspectroscopy in dental research

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Raman spectroscopy is very useful method to study the biological materials including teeth. In our research we used the Raman microspectroscopy to study the compositional and structural analysis of raw and prepared dental hard tissues. All the measurements were carried out on inVia Renishaw micro-Raman system with diode pumped laser emitting 785 nm near-infrared wavelengths. Raman microscope was helpful in the research of total surface energy values of teeth fragments (enamel, crown dentin and root dentin) with the use of inverse gas chromatography, to determine the surface changes of wet and dry bovine teeth tissues at microstructural level. In Raman spectra of wet and dry enamel, root and crown dentin some slight differences connected with water occurring are visible. For wet tissues, broad but weak band in region from 3000 to 3600 cm⁻¹ assigned to stretching mode of OH⁻ groups is observed. Moreover, Raman microscope was effective for enamel and dentin characterization after surface preparation with the use of commercial 3-component etch-and-rinse bonding system. Raman spectroscopy allowed to determine the surface changes of hard tissue after each step of preparation (application of etchant, primer, adhesive and photopolymerization). There are no changes observed in the Raman spectra of dentin and enamel after etching. In the Raman spectra of all analyzed teeth tissues after application of primer and adhesive bands corresponding to functional groups present in compounds of these both bonding system components are observed. Presented analysis of surface composition changes after each step of enamel and dentine preparation confirms that the process was successfully conducted.

Biography

Tomasz Buchwald has worked as a Research Assistant in the Faculty of Technical Physics at Poznan University of Technology (Poland). A major area of his interest focuses on the application of spectroscopic methods, especially Raman spectroscopy, in analysis of biological materials and biomaterials properties. His current research interest is dental materials and human teeth affected by caries. He has published 16 articles in SCI Journals concerning mainly the determination of materials properties by use of Raman microspectroscopy.

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Inverse gas chromatography - A novel method for the examination of bond strength between tooth hard tissues and restorative materials

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Strong and durable connection between the remaining tooth hard tissues (dentin and enamel) and artificial materials applied to fill the cavity after caries removal is crucial to restore the teeth functions, e.g. biting or chewing. This bond strength is usually measured with the use of shear bond strength (SBS) tests that require a large number of healthy tooth hard tissues directly connected with the restorative material. The alternative proposed possibility consists of estimating the work of adhesion between dentin or enamel and restorative material with the use inverse gas chromatography (IGC). This method exploits the dependency between the values of surface energy of both connected materials and the strength of this connection. In this work the connection strength between bovine dentin and enamel and an exemplary restorative material was investigated by means of direct (SBS tests) and indirect (IGC) methods. For this purpose raw bovine tooth hard tissues were prepared according to the standard dental procedure with the use of commercial etch-and-rinse 3-component bonding system and characterized. After that procedure dentin and enamel samples, as well as restorative material samples were placed inside the chromatographic column and their surface energy values were measured. The same materials were also connected together and subsequently disconnected in SBS test giving the direct bond strength values. The obtained results show a clear dependency between the bond strength values measured by these two methods what show a great potential of inverse gas chromatography in bonding strength tests. IGC can also play a significant role in the designing of the dental materials and bonding system properties.

Biography

Zuzanna Okulus has completed her PhD in Chemistry from Poznan University of Technology (Poznan, Poland) in 2017. She is interested in materials science and engineering, especially for dental applications. Her research is focused on the preparation and characterization of new composite materials for potential dental applications. Her current research interests are tooth hard tissues characterization, inverse gas chromatography and spectroscopy, especially the application of these methods in the biomaterials research. She has published 10 papers in SCI journals concerning mainly the characteristics of experimental dental composites with calcium phosphates fillers, characterization of tooth hard tissues and application of Raman spectroscopy and inverse gas chromatography in dental materials research.

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Study on deposition rate and microstructure of niobium coating prepared by CVD from niobium pentafluoride

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Niebium is a metal with high thermal conductivity, high melting point, corrosion resistance, and low neutron capture cross section, which is a kind of material which is very suitable for atomic energy reactor. Adding a layer of niobium to the metal inner tube wall allows it to get a better performance for a wider range of applications. The study of the deposition rate and morphology of niobium deposition in the inner wall of the metal is of great significance for the application of niobium. In this experiment, we used niobium pentafluoride as a precursor to prepare a pure niobium coating in the inner wall by chemical vapor deposition, which was carried out in a stainless steel tube. By hydrogen reduction of niobium pentafluoride, we got a pure niobium coating on the stainless steel inner tube wall, as shown in Figure 1. After microscopic observation and SEM scanning analysis of the niobium coating, we confirmed that the niobium coating prepared was dense, high purity and uniform thickness. And it is easy to find that there was a transition layer between substrate and niobium coating, which means the coating and the substrate tightly bonded. The microstructure of niobium coating showed irregular fine grain substrate closed region and more regular columnar region and it showed a typical preferred growth mechanism. After experiment, we cut the tube along its axis to measure the thickness or deposition rate of the niobium coating at different parts of the inner wall. Figure 2(a) showed the distribution of deposition rate and temperature along the airflow direction, which was obtained by optical microscopy and thermocouple. The data obtained illustrated that the deposition rate of the coating was not only closely related to the temperature but also with the gas environment, the fastest deposition rate and dense niobium coating were obtained in the area 40-55 mm of the inner wall.

Biography

Mingmin Zheng has his expertise in the preparation of protective coating on metal surface. His major study is based on metal inner tube wall with deposited niobium coating and its kinetics and nucleation mechanism during the deposition. He has successfully obtained a pure thickness of niobium coating by hydrogen reduction of niobium pentafluoride chemical vapor deposition.

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MATERIALS SCIENCE AND ENGINEERING

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Effect of reduced graphene oxide on the mechanical, thermal and electrical properties of epoxy

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Graphene has attracted intense scientific interest over the last decade due to its outstanding electrical, mechanical and thermal properties. This work aims to investigate the effect of reduced graphene oxide (RGO) on the structure and properties of epoxy. Graphite powder was oxidized and exfoliated to produce graphene oxide (GO). GO was then reduced to RGO by a thermal reduction procedure using a high temperature. Epoxy-RGO nanocomposites were prepared by mixing epoxy resin with RGO in the presence of a solvent, tetrahydrofuran. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM) were performed to characterize the structure and morphology of the graphene-based nanosheets and nanocomposites. The characteristic peaks for the functional groups of both RGO and the polymer matrix were found in the FT-IR spectra of nanocomposites. The interlayer spacing of RGO increased in nanocomposites according to the XRD results. SEM images elucidated that there was a relatively good dispersion of graphene in epoxy matrix. The incorporation of graphene into epoxy matrix raised the Young's modulus from 2.71 GPa up to 3.56 GPa (ca 35%) at 1.0 wt.% RGO. It increased the degradation temperate at 50% weight loss from 412 to 433°C. The thermal conductivity of epoxy was improved by up to 85%, reaching the maximum value of 0.36 W m⁻¹ K⁻¹ at 1.0 wt.% RGO. The same addition also significantly improved the electrical conductivity of epoxy. These epoxy-RGO nanocomposites could be explored for applications such as anti-corrosive, electrostatic-dissipative, electromagnetic interference shielding and sensing applications.

Biography

Ahmed Alzahrany is a PhD student in the Department of Materials Science and Engineering at the University of Sheffield. He received a BS degree in Mechanical Engineering from King Saud University and the MSc in Mechanical Engineering from the University of Portsmouth in 2009. He has been active in the area of materials science for over 10 years and has worked at Saudi Standards, Metrology and Quality Organization for 18 years. He was the Director of Laboratories in SASO. His current research involves the study of the integration of graphene nanosheets into polymer to improve their properties.

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MATERIALS SCIENCE AND ENGINEERING

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Solar cell: Photochemical cells based on dye sensitization of titanium dioxide and with indium tin oxide as a conductor

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The dye sensitized solar cell (DSSC) is a new type of solar cell which converts the visible light into electricity, by using indium tin L oxide (ITO) and photo electrochemical system. A photo electrochemical solar cell that is based on the dye sensitization of thin microcrystalline films of titanium dioxide (TiO₂) nanoparticles in touch with a liquid electrolyte solution is tested. The main task of the project is to build a photochemical dye sensitized solar cell based on materials that are inexpensive and highly efficient in solar energy conversion by using ITO and TiO₂. The building process of the cell was started with the two conductive glass plate coated with ITO. However, a thin layer of Titanium dioxide TiO, is applied on the conductive side of one glass plate and the other side of the conductive glass plate is coated with graphite. A number of dyes such as natural strawberry and blue berries has been tested and then applied on the thin layer of TiO, and then the two conductive glass plates are stacked together to be a complete cell. A few drops of electrolyte solution such as pure iodine crystal, potassium iodide as well as ethylene glycol been added between the two conductive glass plates, a thin layer of titanium dioxide and a layer of graphite. The operational principle of the cell has been recorded through the measurement of the cell by emitting all wavelengths in the visible spectrum propagating from sunlight and exhibited steady voltage and current at much higher level for approximately 230 mv for the cell dimension 2.5 cm x 2.5 cm. During the testing cell we have got a problem with the nature of the electrolyte solution can undergo evaporation, leaking, charge separation at the titanium dioxide. For this kind of cells we recommend to use filters to decrease the amount of heat reaching the cell. However, recommendations for the future to improve the cell are made with using quantum dots. Quantum dots have the advantages of providing tunable band gaps and the ability to absorb specific wavelength from the solar spectrum.

Biography

Ari A Mohammed received his BSc degree in Physics from the University of Duhok, Iraq, in 2008, and started teaching physics for multiple academic levels including high school. In 2012, he earned his MSC degree in Physics from the University of Pune, India. He has joined the Department of Physics from the University of Zakho as a Lecturer to teach physics for the undergraduate students and has joined a team of researcher in the field of Material Science. His researches focus in the field of material science and nuclear physics; he has a special interest in the field of Astronomy and Astrophysics also.

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Preparation and properties of protective coating on inner surface of nickel-based alloy tube

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Thorium molten salt reactor (TMSR) is one of key reactors of the generation IV in nuclear power system, and molten salt is used as fuel and coolant in TMSR, therefore it has been put forward a higher requirement for the anti-corrosion ability of tubular structural components in molten salt. In this study, the pulse electroplating was used to obtain pure nickel coating on the inner surface of tubular structural material to improve the corrosion resistance of nickel alloy, however, electroplating on the inner surface of tube is not easy to implement, for example the current is shielded and the anode is deactivated easily, in order to solve these problems we used the inner anode and controlled the deposition time at the same time. Pure nickel coating was successfully obtained and the microstructure and properties of coating were analyzed simultaneously. The thickness, hardness and microstructure of coating were observed by metallographic microscope, macro-hardness tester and field emission scanning electron microscope, and the influence of different deposition durations and annealing treatment durations on properties were analyzed, in the meantime, the thermal shock test was investigated that aim to analyze the adhesion of coating. The results showed that the coating became rough as well. The hardness of coating increased at first but decreased finally with the increased of duration. However, the change of hardness was not obvious after annealing. The thermal shock test showed that the coating had good thermal shock resistance and good bonding strength.

Biography

Yanhong Liu has her expertise in surface technology and materials about coating. Her research is based on surface and coating technology for improving the overall performance of materials. She used electrochemistry method to get surface protective coating on energy materials. She was doing research on the surface technology used in the field of nuclear power and new energy field as well. She and her team aims to improve the properties of anti-oxidation and anticorrosion of zirconium alloy cladding using surface technology.

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MATERIALS SCIENCE AND ENGINEERING

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SPECIFIC POLYMERS – Value your research work in functional polymers. From your proofs of concept to hundred grams' polymers

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ver the past decades, intensive academic research work has been achieved in the field of polymer chemistry in order to developed tomorrow's materials. Researches focussed on new polymerization technics (ARTP, RAFT, NMP controlled radical polymerizations), new architectures (block, graft, stars, etc.), innovative crosslinking reactions, hybrid materials, biobased and sustainable materials, smart responsive materials, etc. Even if most of the studies performed at the academic level highlight the most brilliant ideas and reveal outstanding results, there development towards higher technology readiness level is often blocked or slowed by the inability of the research laboratory to produce enough matter to validate proof of concept at pilot, semi-industrial or industrial scale. SPECIFIC POLYMERS company has been built up in 2003 to fill the gap in between academic and industrial researchers. For more than 14 years, the company has performed research and development services, on-demand synthesis and up-scaled production from grams to kilograms. The main goal of the innovative product developed by SPECIFIC POLYMERS is to support academic and industrial partners in the production of functional (macro)molecules to validate proof of concepts. During this period, the company has developed the synthesis of more than 10.000 functional building blocks, monomers and polymers and is now working with more than 500 customers and partners in more than 35 countries worldwide. Main research topics of the company are Polymer Science, Biobased Materials, Hybrid Materials and Composites, Polymers for Biomedical Applications and Polymers for Opto-Electronic. Thus, SPECIFIC POLYMERS is involved in all field of applications such as surface finishing (glass, metal, nanoparticles, plastics), aeronautic, automotive, pharmaceutical industry, cosmetic, electronic, optic or energy. SPECIFIC POLYMERS exists to help you bringing your ideas one step further.

Biography

Cédric Loubat earned his PhD degree in Polymer Chemistry from University of Montpellier (Pr B. Boutevin FRANCE) in 2000. In 2003, Dr. Loubat created SPECIFIC POLYMERS with the aim to fill a gap between academic and industrial researches in the field of polymer chemistry. Indeed, most of the scientific innovations generated within academic researchers were often nipped in the bud since these laboratories do not have the abilities to produced intermediate-scales batches to validate proofs of concept.Nowadays, Dr. Loubat is still heading SPECIFIC POLYMERS (www.specificpolymers.fr) and the company has 12 employees. SPECIFIC POLYMERS works with more than 500 customers located all over the world. In 15 years, SPECIFIC POLYMERS synthesized functional monomers, oligomers and polymers at the grams to kilograms scale (more than 10 000 (macro)molecules have been synthesized in 15 years and 1 000 are now part of SPECIFIC POLYMERS catalog) in all fields of application.

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MATERIALS SCIENCE AND ENGINEERING

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Response of S-phase to Rapid Annealing

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A ISI 316 stainless steelis commonly used in many fields due to its excellent corrosion resistance and good bio-compatibility. However, AISI 316 stainless steel has limitations with regard to low hardness, poor tribological and tribochemical performances. Low temperature plasma nitriding treatment provides an opportunity to significantly improve its hardness and wear resistance without affecting the corrosion resistance by the formation of S-phase. However S-phase is thermodynamically metastable and will decompose into stable phases under certain conditions(Thaiwatthana, Li et al. 2002). Thus, the aim of this study is to investigate the response of S-phase to rapid annealing and to explore the possibility to develop new materials by intentional, controlled decomposition of S-phase. Nitrogen S-phase was formed by low temperature plasma nitriding. Rapid annealing in Gleeble machine was carried on at 440°C, 490°C,540°C and 590°C respectively. The annealed samples were characterised by XRD, SEM and GDS and its properties were evaluated by hardness, electrochemical corrosion and reciprocating wear tests. The results showed that nitrides precipitation began at 540°C for the nitrogen S-phaseafter rapid annealing.Rapid annealing could maintain high nitrogen content at the surface of S-phase. Hence the annealed samples still possessed a relatively high hardness in comparison to untreated samples.No discernible change was observed on the thickness after rapid annealing.Due to the influence of the oxide film covering on nitrogen S-phase, the corrosion resistance deteriorated following rapid annealing. However, little change in the wear ratewas observed, prior to precipitation of nitrides. Although a new material with superior properties did not obtained by this feasibility study, the systematic investigation has advanced scientific understanding on the stability of S-phase.

Biography

I graduated with a master's degree in Material Science from the University of Birmingham in 2015 worked on the stability of S-phase. I am now working towards my PhD in the IMPaCT Doctoral Training Centre under the supervision of Professor Hanshan Dong. My project is focussed on the surface multi-functionalization of carbon fibers using active-screen plasma treatment. The hope is that this work can help to enhance the fibre/matrix interfacial adhesion and the interfacial shear strength (IFSS) between the reinforcing fibres and the matrix in composites

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Functional surfaces - Development of innovative products

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Surfaces and their properties are playing an increasingly important role in industry application. In general, materials are used according to their property requirements such as elasticity, strength, heat resistance or to meet other requirements such as corrosion resistance. However, traditional surfaces are often not able to meet the ever increasing demands of today's applications in automotive, textile, medical and food industry. Thus, in recent years, advances have been made using functional coatings to exceed limitations of material to make surfaces more attractive for specific industry applications. Hygienic and efficient automation technologies are key aspects for a successful production process for example in the food and beverage industry. Requirements regarding the cleanability and durability of surfaces that are in food contact are important factors. The approach of this study was to design functional surfaces with easy to clean and/ or self-cleaning coatings that enable automation components to be easily or less cleaned. For coating procedure physical vapor deposition was carried out in order to facilitate separation of the vaporized coating material to the substrate. Substrates used are aluminum, stainless steel and plastics for example polyamide or polyethylene. Analytical description of surface characteristics was performed using scanning electron microscopy, contact angel and roughness. Different surfaces were successfully coated with easy to clean coatings and characterized analytically. In addition, coating of automation components consisting of different materials was realized and coating adhesion was improved. First application tests showed a clear improvement of material properties relating to chemical resistance and cleanability compared to today's standard materials used.

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Coupled thermal-mechanical simulation for continuous casting of lightweight alloys

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The numerical simulations of industrial continuous and semi-continuous casting process for lightweight alloys have been used L extensively to investigate the optimization of casting billets with high quality within relatively low operating cost and energy. The thermal evolution during the casting process and the industrial trend to control the rate of heat transfer coefficient (HTC) during both start-up and during-casting phases has been broadly studied. However, the estimation of HTC values during air, contact and water/oil cooling and the implementation of thermal and mechanical phenomena during casting process have relatively received little attention. The development of advanced numerical techniques (including multi-physical and evolving domain techniques) for thorough process simulation of the melt flow, heat transfer and evolution of stress/strain and damage during casting process has promoted many new opportunities. However, smarter and broader improvements are needed to capture the underlying physical and chemical phenomena including multi-physical transient fluid-thermal-mechanical coupling and heat-transfer changes during the process. For the starting-cast condition where most of mechanical cracking and damage are initiating, there have been many efforts to control mechanical defects by optimizing casting recipes. The concerns about cast billet quality and the minimization of hot tearing, cold cracking, and shrinkage dimensional control are part of casting quality control. Within this framework, the cooling system numerical simulation including its fluid flow and its characteristics (turbulence, free surface boundaries, etc.) heat transfer have to be modeled. In the research work herein, parallel experimental-numerical studies of coupled transient thermal-mechanical phenomena including HTC estimation using empirical and reverse analyses are presented. The phase change modeling during semi-continuous casting process including liquid and solid interface, and also implementation of dynamic HTC curves are also considered. One of the main contributions of this paper is to show the applicability and reliability of newly developed coupled thermal-mechanical numerical simulation approach for the optimization of continuous and semi-continuous casting process.

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MATERIALS SCIENCE AND ENGINEERING

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Low-cost, high-performance, single-crystal-like device layers and controlled self-assembly of nanostructures within device layers for wide-ranging energy and electronic applications

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 \mathbf{F} fabrication of single-crystal form of the relevant material is too expensive. In addition, for many applications, very long or wide materials are required a regime not accessible by conventional single-crystal growth. This necessitates the use of artificially fabricated, large-area, single-crystal-like substrates suitable for heteroepitaxial growth of the relevant advanced material for the electronic or energy application in question. In this talk, details of the fabrication of such substrates will be provided. Heteroepitaxial growth of nanolaminate multilayers and devices on such substrates using a variety of deposition techniques such as pulsed laser ablation, sputtering, e-beam evaporation, MBE, MOCVD, and chemical solution deposition will be reported upon. Application areas that have been demonstrated via the use of such artificial substrates include – oxide high-temperature superconductors, semiconductor materials (Si, Ge, GaAs, CdTe and Cu₂O), ferroelectrics (BaTiO₃), multiferroics (BiFeO₃), etc. In addition, strain-driven self-assembly of second phase nanomaterials at nanoscale spacing has been demonstrated within device layers. Control of heteroepitaxy in lattice-mismatched systems and the effects of strain on self-assembly will be discussed. Such heteroepitaxial device layers on large-area, single-crystal-like artificial substrates are quite promising for a range of electrical and electronic applications.

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Cell loaded hydrogels as advanced bioinks for 3D printing

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Inree-dimensional bioprinting is the process of extruding cells with or without the addition of materials in a precise spatial arrangement towards tissue substitutes. Yet bioprinting bears some limitations, mainly the selection of materials to be used as bioinks. Among others, bioinks must be able to mimic native tissue microenvironment and protect cells from the shear-stress to which they are submitted during printing process, without compromising the resolution, shape and stability of the tissue construct. These features are common for injectable hydrogels, which are 3D hydrophilic networks that facilitate oxygen, nutrients and growth factors diffusion and partially mimic tissue physical characteristics. Some examples of natural-derived materials include decellularized tissue, gelatin, fibrin, collagen and alginate. Nevertheless, the gelification kinetic of current proposed bioinks is impairing the printability of tissue constructs. Pectin can be considered a novel and versatile biomaterial as its favorable properties, including swelling, degradation, cell immobilization, and binding or release of bioactive molecules can be tailored by the crosslinking mechanisms and agent. Herein, an innovative injectable pectin hydrogel encapsulating human adipose stem cells is proposed. Gelation kinetics, viscosity and shear-thinning properties could be finely tailored by controlling pH, pectin concentration and gelifying methods. Gelification time of the developed hydrogels ranged from seconds to 20 minutes, accordingly with the adopted conditions, therefore offering a suitable time window to prevent the collapse of the gel post-printing. Additionally, the obtained viscosity is within the range of the different bioprinting techniques, namely inkjet, orifice-free and extrusion. Their injectable potential was confirmed through rheological analyses. Upon extrusion through 20G and 25G needles, cells encapsulated within pectin hydrogels were viable and kept their stemness capability up to 7 days after extrusion, indicating that the presence of 3D pectin hydrogels protects cells from damaging during the printing process. In this sense, a ready-to-use and inexpensive pectin hydrogel is herein proposed as a bioink for 3D bioprinting tissues.

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MATERIALS SCIENCE AND ENGINEERING

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NIR-triggered, on-demand drug delivery using lanthanide-doped upconverting nanolamps

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Localized and recurring delivery of drugs in the hour of need is of great importance in many clinical conditions such as in the treatment of solid tumors, post-surgical wounds and localized infections. This helps increase the drug efficacy and minimize the side effects of anesthetics. Lanthanide-doped upconverting nanoparticles (UCNPs) have emerged as excellent nanotransducers for converting longer wavelength near-infrared (NIR) light to shorter wavelengths spanning the ultraviolet (UV) to the visible (Vis) regions of the spectrum via a multiphoton absorption process, known as upconversion. Here, we report the development of NIR to UV–Vis–NIR UCNPs consisting of LiYF₄:Yb₃/Tm₃@SiO₂ individually coated with a 10±2 nm layer of chitosan (CH) hydrogel cross-linked with a photocleavable cross-linker (PhL). We encapsulated fluorescent-bovine serum albumin (FITC-BSA) inside the gel. Under 980 nm excitation, the upconverted UV emission cleaves the PhL cross-links and instantaneously liberates the FITC-BSA under 2 cm thick tissue. The release is immediately arrested if the excitation source is switched off. The upconverted NIR light allows for the tracking of particles under the tissue. Nucleus pulposus (NP) cells cultured with UCNPs are viable both in the presence and in the absence of laser irradiation. Controlled drug delivery of large biomolecules and deep tissue imaging make this system an excellent theranostic platform for tissue engineering, biomapping, and cellular imaging applications.

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The influences of surface molecular structure of carbon nanotubes on the stability of thermal conductivity enhancement of CNT NFs

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Statement of the Problem: Pristine CNT, which have a strong tendency to entangle with each other and to rapidly aggregate due to large hydrophobic surface area. CNT in the CNT-based NFs tend to quickly stratify and precipitate to the bottom of the container. Such rapid sedimentation, which can clog any flow channels, seriously decays heat transfer effectiveness, and renders practical engineering applications infeasible. Therefore, improving the stability is the key challenge to enable successful engineering applications of the CNT-based NFs. The purpose of this study is to reveal the influences of surface molecular structure changes of CNT on the stability of suspension and thermal conductivity enhancement of CNT NFs.

Methodology & Theoretical Orientation: In this study, multi-walled carbon nanotubes (CNT) was used as the objects of study, a mixed acid composed of nitric acid (HNO3) and sulfuric acid (H2SO4) was used as oxidative modification agent, and different oxidation acid treatment times were adopt to investigate the effect of structural changes of CNT on the stability of suspension and thermal conductivity enhancement of carbon nanotubes/ethylene glycol (EG) nano-fluids (CNT/EG NFs). The effects of oxidative acid treatment on the morphology and surface molecular structure of CNT were investigated by SEM, TEM, FTIR, respectively; and the influence of structure changes of CNT on the stability of suspension and thermal conductivity enhancement of CNT/EG NFs was evaluated by sedimentation observation method, centrifugation method and optical microscopy method and transient line heat source method.

Findings: The stability of suspension is proportional to the abundance of functional carboxyl group –COOH on CNT.

Conclusion & Significance: The formation of carboxyl group COOH plays a major role in improving the stability of suspension and thermal conductivity enhancement of CNT/EG NFs.

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Preparation of hydroxyapatite from industrial waste phosphogypsum by hydrothermal method, its application in waste treatment

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Phosphogypsum (PG) is an industrial waste derived from the production of phosphoric acid where the phosphate ore is dissolved in sulfuric acid. About 5 tons of phosphogypsum are produced for every ton of P_2O_5 manufactured. Worldwide PG production is huge, and it is estimated that 200,000 tons are produced annually in phosphoric acid plants. In fact, 85% of the worldwide production remains at present stored into piles near the factory that occupy considerable land resources, or completely discharged into water, which lead to serious contamination. In consequence, valorizing and minimizing the negative effects of this hazardous waste increasingly grab the attention of researchers all around the world. In the present work, the conversion of an industrial sub-product phosphogypsum (PG) into hydroxyapatite (H-Ap) was investigated. Hydrothermal synthesis was applied by reacting PG with a salt at different times, temperatures, while adjusting pH using sodium hydroxide solution NaOH (1 M). The obtained H-Ap exhibited a hexagonal structure, a high purity and nanorod- like shaped of 44 nmx12 nm. The prepared nano-hydroxyapatite was characterized by X-ray diffraction (XRD), Fourier transformed-infrared spectroscopy (FT-IR), transmission electron microscopy (TEM) and scanning electron microscopy (SEM). The findings showed that PG recycling could be accomplished using an easy synthesis route with relatively cheap reactants in order to produce nano-crystalline H-Ap. The elaborated hydroxyapatite powder was used as en effective adsorbent of organic dyes/heavy metals from wastewater.

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Designing novel gelatin-based hydrogels for soft tissue engineering

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Driven by enormous potential of hydrogels, novel gelatin-based biocompatible hybrid hydrogels were developed under mild condition using poly(ethylene glycol) diglycidyl ether (PEG) as a cross-linking agent. Chitosan (CH) and hydroxyethyl cellulose (HEC) were added to tune the structural stability, mechanical properties and degradation resistance as well as to better mimic the native extracellular matrix (ECM). Post-curing was essential to achieve suitable structural stability, tunable mechanical strength and controlled degradation resistance of the hydrogels. Structural features and cross-linking interaction of the hydrogels were confirmed by infrared spectroscopy. Mechanical properties were measured by uniaxial tensile tests, and the characterization revealed non-linear and J-shaped stress-strain curves for all hydrogels, similar to those found for native ECM. Structural integrity of these hydrogels was confirmed by the hydrolytic degradation test as well as by the variation of mechanical properties over time. Degradation study demonstrated that the mass loss and change in mechanical properties were dependent on hydrogel compositions and cross-linking. Biological evaluation of the hydrogels was conducted using rat myoblasts and human fibroblasts cell lines. The results showed that the hydrogel scaffolds were not toxic to cells; all of them allowing cell adhesion and proliferation. Hence, these hydrogels might have a great potential for use in the soft tissue engineering applications.

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MATERIALS SCIENCE AND ENGINEERING

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Energy efficiency and building environment

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 $\boldsymbol{\gamma}$ ith the environmental protection posing as the number one global problem, man has no choice but reducing his energy consumption, one way to accomplish this is to resort to passive and low-energy systems to maintain thermal comfort in buildings. The conventional and modern designs of wind towers can successfully be used in the hot arid regions to maintain thermal comfort (with or without the use of ceiling fans) during all hours of the cooling season, or a fraction of it. Climatic design is one of the best approaches to reduce the energy cost in buildings. Proper design is the first step of defense against stress of climate. Buildings should be designed according to climate of the site for reducing the need of mechanical heating or cooling hence maximum natural energy can be used for creating pleasant environment inside the built envelope. Technology and industry progress of the last decade diffused electronic and informatics' devices in many human activities and now appear also in building construction. The utilization and operating opportunities components, increase the reduction of heat losses by varying the thermal insulation, optimize the lighting distribution with louver screens and operate mechanical ventilation for coolness in indoor spaces. In addition to these parameters the intelligent envelope can act for security control and became an important part of the building demotic revolution. Application of simple passive cooling measure is effective in reducing the cooling load of buildings in hot and humid climates. 43% reductions can be achieved using a combination of well-established technologies such as glazing, shading, insulation, and natural ventilation. More advanced passive cooling techniques such as roof pond, dynamic insulation, and evaporative water jacket need to be considered more closely. The building sector is a major consumer of both energy and materials worldwide, and the consumption is increasing. Most industrialized countries are in addition becoming more and more dependent on external supplies of conventional energy carriers, i.e., fossil fuels. Energy for heating and cooling can be replaced by new renewable energy sources. New renewable energy sources, however, are usually not economically feasible compared with the traditional carriers. In order to achieve the major changes needed to alleviate the environmental impacts of the building sector, it is necessary to change and develop both the processes in the industry itself, and to build a favorable framework to overcome the present economic, regulatory and institutional barriers.

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MATERIALS SCIENCE AND ENGINEERING

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Fundamental limitations and development perspectives of quantum nanoelectronics

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ver several decades the tendency for miniaturization of micro- (or nanoelectronic) components has followed the Moore's law: doubling of the number of elements per chip over each 18 months. However, nowadays all authorities come to conclusion that the progress in miniaturization of commercial nanoelectronic circuits will come to saturation very quickly (in 2017-2019), based on different estimations. Typically, two main reasons are provided. First, is purely technical: the dramatic increase of energy dissipation per unit volume of a processor. Second problem is of fundamental origin: below a certain size limit (rough estimation ~10 nm) the electron transport does not follow the laws of classic physics, but is rather described by quantum mechanics. The behavior of an ultra-small system (e.g. transistor) becomes qualitatively different from behavior of a "classic" (macroscopic) device. Some potential solution of the first problem might be the rejection of CMOS technology and utilization of superconducting materials in critical elements of the circuit. However, contrary to the first problem, the second one does not have a solution in foreseen future. All solid conductors like metals, semiconductors or superconductors (the last being already by the very nature the macroscopic quantum objects) - below certain scales exhibit various quantum size effects. Those quantum size phenomena dramatically alter properties of electric conductors: with reduction of electric conductivity and transition to insulating state being a typical manifestation. Obviously the mentioned size limitations should be carefully taken into account in designing ultra-small nanolectronic devices of the next generation. However, beside the negative influence, quantum effects can be used for building the qualitatively new generation of nanoelectronic devices essentially based on quantum physics: e.g. qubits - elements of quantum logic, to be used in quantum information and processing systems. Utilization of such quantum devices opens up qualitatively new horizons for such disciplines as informatics, telecommunication, metrology and computing. In addition to applications in such crucial fields as space and defense industry, national security, quantum nanoelectronics opens-up new fields of research in basic studies. Quantum nanoelectronics cross-fertilize interdisciplinary links between subjects like linguistic and quantum cryptography, brain research and quantum informatics. Here, we outline the mentioned technical and fundamental limitations for miniaturization of nanoelectronic elements, as well as suggest certain alternatives for the field development.

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MATERIALS SCIENCE AND ENGINEERING

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Carbon-based nanostructures for single-molecule investigations

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We present a universal approach for the generation of multifunctional nanomaterials that employ molecular building blocks assembled on carbon nanotube (CNTs) electrodes. We will demonstrate single-molecule control in the formation of nanohybrids via the in-solution assembly of classes of molecular materials (organic, inorganic, and biological with promising attributes) to DNA wrapped CNTs. We have linked in solution metallic single-walled CNTs (SWCNTs) with different conjugated molecular wires, and measured the molecular conductance in these molecular transport junctions, highlighting the potential of an all-carbon based approach for solution-processable molecular electronics (see image). Additionally, we produced organic-inorganic heterostructures consisting of single quantum dots (QDs) univocally linked at the terminal ends of individual SWCNTs. Monofunctionalized SWCNT-QD heterostructures were obtained and photo physical investigations at the single nanohybrid level showed evidence of electronic coupling. Studies in this context are critical in the design of novel QD-based optoelectronic and light-energy conversion devices. Finally, we will demonstrate site-specific assembly of single proteins on individual SWCNTs. As a proof of concept, we investigated different CNT-protein configurations and obtained evidence of site-specific coupling between SWCNTs and specific proteins of interest. Notably, only the right bioengineered system exhibited the expected direct protein-nanotube communication, paving the way to selective electrical addressability of proteins via the use of carbon nano electrodes.

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Physicochemical and mechanical evaluation of a novel theophylline and 4-aminobenzoic acid pharmaceutical co-crystals

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Statement of the Problem: Pharmaceutical cocrystals are solids that are crystalline materials comprise of two or more components held together by non-covalent forces. In recent years co-crystals are being studied intensively due to the potential for improved pharmaceutical properties such as increased solubility, bioavailability, chemical stability and hygroscopicity of active pharmaceutical ingredients. A crystalline particle is characterized by definite crystal habit which relates to the external structure (such as shape and size) and crystal lattice describes the internal structures. Change in crystal forms has significant effect on drug particle mechanical properties (particle strength, flowability, miscibility and tableting) dissolution rate and stability. To enhance understanding of co-crystallization process on mechanical properties of Theophylline (active pharmaceutical ingredient) in the present study the impact of crystal structure and its relationship with powder compaction has been investigated.

Methodology: Novel theophylline and 4-aminobenzoic acid pharmaceutical co-crystals at molar ratio of 1:1 were synthesized by solvent evaporation and mechano-chemical synthesis techniques. Co-crystals were mainly characterized by powder X-ray diffraction (PXRPD), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR) and single crystal X-ray diffraction. Theophylline cocrystals were also subjected to powder flow, powder compaction and relative humidity stability testing studies.

Findings & Significance: The molecular structure of the novel theophylline and 4-aminobenzoic acid pharmaceutical cocrystal was further confirmed using single crystal X-ray diffraction analysis. Finally crystal structure and its relationship can be considered for improving mechanical properties of API.

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MATERIALS SCIENCE AND ENGINEERING

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Ab-initio investigation of metallic dopant segregation and embrittlement in molybdenum grain boundaries

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Mo is widely used as a refractory material due to its excellent high temperature properties, but a critical limitation is its room temperature brittleness resulting from its ductile-to-brittle transition temperature (DBTT). Doping the grain boundaries (GBs) of Mo with metals such as Zr, Re or Al have previously been demonstrated as a promising approach to remedy this limitation, whereas other alloy elements are known to exacerbate it. In this work we investigated the segregation and strengthening/embrittling effects of 29 metallic dopants at the $\Sigma5(310)$ tilt and $\Sigma5(100)$ twist Mo GBs using density functional theory (DFT) calculations. We show that GB segregation for most dopants is independent of the type of GB. Based on previous works for other metals, we also developed a model that uses radius and cohesive energy of the dopants relative to that of Mo as a good predictor of the strengthening/ embrittling effect. However, when comparing our values to previous empirical continuum models, we find that dopant chemistry for elements such as Ni also plays a significant role in affecting segregation behavior at GBs, particularly in driving the formation of intermetallic precipitates or 2-D interfacial phases (complexions). We also show that the site preference of a dopant in the GB can lead to strengthening effects that deviate from those predicted using simple bond-breaking arguments. Under a fast cleavage model of fracture, Ta, Re, Os and W are predicted to have a weak strengthening effect on Mo for the $\Sigma5(310)$ tilt GB.

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Nanoplasmonic upconverting nanoparticles as orientation sensors for single particle microscopy

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Statement of the Problem: Protein-DNA interactions are the center of many important biological pathways including DNA replication, transcription, recombination, and repair. Dynamic movements of proteins on DNA include jumping, hopping and quasi-1D curvilinear movement during which the protein maintains continuous DNA contact (Fig. 1). While some work has been done on translational motion of proteins on DNA, the 3D rotational motion of the proteins on DNA, is less explored, due to limitations in current nanoprobes. Recent studies have shown that rare earth upconverting nanoparticles (UCNP) offer an attractive alternative method for tracking orientation due to their inherent excitation polarization dependence. UCNPs are excited in the near infrared and fluoresce via anti-stokes emission in the visible energy range (400-800 nm), making them attractive for use in biological settings due to their low-energy excitation photon energy. UCNPs are excellent fluorescent probes, as they have no blinking, bleaching, or fluorescence background due to their near infrared excitation. These properties allow dynamic molecular interactions to be tracked continuously in real time. By coating disk-shaped UCNPs with a metal layer (NP-UCNP), they gain a large anisotropy in the fluorescence yield if illuminated with polarized light. This fluorescence anisotropy of the NP-UCNP probe renders them as excellent orientation probes in both linear and 3D tracking.

Methodology & Theoretical Orientation: We have designed and demonstrate proof of concept of single particle orientation and rotation tracking of NP-UCNP probes. We apply 1) predictive modeling to design and optimize NP- UCNPs for anisotropic fluorescence intensity with orientation, 2) perform correlated structural and optical single nanoparticle spectroscopy of nanofabricated NP-UCNPs to validate model predictions, and 3) analyzed the diffusional characteristics of a single NP-UCNP tumbling in solution between coverslip and slide to confirm that the orientation dependent fluorescence of the single NP-UCNP can be used to track single molecules.

Findings: It was found that the shape asymmetry of the UCNP itself contributes strongly to the orientation and excitation polarization dependence of the emission intensity. The presence of a gold shell enhances the intensity contrast between flat and edge orientations. We analyzed a particle tumbling in solution to show that the diffusional constant of a single particle can be determined.

Conclusion & Significance: The proposed new orientation sensitive platform based on NP-UCNP probes that can be coupled to proteins has wide-ranging applications in the future analysis and compilation of protein dynamics in any biological system. This model will open new opportunities for the biomedical research community to develop novel technologies for early diagnosis, control, and treatment of a wide-range of human diseases.

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MATERIALS SCIENCE AND ENGINEERING

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Design of frequency-tunable triple-mode filter based on ceramic substrate integrated waveguide

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A novel triple-mode filter based on ceramic substrate integrated waveguide structure designed for compactness is proposed. The operating filter can tuned from 1.8 GHz to 2 GHz by adjusting the capacitance at tuning point from 6pF to 2pF. For the triple-mode, the circular cylindrical cavity has been constructed in the form of the substrate integrated waveguide (SIW) structure since it could be made to easy in a low cost. The thickness of substrate is 10 mils and the dielectric constant is 2.2. The whole eight tuning points are placed inside the circular cavity. Each tuning point has a thru-hole connected to the other side conductor and has four variable capacitors. The diameter of via is 0.8 mm. This design has one TE_{011} mode and two orthogonally generated TM_{110} similar modes, and the mode characteristics of the proposed filter are analyzed using a full-wave electromagnetic (EM) simulation. The frequency variation was verified using the eigenvalue simulation embedded in EM simulator.

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Nanotechnology: General and biomedical applications

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N anotechnology represents the most important issue in the development of different scientific and practical fields. For example, the urgent task of modern care of public health is developing completely brand-new, "smart" drug formulations that can provide a superior therapeutic efficacy with minimum side effects. Moreover, the research in this direction might able to achieve the unexpected decisions when choosing therapy for various, including widespread and extremely dangerous, diseases. In particular, biodegradable nano-containers with stipulated physical and chemical, as well as biological (biomimetic) properties of surface, which smoothly invaded in the natural processes of human body, enable to provide such results. Thus, the special attention is paid to the application of nano-technology to biology, biotechnology and medicine. The problems of the creation of carefully designed smart biomaterials and nanodevices will be discussed using the examples of the projects realized in presenting department. The prospectives of nano-approaches in biomedicine will be demonstrated.

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MATERIALS SCIENCE AND ENGINEERING

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EAF long term industrial trials of utilization of char from biomass and waste residues as fossil coal substitute

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Diomass is a renewable resource having a steady and abundant supply, especially those biomass resources that are by-products Dof agricultural and industrial activity. Its use is by supplying neutral carbon, can displace fossil fuels, and help reduce GHG emissions while closing the carbon cycle loop. Every year End of life vehicles (ELVs) generate about 8 M tons of waste of which the ferrous fraction represents about 70-75%, nonferrous metals about 5%. The remaining 20-25%, the ASR, contains rubber, ferrous and non-ferrous metals, textile, fiber material, wood, glass and a relevant fraction (~40% wt) of polymers with high calorific value (~25 MJ/kg). With a start date of January 1st 2015, the EU directive 2000/53/EC establishes the reuse and recovery of a minimum of 95% ELV total weight. Therefore different ASR management options, such as further material and energy recovery, must replace the landfilling. Steel produced starting from scrap, already needs less energy with beneficial effects on environment and economy that are greater as increases the share of fossil fuels in total energy feeding. The replacement, in EAF practice, of fossil fuels with char and syngas obtained from biomass, waste residues (i.e. plastics, automotive shredder residue (ASR), petrochemical sludge, etc.) can further improve the environmental performance and the attractiveness of the EAF based route, eventually increasing the amount of chemical energy respect electrical one, with beneficial effects on environment, economy and flexibility of the EAF process. The feasibility of biochar as fossil coal substitute as charge material in EAF has already been proved in two previous European projects (GREENEAF and GREENEAF2) were an intensive industrial utilization of biochar was foreseen. A test sequence of six consecutive heats was carried out replacing standard anthracite with biochar. The results of the industrial tests indicate that utilization of char as charge material can be done, but operating practice, environmental evaluation of off-gas emissions, for these new applications needs to be optimized with long term experimentation. The results of industrial long term trials confirmed the feasibility of the use of biochar as charge material, without significant modification in steel and slag analysis. This paper describer the industrial long term trials with biochar in EAF, with the final target to replace fossil coal and new laboratory trials with plastic, ASR and petrochemical sludge.

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Effect of surface treatment on oxidation behavior of Ni-base superalloys

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The materials used at high temperature, like in gas turbines or jet engines, need to fulfill a number of requirements, e.g. high creep strength and oxidation resistance at a wide range of operating temperatures, environments and loading condition as well as a suitable ductility at low temperature. Such properties are obtained in Ni-base superalloys, due to their microstructure consisting of thermodynamically stable γ -Ni matrix with combination of strengthening γ' -Ni₃Al phase. However, when one exposes the alloys at high temperature, an oxidation process occurs and the material starts to form an oxide scale. The Ni-Cr-Al based alloys can be classified into the three groups of materials in term of formed oxide scales: NiO-forming, chromia layer forming and an alumina forms alloys. Formation of protective oxides like Al₂O₃ or Cr₂O₃ substantially increase the lifetime of the component exposed at high temperature. To provide a resistance against oxidation a protective coatings such as MCrAlY (where M is mainly Ni or Co) or β -NiAl which are an alumina forming materials are applied. However, coatings production is time consuming, results in additional component costs, and can negatively affect alloy mechanical properties, such as fatigue strength. Therefore, another method to force material to form a protective oxide scale is proposed in the present study. Namely, a different surface preparation of Ni-base superalloys, like grinding, polishing, sand blasting, etc., on oxide scale formation during exposure at high temperature in Ar-O₂ atmosphere will be presented. It was found that material ground material formed less non-protective NiO compared to polished one (Figure 1). The effect of surface treatment on oxidation kinetics and oxide scale formation will be described as well.

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MATERIALS SCIENCE AND ENGINEERING

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Self-healing capacity of nuclear glass observed by NMR spectroscopy

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B orosilicate glasses have been recognized as valuable materials for the conditioning of nuclear wastes. An important issue for their long-term behavior is radiation effects which may impact their performance and stability. To address these concerns, a fundamental understanding of the origin at the atomic scale of the macroscopic property evolutions must be established. To this aim, magic-angle spinning nuclear magnetic resonance (MAS NMR) has firmly established itself as one of the most powerful tool to investigate glass structure. Recently, using external heavy ions irradiation (Xe, Au and Kr) to simulate alpha decays, dramatic changes in the local network structure were evidenced: Conversion of tetrahedral BO₄ units into planar trigonal BO₃ units (¹¹B), appearance of high-coordination aluminum units (AlO₅, AlO₆); glass depolymerization (²⁹Si) and changes in the distribution of alkali cations (²³Na). Additionally, the spectra broaden globally which supports the hypothesis of an increased topological disorder after irradiation. All these structural changes are similar to those observed with increasing the glass temperature or quenching rate and support therefore the model of ballistic disordering fast quenching events which induce a new glassy state with higher fictive temperature. Until recently, such studies were limited to externally irradiated samples (enabling the different components of irradiation to be dissociated for their precise investigation), but recently, the first MAS-NMR experiments could be performed on radioactive glasses (doped with ²⁴⁴Cm 0.1 % mol.) paving the way for future MAS NMR examinations of self-irradiation damages in glasses. Experiments were performed at the Joint Research Centre Institute for Transuranium Elements (JRC-ITU) where a commercial NMR spectrometer were integrated with a radioactive glovebox and a MAS commercial probe. First results will be presented. Competitive effects between the recoil nuclei and alpha decays were evidenced and the high resistanc

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Bioinspired wettability-controlled surfaces with gradient micro- and nano-structures

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Biological wettability surfaces with various-style gradient micro- and nanostructures (MN) greatly provide with excellent functions by a natural evolvement. In nature, a combination of multiple gradients in a periodic spindle-knot structure take on surface of spider silk after wet-rebuilding process in mist. This structure drives tiny water droplets directionally towards the spindle-knots for highly efficient water collection. Inspired by the water collecting ability of spider silk, a series of functional fibers with unique wettability has been designed by various as-inspired techniques. Various geometrically-engineered thin fibers with the bead-on-string structures achieve droplet driving, transport of droplet for water collection in efficiency, etc. Besides, inspired by gradient effects on butterfly wing and lotus leaves, the surfaces with ratchet MN, flexible lotus-like MN are fabricated successfully by improved methods, which demonstrate that the gradient MN effect rises up distinctly anti-icing, ice-phobic and de-ice abilities. These multifunctional materials can be designed and fabricated for promising applications such as water-collecting, anti-frosting, or anti-fogging properties for practical applications in aerospace, industry, etc.

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MATERIALS SCIENCE AND ENGINEERING

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A study on recent developments in natural fiber composites and their mechanical performance

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R ecently, there has been a rapid growth in research and innovation in the natural fiber composites (NFCs) area. The mechanical performance of NFCs is affected mainly based on the fiber selection where fiber type is commonly categorized based on its origin, whether it is a plant, animal or mineral. The use of natural fiber from both resources, renewable and nonrenewable such as oil palm, sisal, flax, and jute to produce composite materials, gained considerable attention in the last decades. The plants, which produce cellulose fibers can be classified into bast fibers (jute, flax, ramie, hemp, and kenaf), seed fibers (cotton, coir, and kapok), leaf fibers (sisal, pineapple, and abaca), grass and reed fibers (rice, corn, and wheat), and core fibers (hemp, kenaf, and jute) as well as all other kinds (wood and roots). The matrix selection is an important part of a fiber-reinforced composite. It provides a barrier against adverse environments, protects the surface of the fibers from mechanical abrasion and it transfers load to fibers. The most common matrices currently used in NFCs are polymeric as they are light weight and can be processed at low temperature. Matrix selection is limited by the temperature at which natural fibers degrade. Interfacial bonding between fiber and matrix plays a vital role in determining the mechanical properties of composites and good interfacial bonding is required to achieve optimum reinforcement. The best mechanical properties can generally be obtained for composites when the fiber is aligned parallel to the direction of the applied load. Regarding the degree of influence of orientation on mechanical performance of NFCs, similar large reductions of strength and Young's modulus to those seen with synthetic fibers have been obtained with increasing fiber orientation angle relative to the test direction. Natural fiber reinforced polymer composites have beneficial properties such as low density, less expensive, and reduced solidity when compared to synthetic composite products, thus providing advantages for utilization in commercial applications (automotive industry, buildings, and constructions). Using natural fibers as reinforcement for polymeric composites introduces positive effect on the mechanical behavior of polymers, but it has high moisture absorption which results in swelling which can be further enhanced through the chemical treatment, while moisture absorption of the NFPCs can be reduced through surface modification of fibers such as alkalization and addition of coupling agents.

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Biodegradable natural fiber polymer composites- A review

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A s per environmental prospect natural fiber has many advantages such as lower pollutant emissions, lower green house gas emissions and end of life biodegradability of components. Recently studies had proven that performance of natural fiber as per environment prospect is far better than glass fiber over its specific applications, Where the polymer matrices are derived from renewable resources such as poly lactide (PLA), thermoplastic starch (TPS), cellulose and polyhydroxyalkanoates (PHAs). TPS composites modulus displays a regular behavior where reinforcement effect increases with the fiber length from short length fiber (SF) to medium length fiber (MF) and fiber content. While elongation at break decreased with the increase in fiber contents and length. These composite materials with its various interesting properties may soon be competitive with the existing fossil plastic materials. This can be applied to various fields such as household items, automobiles and food packaging systems. By using this type of polymers an ecofriendly atmosphere can be created and thus hazardous effects can be reduced. However, the present low level of production and high cost restrict them for to be applied in industrial application. In addition, its hydrophilic properties make the real challenge to design the product which can be good candidate for outdoor applications.

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