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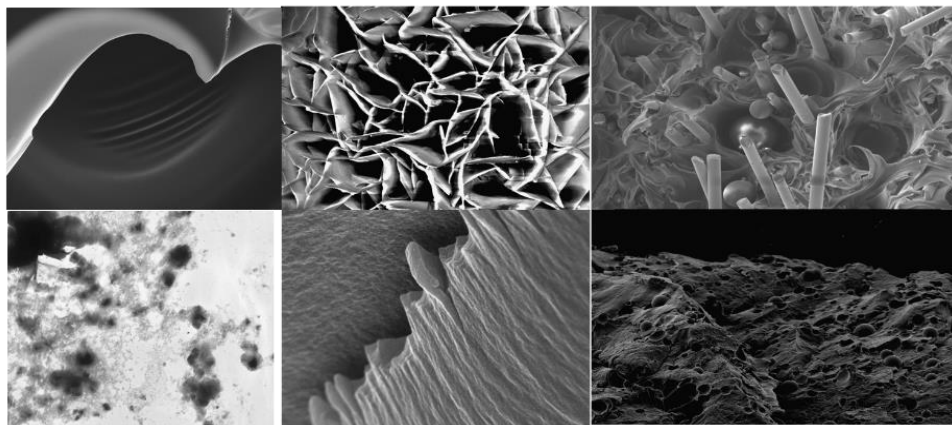
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NANOSTRUC 2018

International Conference on Structural Nano Composites
23rd - 24th May 2018, Berlin Germany

Abstract Book



Conference Programme



Hochschule für Technik
und Wirtschaft Berlin

University of Applied Sciences

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Preface

Dear Colleagues,

Welcome you to Berlin. It is our great pleasure to welcome you to NANOSTRUC 2018 at HTW Berlin. NANOSTRUC2018 brings together an international community of researchers in Berlin (Germany) on 23-24 May 2018. The aim is for these stakeholders to discuss the state-of-the-art, new research results, perspectives of future developments, and innovative applications relevant to structural materials, engineering structures, nanocomposites, modelling and simulations, and their related application areas.

The recent developments in understanding and improved manufacturing techniques of nanoparticles have rapidly introduced engineering nanomaterials across the commercial industry. Manufacturers can now disperse nanoparticulate nanotubes, metals, layered silicates, oxides and other nanomaterials with polymers, metals and ceramics to optimize the composite's properties.

This in turn provides proprieties and performances while opening doors for new inventions. We have 8 sessions including 2 Keynote sessions focusing on Automotive & Aerospace Materials, Nanosensors, Hybrid Composites, Biomaterials and Biomedical Devices, Functional Nanocomposites.

We would like to acknowledge the hard work, professional skills and efficiency of the Organising Committee and Steering Committee which ensured the successful organisation. Most importantly to the conference contributors authors, delegates, sponsors and supporters.

Welcome to the NANOSTRUC 2018 and wish you a stimulating Conference and a fruitful time here in Berlin.

Yours sincerely,

Ha-Duong Ngo & James Njuguna
Conference Co- Chairs

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Session Chairs

Session 1.1: Keynote 1 (Room G001) - *Ha-Duong Ngo, HTW Berlin University of Applied Sciences, Germany*

Session 1.2: Automotive and Aerospace Materials (Room G001) - *Sérgio Henrique Pezzin*

Session 1.3: Nanosensors (Room H001) - *Mária Omastová, Polymer Institute, Slovak Academy of Sciences, Slovakia*

Session 1.4: Keynote 2 (Room G001) - *Fengge Gao, Nottingham Trent University, United Kingdom*

Session 2.1: Keynote Lectures (Room G001) - *Raquel Verdejo, CSIC, Spain*

Session 2.2: Hybrid Composites (Room G001) - *Theodora Krasia-Christoforou, University of Cyprus, Cyprus*

Session 2.3: Biomaterials and Biomedical devices (Room H001) - *Radhakrishna Prabhu, Robert Gordon University, United Kingdom*

Session 2.4: Functional Nanocomposites (Room G001) - *Krzysztof Pielichowski, Cracow University of Technology, Poland) & Alina Adriana Minea, Technical University Gheorghe Asachi, Romania*

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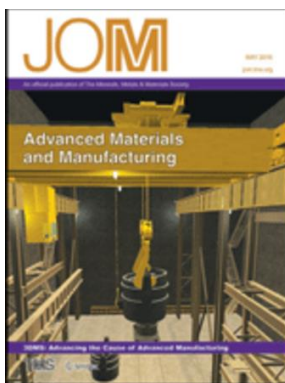
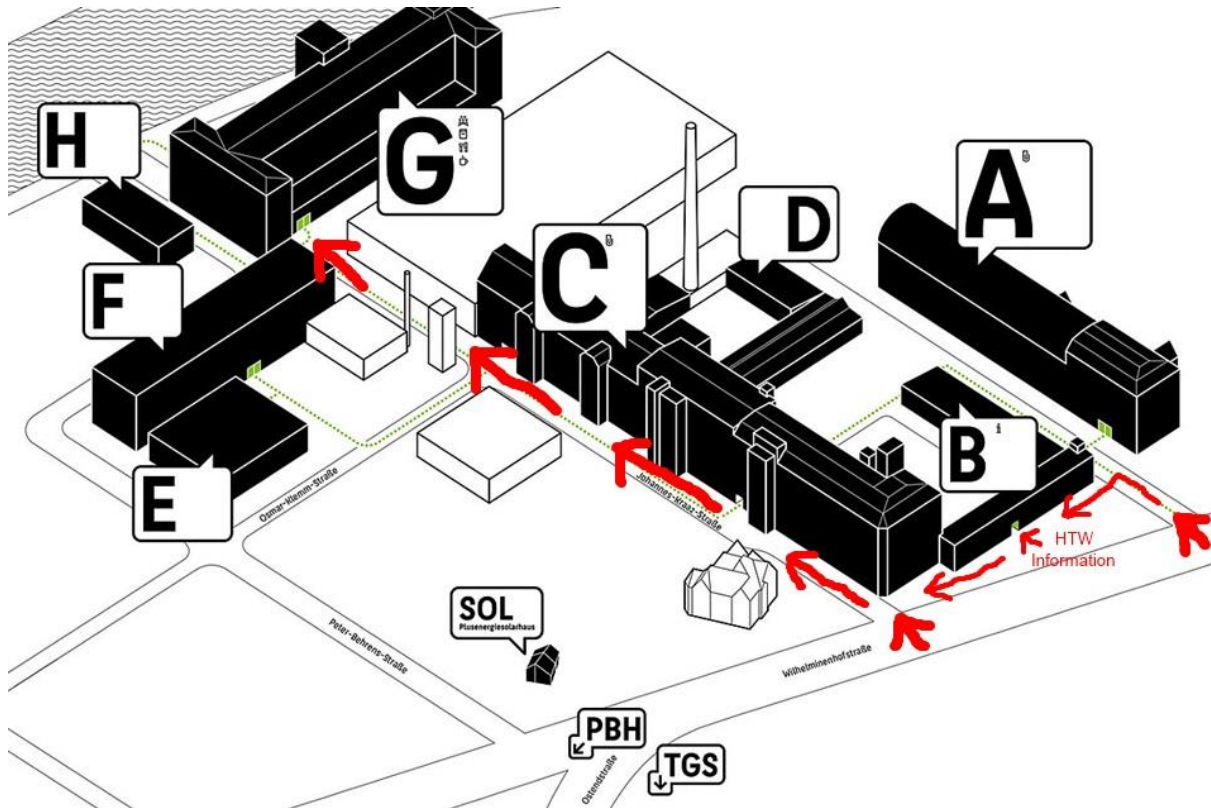
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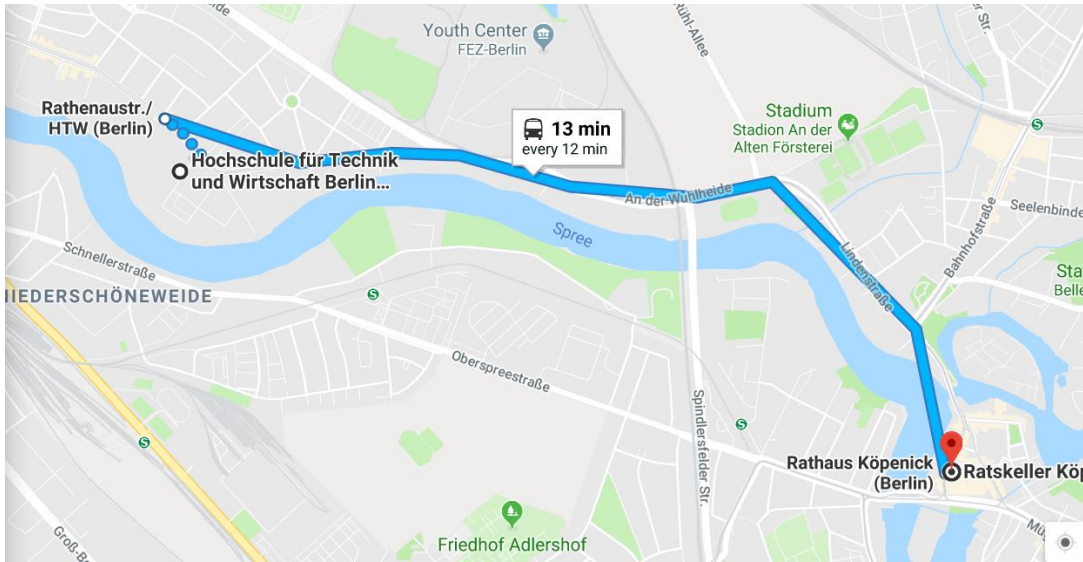


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Wednesday 23th May 2018

08:00 – 09:00	Registration (Room G007/008)	
09:00- 09:15	Welcome (Room G001)	
	Session 1.1: Keynote 1 (Room G001) Chair- <i>Ha-Duong Ngo</i>	
09:15- 09:55	Optical grating technology <i>Marcus Lörger</i>	
09:55 -10:30	Smart electrically conductive polymeric nanocomposites <i>Matej Mičušík, Eliška Číková and Mária Omastová</i>	
10:30- 11:00	Coffee/Tea Break (Room G007/008)	
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12:30- 13:00	The role of the acetalization degree on the dynamical mechanical properties of polyvinylbutyral nanocomposites <i>Sergio Pezzin and Jean Hoepfner</i>	Nanosilicon as a material for sensors and thermoelectrics <i>Androula G. Nassiopoulou and Manolis Hourdakís</i>
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	Chair – <i>Fengge Gao</i>
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14:40-15:10	Functional polymer-based nanocomposite fibers via electrospinning <i>Theodora Krasia-Christoforou</i>
15:10-15:40	Numerical approaches in the study of hybrid nanofluids and their possible applications in solar energy <i>Alina Adriana Minea</i>
15:40-17:00	3 mins Poster Presentation (for Each Poster) WILEY
17:00	Posters and Coffee/Tea Break (Room G007/008)
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11:30-11:50	Influence of graphene oxide on mechanical and hydrophilic properties of epoxy/banana fiber composites	Investigations on sensitivity enhancement of SPR biosensor using tunable wavelength and graphene layers
	<i>Preetam Bharadiya, Mukesh Singh and Satyendra Mishra</i>	<i>Kaushalkumar Bhavsar and Radhakrishna Prabhu</i>
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Optical Grating Technology

Marcus Loergen*

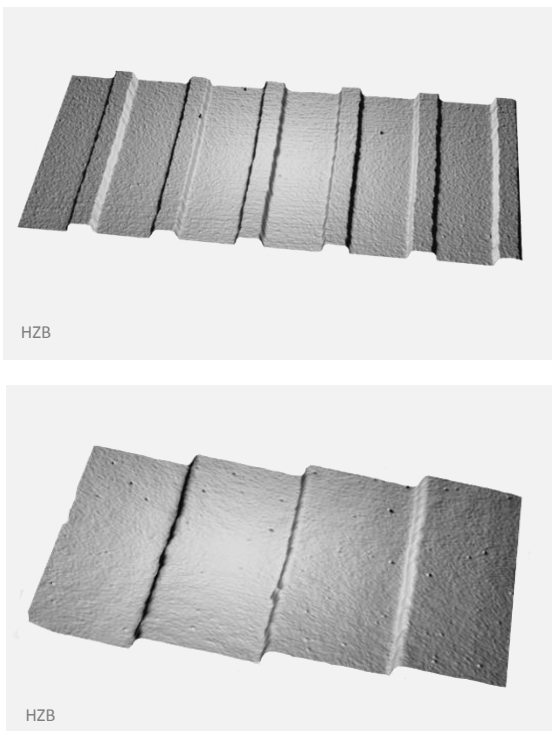
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Almost ten years ago, an important supplier company for precise optical diffraction gratings used for scientific synchrotron experiments worldwide, took the decision to close its activities in that field. The Helmholtz-Zentrum Berlin (HZB), as operator of one of the soft X-ray synchrotron radiation source in Europe namely BESSY II, faced a shortage of precision gratings for its beamlines and experiments. It was then when internal decisions have been made to take over the production facilities from the company. Major efforts have been taken in order to get the equipment back to operation. In 2013, HZB was able to announce the first diffraction grating being manufactured with own resources for one of the beamlines at BESSY

II. Since then, more than 40 gratings have been manufactured not only for the synchrotron in Berlin but also for light sources in Europe (UK, Sweden, France amongst others) and in Asia.

The spectrum of synchrotron radiation created by accelerated electrons is very broad ranging from THz, Visible to X-rays. Synchrotron sources gained relevance in the early fifties of last century with a soaring in number and usage worldwide during the nineties. Particularly, because of the Soft X-ray regime which makes the element specific probing of core shell electrons possible.



*Figure 1: Typical profiles of optical gratings.
Top: AFM image of a laminar grating.
Bottom: AFM image of blazed grating.*

In order to control the specific photon energy for exciting shell electrons, diffraction gratings are necessary that allow for the appropriate energy resolution and photon flux.

At HZB there exist two production lines, one for gratings with rectangular profiles, so called laminar gratings, and one for so called blazed gratings with saw-tooth profiles. While laminar gratings allow for efficient reduction of stray light and high spectral resolution, blazed gratings are optimized for high flux.

The production of diffraction gratings makes use of typical micro- and nanotechnology processes including thin film deposition, ion etching, lithography and the corresponding analytics, mainly Atomic Force Microscopy. The production process consists of over 20 steps grouped into the masking step, the texturing step and the finishing step including measuring processes for quality control. Typical line structures for the diffraction gratings have periods of 600 nm to 3 μm with extreme values of down to 250 nm. The height of laminar line profiles is in the range of 5 nm to 50 nm. Angles for blazed gratings are typically specified between 0.3° to 2° with respect to the optical surface. These microstructures have to be applied on surfaces of 200 mm x 40 mm size in order to ensure sufficient illumination of grating structures inside the monochromator of the synchrotron beamlines.

The work of HZB in this field combines micro-technology and surface structuring techniques with the demand for comparatively large optical devices, which make cutting edge scientific experiments with soft X-ray photons available to an international user community.

Smart Electrically Conductive Polymeric Nanocomposites

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Electrically conductive composites with polymeric matrices are usually designed by mixing insulating polymeric matrix with electroconductive fillers. Recently also a number of new nanofillers have been used, such as carbon nanotubes, graphene, metal nanoparticles, etc. The most important challenge in the production of electrically conductive polymeric composites is creating conductive paths through non-conducting polymeric matrix. For that a certain filler concentration is necessary, the so-called percolation threshold or percolation concentration (PC). Carbon nanotubes (CNT) have drawn tremendous attention due to their extraordinary electrical, mechanical and thermal properties and many research teams work in the field of composite preparation with CNT nanofillers [1].

Nanocomposites using styrene butadiene rubber (SBR) as the polymeric matrix and two types of carbon nanofillers, carbon black (CB) and CNT were prepared. The ability of prepared composites to act as sensors for three organic gases, toluene, THF, and n -hexane, by the changing of their electrical properties was studied. The degree and rate of response depends on filler type and concentration, type of analyte, and analyte concentration. Response of SBR/CB composites to the presence of all three studied gases compared to SBR/CNT composites was faster. When polymeric matrices start to swell, the disconnection of smaller CB particles can occur much faster than in case of long cylindrical CNT particles [2].

Next part of the presentation is devoted to preparation of electrospun polycaprolactone (PCL) fibers at a nano and submicron scale. These electrospun mats were coated with conducting polymer, polypyrrole (PPy). We studied the influence of polymerization conditions, including used combination of oxidant and surfactant during chemical oxidative polymerization of pyrrole monomer on quality of depth penetration of conductive polymer into fibrous mats. Various analytical methods e.g. ToF-SIMS, XPS, SEM were used for characterization of the morphology and structure of prepared fibrous composite. The PCL/PPy nanofibers were also

characterized in terms of morphology, electrical conductivity, and stability. Selected samples were tested for biological activity and toxicity on mouse fibroblastic cells.

The rapid increase in the number of methods for the preparation of conducting polymeric composite, as well as the range of their combinations with other materials, affords the possibility of various kinds of applications. Prepared new type of conducting nanofibers are important materials for the rapidly growing technology development such as tissue engineering, scaffold materials, or flexible solar cells applications and many others.

ACKNOWLEDGMENTS

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Reduced Order Modeling for Complex, Time Dependent and Multi-scale Modelling

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In this presentation we will provide a general purpose, innovative and simple approach in order to develop “reduced order models” of large, time dependent and CPU-consuming applications which may even involve multi-physics or multi-scale applications (such as material characterization). These models have the advantage of being re-employed in a “solver independent” environment as sub-parts or components which need not be recomputed at every cycle but can simply reconstructed from existing results. The computation time is efficiently improved and off-the-shelf models may be optimally exploited in a wide variation of scenarios, including real-time computing. A major advantage of this approach is that a reduced order model generated by any FE code or experimental test could easily be used for coupling with any other commercial FE code or existing real-time solver. Examples of applications for biomaterial modelling will be provided.

In situ mechanical synthesis of Al-Ti nanointermetallic reinforcements in AA 5052 alloy

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Friction Stir Welding (FSW) is a solid state joining method using a non-consumable pin tool that heats and plastically deforms the materials to be welded. During the welding, a cylindrical tool is inserted in high rotation in the middle of the junction between the materials. Through the tool rotation, intense heating and plastic deformation in the bonding interface results in a mechanical mixing. Recently, a technique was developed to use the passage of a FSW tool to modify composition and microstructure by mechanical synthesis of nanoparticles for structural reinforcement. After this process, it is obtained a composite with improved properties of hardness, wear resistance and ultimate tensile strength (UTS). This modification is as better as smaller and more homogeneously dispersed the nanoparticles are. Because of its importance for the aerospace industry, aluminum has been the most used matrix for composite generation through friction processing. Alloying a low density and ductile base metal with hardening and strengthening materials is of extreme interest, since it is possible to reinforce specific parts of the structure, either regions of higher demand (higher loads applied) or the surface, providing surface hardening and maintaining a ductile and light core. Here we report the results of friction stir alloying using an AA 5052 matrix and Ti for in situ mechanical synthesis of Al-Ti nanometric intermetallics. The composite is 20% harder than the base metal, has better UTS and presented evenly distributed nanoparticles. In addition to the mechanical characterization, the composite Al matrix/nanointermetallics was characterized by DRX, SEM and TEM.

Processing and Yield Strength Increase of an AM60-Based Metal Matrix Nanocomposite (MMNC)

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Magnesium high pressure die cast (HPDC) alloy AM60 was reinforced with 1 wt.-% AlN nanoparticles of 80 nm diameter. To break up the particle clusters in the melt we used an ultrasound assisted casting process, using the cavitation from sonification and acoustic streaming in the melt. However, applying an indirect chill casting method subsequently leads to pore-free casting. Microstructure and tensile mechanical properties were examined. It was found that the nano-AlN addition refines the microstructure significantly. Mechanical testing shows an outstanding increase in tensile yield strength, ultimate tensile strength and ductility. For industrial use this material requires good castability. Casting using a casting spiral was performed with both materials in order to assess the solidification length. The casting length was expected to indicate the castability of a nanoparticle reinforced magnesium alloy, because the viscosity of the melt influences this property. The properties of the material were found to be comparable to HPDC AM60. Unlike high pressure die cast materials, this material is free of pores and can therefore be heat-treated. Remelting trials were performed as well and these showed that the nanoparticles remain in the melt with only a marginal loss of grain refinement and loss of strength occurring for each remelting.

Thermal diffusivity behaviour of multi-walled carbon nanotube reinforced Ti6Al4V metal matrix composites

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This study investigated the thermal diffusivity behaviours of spark plasma sintered (SPS) multi-walled carbon nanotubes (MWCNTs) reinforced Ti6Al4V composites containing 0, 1, 2 and 3 wt. % of the reinforcement respectively, over a range of 50 – 300 °C. The MWCNTs were dispersed into the Ti6Al4V matrices by high-energy ball milling (HEBM) technique and the milled composite powders were consolidated by SPS under a vacuum atmosphere. The sintering conditions employed were heating rate (100 °C/min), holding time at temperature (5 min), sintering temperature (850 °C) and applied pressure of 50 MPa. The relative densities of the composite discs were measured according to Archimedes' principle while the thermal diffusivities of as-sectioned composite samples were measured using the Laser Flash equipment. Relative densities of the synthesized nanocomposites deteriorated with increase in the weight fraction of MWCNTs added to Ti6Al4V.

The thermal diffusivities of the composites containing 1 and 2 wt. % MWCNTs improved with increase in temperature and weight fraction of MWCNTs contents. A reverse trend was observed in the composite containing 3 wt. % MWCNTs, as the measured thermal diffusivities continued to drop with increase in temperature. Although this composite exhibited the best thermal diffusivities compared to the other composites up to 200 °C, a significant drop in

thermal diffusivity was recorded between 250 and 300 °C respectively with the values lower than that of the unreinforced Ti6Al4V alloy. However, the thermal diffusivities of MWCNTs/Ti6Al4V composites were generally not dependent on their densification as the composites with higher weight fractions of the reinforcement had higher thermal diffusivities in spite of their lower relative densities.

The role of the acetalization degree on the dynamical mechanical properties of polyvinylbutyral nanocomposites

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This work describes the preparation of polyvinylbutyral (PVB) nanocomposites reinforced with pristine and oxidized carbon nanotubes (CNT), graphene oxide (GO) and graphene nanoplatelets (GNP), via 'in situ' polymerization, at concentrations varying from 0.1 to 2.5 wt%. It was found that the presence of nanoreinforcements during the synthesis altered the degree of acetalization of PVB, since CNT and GO-reinforced samples had acetalization degree values between 50 and 77 mol%, whereas pure PVB and GNP-reinforced samples had values close to 65 mol%. FTIR, Raman and ¹H NMR results indicated interfacial interactions between oxidized CNT and PVB, while XRD results showed exfoliation of GO in PVB for all concentrations. GNP-reinforced nanocomposites presented exfoliation only for the lower concentrations. DMA analyses showed that the storage modulus increases 38.5, 20.5 and 20% for samples reinforced with 2.5 of GO, 0.5 of 'pristine' CNT and 1.0 wt% of oxidized CNT, respectively. Increases of 10, 12 and 7 °C in T_g were also observed for the same samples, respectively. DMA analyses of samples with higher degrees of acetalization show the presence of two Tan δ peaks, attributed to PVB and to PVA, characterizing a material with two immiscible phases. The entanglement degree, reinforcement efficiency factor ('C' coefficient) and 'A' adhesion factor, calculated from DMA results, evidenced higher degrees of dispersion, adhesion and reinforcement efficiencies for nanocomposites with 2.5 of GO, 0.5 of pristine CNT and 1 wt% oxidized CNT. The results showed that the 'in situ' polymerization method can improve the dispersion and final properties of the nanocomposite only if the nanoparticles are able to form relevant interfacial interactions during the PVB synthesis process. In addition, it was verified that the presence of nanoreinforcements altered the degree of acetalization of PVB, which also contributes to influence the final properties of the nanocomposites.

Recovery of copper nanoparticles from waste printed circuit boards by using high voltage and chemical reduction technology

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According to recent global reports, about 55 million tons of electronic waste are generated in 2017 around the world. Waste Printed Circuit Boards (WPCBs) represent about 10% of total mass of electronic waste (5.5 million tons in 2017). WPCBs are composed of approximately 30% metals (including precious) and 70% non-metals (fiberglass and epoxy resin). Copper is considered the base metal in WPCBs and typically represents approx. 22 wt.% from their total weight. In order to achieve the maximum environmental and economic benefits, this research aims to liberate copper foils and other components from WPCBs by using dissolution-ultrasonic treatment. The recovered copper foils were reprocessed into copper nanoparticles with average size 8nm by using high voltage and chemical reduction technology. SEM-EDS, TEM, FTIR, and XRD were used to examine the recovered components as well as the structure of produced copper nanoparticles. The results showed that the developed approach seems to be promising in terms of profitability and can be applied on the industrial scale.

Effect of CrC-Ni on the tribological properties of WC

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Tungsten carbide (WC) is extensively used in industrial processing as cutting tools, wear resistant components and drilling tools owing to the good combination of phenomenal properties. The binder phase of WC is usually cobalt (Co) as a result of good wetting behaviour and excellent solubility with regards to WC particles. However, degradation of WC-Co components when subjected to harsh environmental conditions often results in premature failures during application. In this study, the effect of CrC-Ni on the microstructure, mechanical and tribological properties of WC based cermet produced by spark plasma sintering was investigated. Sintered samples were then analysed and characterized by SEM and EDS. Macro hardness of the sintered compacts were evaluated using Rockwell hardness machine at 150kg load. Subsequently, comparative studies on the tribological behaviour of the experimental samples were performed using a reciprocating wear set up at 200°C. The area of the wear track cross-section was measured using optical profiler and the wear rate in terms of volume loss was calculated. Results showed improved mechanical and tribological properties on WC-20CrC-7Ni sample as compared to WC-Co cemented carbide sample.

Synthesis and applications of monolithic quasi 1D metal-semiconductor nanowire heterostructures

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Due to physical limits and short channel effects a shift towards the adoption of new materials and novel design architectures is predicted to insure further improvement of modern integrated circuit technology with respect to integration densities, power dissipation and performance.

Nanowires (NWs) are predicted to be one of the most promising building blocks for future ultra-scaled high-speed nano- and opto-electronics. Out of the wide range of NWs, germanium (Ge) combines a high carrier mobility, with a more than five times larger exciton Bohr radius compared to silicon. Hence, Ge is of particular interest especially for the development of high speed and novel quantum devices.

A novel synthesis approach for semiconductor-metal NW heterostructures is presented and discussed. The synthesis employs millisecond flash lamp annealing (FLA) along with several standard techniques of semiconductor manufacturing like sputtering and plasma enhanced chemical vapor deposition (PE-CVD).

We recently demonstrated the formation of axial Al-Ge-Al NW heterostructures with abrupt interfaces and monocrystalline aluminum (Al) leads by using a thermally initiated exchange reaction. This enables the formation of an in line contacted Ge quantum dot without requiring precise lithographic alignment of the contacts, which is one of the most challenging issues of fabricating quantum dot based devices. Unambiguous signatures of quantum ballistic transport and electrostatically tunable negative differential resistance even at room temperature are demonstrated and attributed to intervalley electron transfer. Modulation of the transfer rates, manifested as a large tunability of the peak-to-valley ratio and the onset of impact ionization is achieved by the combined influences of electrostatic gating, geometric

confinement, and surface tuning on hot electron transfer and by electron–electron scattering rates that can be altered by varying the charge carrier concentration in the NW FETs.

CNT-based sensors for strain monitoring/sensing applications

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In the last decades, carbon nanotubes (CNT) have been used for structural health monitoring of composites with possible applications in aerospace, aeronautic and naval industries. These nanostructures can be used as conductive matrix filler [1] or aligned forests [2]-[3] in polymer-based sensors. However their manufacturing processes issues are a drawback.

This paper presents an alternative CNT-based sensor for strain monitoring for composite structures. Vertical aligned carbon nanotubes (VA-CNT), synthesized by chemical vapour deposition (CVD), were knocked down onto a polymeric film, in order to obtain a thin 10x10 mm CNT patch. A MATLAB software with an adapted Van der Pauw method for anisotropic conductor [4] was developed to determine the electric properties of the obtained samples, which were strained in the parallel (1) and transverse (2) directions of the CNT alignment. The electric anisotropy, defined as electric resistance ratio between obtained measurements in direction 1 (R_{xx}) and 2 (R_{yy}), decreases when the sample was strained in direction 1, while it increases when strained in direction 2 with deformation increment (Figure 1 - A). Moreover, the obtained Gauge factor's values showed a much sensitive response to deformation when the samples were strained transversely to CNT alignment direction (Figure 1 - B).

Keywords: CNT, large strain sensor, strain monitoring, anisotropy

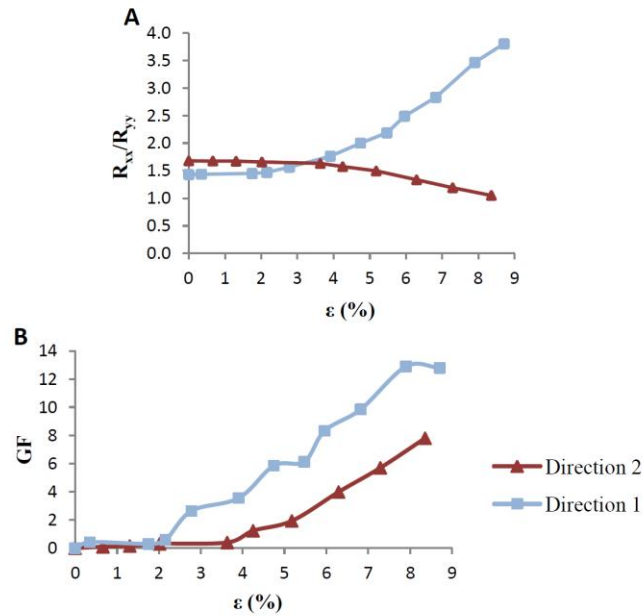


Figure 1 – Samples' results of electric anisotropy (A) and Gauge factor (B) of CNT when strained parallel (direction1) and transverse (direction2) to CNTs' alignment direction

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Structural, Morphological and Optical Properties of BaSnO₃ films prepared by pulsed laser ablation

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Surface modification of carbon nanoparticles (CNPs) by plasma polymerization of propylene was studied aiming to enhance affinity to produce polymer nanocomposites with high thermal conductivity. For this purpose, carbon nanofibers (CNF), graphene platelets (GP) and mixtures CNF:GP (using ratios of 9:1, 8:2 and 7:3) were modified. The power of the plasma reactor (60 w), reaction time (60 min) and reactor pressure of 2×10^{-1} mbar, were constant through all experiments, while the surface area and sp² hybridization spots were the studied variables. The CNPs were previously treated by sonication in gas phase, the process of deagglomerated particles was evaluated by dynamic light scattering (DLS). Meanwhile, the surface modification was characterized by transmission electron microscopy (TEM), infrared spectroscopy (IR), Raman spectroscopy, solvent dispersion tests and thermogravimetric analysis (TGA). Such characterizations indicate a significant deagglomeration by increasing the surface area exposed of CNPs, also, the presence of crosslinked polypropylene clusters generated on the surface of the CNPs after treatment was observed. All NPs exhibit similar modification percentages (4-5 wt-%), however, while an increment occurs in the surface area and sp² hybridization spots (with increasing GP concentration), the ratio I_D / I_G shows an increase in the covalent modification.

Synthesis, structural and morphological property of a novel Pd/g-CN nano composite for gas sensing application

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In this paper graphitic carbon nitride (g-CN) was synthesized using urea as a precursor at temperature 550 °C in a muffle furnace. Palladium Nano-particles were introduced in the graphitic carbon nitride matrix by fairly new chemical sol-gel process followed by filtering and drying. Material characterization such as X-Ray Diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM) and Energy-dispersive spectroscopy (EDS) were performed. XRD indicates the formation of polycrystalline material. SEM and TEM analysis indicate the uniform Palladium nanostructures impregnated g-CN matrix. EDS analysis justifies the presence of all the elements.

Nanosilicon as a material for sensors and thermoelectrics

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Nanosilicon stands for a large variety of materials composed of Si nanostructures, namely arrays of vertical Si nanowires (SiNWs), nanostructured Si thin films and porous Si, composed of a skeleton of interconnected Si nanowires and nanodots. Due to their low dimensionality the above materials show very different properties from those of bulk Si, including a much lower electrical and thermal conductivity, higher Seebeck coefficient and much higher surface area. In this talk we will mainly focus on porous Si and vertical SiNWs on a silicon substrate for two main applications: a) porous Si as a very low thermal and electrical conductivity material on the Si wafer applied as a local platform on Si for the on-chip integration of Si thermal sensors and thermoelectric generators and b) SiNWs used as a means of increasing the Si surface (3-dimensional (3D) structuring) towards high capacitance density on-chip microcapacitors. A state-of-the art Si-based thermoelectric generator with an output of $0.39\mu\text{W}/\text{cm}^2$ will be presented. A thermal Si sensor and a corresponding flow meter for controlling air input in an automobile engine, which rivals state-of-the-art commercial systems, will be also presented. Finally, on-chip 3D capacitors with increased capacitance density, paving the way towards Si-based autonomous sensor systems, will be discussed.

Temperature effect on the mechanical characteristics of niobium nitride thin films

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This paper focuses on revealing the length influence of a group of gold cantilevers on the mechanical behaviour (i.e. bending stiffness, Young modulus, pull-off force) on the one hand and on the investigation of the temperature influence on the pull-off force of thermally actuated microcantilevers, on the other hand. The length was ranged between 200 μm and 350 μm while the temperature was ranged between 20 °C to 100 °C. The tests were performed using an atomic force microscope. A non-linear variation of the bending stiffness of microcantilevers as a function of temperature was experimentally determined. The variation of the pull-off force between microcantilevers and substrate was monitored at different temperatures. The results obtained in the study are important to enhance the design of MEMS devices and to increase their reliability and their lifetime. Moreover, the results are extremely useful in understanding and controlling the mechanical characteristics of sensing/acting micro-components under thermal operating conditions. The results are promising for applications in MEMS devices where accurate properties of the thermally actuated cantilevers are required within the extended temperature range.

Functional bionanocomposites prepared through cellulose mineralization

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Alkaline earth stannates with the general formula RSnO_3 ($\text{R} = \text{Ba}, \text{Sr}$ and Ca) are important material systems in view of their interesting physical properties and perovskite structures. Perovskite-type oxides have a simple and flexible structure that is easy for ionic substitution, carrier doping and oxygen non-stoichiometry, which can form a vast set of technologically important materials for a wide variety of industrial applications. BaSnO_3 is a cubic perovskite-type oxide that behaves as an n-type semiconductor with a wide band gap of 3.4 eV and remains stable at temperatures up to 1000°C. It has wide applications such as thermally stable capacitors, humidity sensors, gas sensors, etc. BaSnO_3 doped with a few percent of La exhibits unusually high electrical mobility of $320 \text{ cm}^2(\text{Vs})^{-1}$ at room temperature and superior thermal stability at high temperatures.

BaSnO_3 powder was prepared by solid state ceramic method. X-ray diffraction pattern of the prepared sample presents the characteristic peaks of cubic phase of BaSnO_3 . The average size of the crystallites, estimated by Debye Scherrer's formula, was found to be 49 nm indicating the nanostructured nature. The SEM image shows a porous surface morphology with grains of cuboidal structure with well-defined grain boundaries. UV-Visible spectra shows BaSnO_3 powder exhibit high reflectance in the 400-700 nm range. The open aperture Z-scan measurements are carried out in the present sample using 5 ns laser pulses at 532 nm from a frequency doubled Nd: YAG laser. The normalized transmission decreases at higher laser intensities indicating an optical limiting behavior. From numerical fitting the effective third order absorption coefficient β_{eff} and saturation intensity I_{sat} are found to be $6.9 \times 10^{-11} \text{ m/W}$ and $9.0 \times 10^{12} \text{ W/m}^2$, respectively. These values indicate a high optical limiting efficiency, comparable to that of graphene and its metal hybrids.

Functional polymer-based nanocomposite fibers via electrospinning

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Polymer fibers with diameters in the nano- and micrometer size range attract high attention nowadays due to their unique properties including high surface to volume ratios, composition tailoring and facile introduction of multifunctionalities. One of the most versatile techniques employed for generating nano- and microfibers is electrospinning. Electrospinning can be used for the fabrication of polymer, ceramic and polymer-based nanocomposite fibers. The latter may be accomplished through the incorporation of inorganic nanoparticles within polymer fibers during electrospinning or via their anchoring onto the fibers' surfaces by following post-modification strategies. This fact renders the technique highly attractive and competitive in biomedical, optoelectronic, environmental, sensing, catalytic and energy-related applications.

In this presentation selected polymer-based electrospun nanocomposite fibrous systems will be discussed, including magnetite-containing electrospun microfibers and microrods with applicability in the biomedical field [1] and in water remediation processes [2] and catalytic electrospun polymer fibers with embedded metal and metal oxide nanoparticles that were successfully employed as effective heterogeneous catalytic supports in organic synthesis [3, 4].

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Numerical approaches in the study of hybrid nanofluids and their possible applications in solar energy

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Numerical and experimental researches on nanofluids and hybrid nanofluids increased promptly over the last few years. In spite of some inconsistent reports—mainly due to the underprovided understanding of the involved mechanisms—nanofluids have been developed as a very good heat transfer fluid, especially in heat exchangers. Recently, hybrid nanofluids were defined as a new class of nanofluids with possible applications in almost all the fields of heat transfer. This is mainly because of the synergistic effect through which they provide promising properties of all of its constituents.

Nonetheless, hybrid nanofluids are a new sort of nanofluid that can be prepared by mixing two nanofluids, by suspending (i) different types (two or more than two) of nanoparticles in a base fluid, or by suspending (ii) hybrid (composite) nanoparticles in a base fluid. Basically, a hybrid material (fluid or solid) is a substance that combines the physical and chemical properties of different materials simultaneously and provides these properties in a homogeneous phase. A significant amount of research has been done in regard to the properties of nanocomposites and hybrid materials consisting of carbon nanotubes (CNTs) to be used in electrochemical-sensors, biosensors, nano catalysts, etc. but the use of these hybrid nanomaterials in nanofluids is at its very beginnings and has not been developed as such.

The idea of using hybrid nanofluids is to further improve the heat transfer characteristics of individual nanofluids and to beneficially combine different properties from oxides, carbon nanotubes, metals, composites etc. Latest research in this area clearly showed that proper characterization may make hybrid nanofluids a very promising heat transfer media. However, a lot of research is still needed in the field of preparation and stability, characterization, and applications to overcome the barriers in implementing these new fluids in real-life applications, especially in solar energy area.

Session 2.1- Keynote Lectures – Chair: Raquel Verdejo

Preparation and characterisation of cellulose nanocrystals for bio-based polyamide reinforcement

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Cellulose nanocrystals (CNCs) are considered as innovative biomaterial with large reinforcing potential and a kind of nanomaterial that can add functional properties of polymer composite materials, including enhanced barrier and mechanical properties. Various methods of CNCs preparation lead to materials with different structure/morphology and characteristics; as standardization protocols are at infancy this issue requires detailed description in regard to substrate sources, reaction conditions, purification routes, etc.

One of the key factors is the thermal stability of CNC since it may limit the processing possibilities with other (synthetic) polymer matrices. The processing temperature of most engineering polymers is close to or exceeds the onset temperature of cellulose degradation. Usually, surface functionalities of CNC undergo thermal degradation at the first stage, then decomposition of cellulose core material follows.

CNC-reinforced bio-polymers produced from renewable raw materials are an environmentally friendly alternative to conventional petroleum-based polymeric composites. Among bio-based polymers bio-polyamides (bio-PAs) are a unique class of engineering polymers showing high growth potential due to their promising mechanical, barrier and thermal properties.

Acknowledgements

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Problems with the current filler-reinforced nanocomposite technology and their solutions

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As filler reinforced nanocomposite technology is progressing into its mature stage, the advantage and shortage of different solutions for structure reinforcement developed so far have become progressively clear. From the point of view of the properties of reinforcing elements, nanofillers have better strength and stiffness than traditional fibres and micro-sized fillers. This is partially due to the size reduction of materials leading to the decrease of the size of pores and cracks. According to the Griffiths theory, strength of a material would increase with the the decrease in pore size. This is typical when comparing carbon nanotubes or nanofibres with traditional carbon fibres. Another reason to make nanofillers better is structural evolution. Using layered-structured clay and graphite as examples, exfoliation of layered-structured fillers into individual silicate and graphene layers would eliminates the weakest link in mechanical properties in micro formed particles, i.e., weak van der Walss force between the layers so that exfoliated silicate and graphene layers have much better mechanical properties. These are the driving force to develop nanocomposite technology for structural reinforcement. Nanofillers are superior over tranditional fibres and micro-fillers.

Matters arise when nanofillers are integrated into matrix to form composite structure. One problem encountered in early stage of development was the restriction of filler loading. Nanofiller reinfrocement is only effective in low filler content in nanocomposites. As filler loading increases, filler aggregation and poor dispersion become more and more significant resulting in rapid reduction in efficincy of reinforcement. In fact, the properties of the best nanocomposites produced using traditional polymer processing techniques are much worse than those of fibre reinforced composites in high fibre content, typically 40-60 vol% of fibre

content. The later stage of development make it possible to produce nanocomposites with high filler loading in well dispersed and oriented nanofillers in matrix through applying layer-by-layer self-assembly and spin coating techniques etc. It has been demonstrated that the strength and modulus of nanocomposites produced in these methods are much high than those of fibre composites with high fibre content. However every individual case shows that these nanocomposite are extremely brittle.

The current situation is that the design of both fibre reinforced composites and the current nano-filler enhanced nanocomposites is not perfect. A fundamnetal change is need by designing a new structure of reinforcement to overcome those problems. This presentation will give a rational analysis of the reasons behind those current problems and the concept of a novel composite structure to give comprehensive reinforcement of strength and stiffness without sacrificing toughness.

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Carbon nanoparticles for epoxy hierarchical composites

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Potable drinking water is essential for the good health of humans and it is a critical feedstock in a variety of industries such as food and pharmaceutical industries. For the first time, chitosan-alumina/functionalised multiwalled carbon nanotube (f-MWCNT) nanocomposite beads were developed and investigated for the reduction of various physicochemical parameters from water samples collected from open wells used for drinking purposes by a rural community in South Africa. The water samples were analysed before and after the reduction of the identified contaminants by the nanocomposite beads. The nanocomposite beads were effective in the removal of nitrate, chromium and other physico-chemical parameters. Although, the water samples contained these contaminants within the WHO and SANS241 limits for no risk, the long-term exposure and accumulation is an environmental and health concern. The reduction of these contaminants was dependent on pH levels. At lower pH, the reduction was significantly higher, up to 99.2% (SPC), 91.0% (DOC), 92.2% (DO), 92.2% (turbidity), 96.5% (nitrate) and 97.7% (chromium). Generally, the chitosan-alumina/f-MWCNT nanocomposite beads offer a promising alternative material for reduction and removal of various physico-chemical parameters for production portable water.

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Influence of graphene oxide on mechanical and hydrophilic properties of epoxy/banana fiber composites

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In this research work, Graphene oxide (GO) was synthesized by improved hummer's method and confirmed by Transmission Electron Microscopy (TEM), Field Emission Scanning Electron Microscopy (FE-SEM), Raman Spectroscopy, Fourier Transform Infrared Spectroscopy (FT-IR), and X-ray Diffraction (XRD). A cationic surfactant, cetyl trimethyl ammonium bromide (CTAB) was used for the dispersion of GO in the epoxy matrix and the influenced was assessed of GO (1.0, 2.5 and 5.0 wt. % loading) on the mechanical properties such as tensile strength, flexural strength, impact strength and surface hardness, and hydrophilic properties of the epoxy/banana fiber composites (EBF). The EBF composites were prepared using hand layup technique, with fiber length in the range of 5-7 mm and constant fiber ratio of 5.0 wt. %. The highest tensile strength of 11 MPa was obtained for 5.0 wt. % GO reinforced EBF as compared to 4 MPa for neat epoxy and 5 MPa for EBF. The lowest flexural strength of 23 MPa was obtained for neat epoxy as compared to 27 MPa for EBF and 55 MPa for 5.0 wt. % GO reinforced EBF. The impact strength increased from 31 J/m to 38 J/m and 92 J/m for neat epoxy, EBF, and 5.0 wt. % GO reinforced EBF respectively. The hydrophilic properties of the GO/EBFs composites also increase with the increase in GO concentrations. It was observed that due to the CTAB treatment, GO dispersed uniformly, resulting from good interactions with epoxy resin and banana fibers; improving the mechanical and hydrophilic properties of EBF with GO concentration.

Flexural and compression strength properties of novel Polyamide 6 nanocomposite materials

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In the manufacture of materials, fillers and reinforcement materials are included to improve the mechanical strength of the original polymer. These novel materials could be known as composites or nanocomposites, a classification based on the size of the fillers. In this research, spent oil based drilling fluid and cutting (ODFC) solid residue (waste-to-resource) was used as fillers to enhance the performance of polyamide 6 (PA6). Other include fillers used include: clay (montmorillonite - MMT and glass fibre. The analytical results shows that the use of nanosized fillers greatly improves the flexure and flexure strength of PA6 materials. The results were compared to those obtained for commercially available (simulated) clay filled PA6 composite which was used as a benchmark. The results demonstrated the importance of the use of the organophilised nanofillers which improved the intercalation of fillers in PA6 and improved failure resistance of PA6 materials.

Material configuration in the die, influences of pultrusion process parameters and part properties

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Pultrusion process is a continuous process for manufacturing of fibre reinforced polymers composites. Designing a material configuration affects the Pull force, encounter during Pulling of the fibres through the pultruded die. For any health process and part properties, optimum pull force at particular Material and heating is crucial to Understand. Governing equation was modelled to predict the entire pull force during scale up operation.

$$\int \int P(x,y,g(x,y)) \sin \theta \, dA_1 + \int \int [P]r(x,y,g(x,y)) \mu(\alpha,T) \, dA_3 + \mu(\alpha,T) du/dh = \mu(\text{static CO-friction}) (Pr + Sdh - G \delta R/\lambda)$$

Pulling force is governed by various parameters like frictional forces at guides and resin tank, the radius of the die, sliding induced shear, length of the die, viscous adhesion force, compact pressure in the die, shrink induced part detached. Sustainability of the smooth process is decided by the ultimate tensile of the part to be pulled in machine direction. The functional parameters which influences properties of the pultruded products are pulling speed, fibre volume fraction, resin release rate, fibre diameter and the configuration of material at die interface, die temperature, resin viscosity, pulling tension. The pulling tension is normally affected by viscosity of resin in tank, resin releasing rate from reinforced fibre, fibre volume fraction, filler ratio, pulling speed and heater position.

Synergistic action of micro and nanofillers on Polylactic Acid mechanical properties

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PLA-based materials are attractive for the manufacture of medical devices, rigid packaging solutions and, more recently, electronic devices and automotive parts. Their renewable bio-based nature, biodegradability and recyclability, are attractive features for their application and potential establishment in various industries. Ongoing research on PLA is mostly targeted on resolving specific drawbacks, such as its low heat-distortion temperature and low toughness. It is well-known that both micro and nanoparticles can potentially improve the mechanical, electrical, thermal, optical, fire-retardant etc. properties of polymeric composites. This study presents and evaluates the synergistic effects of micro and nano-sized reinforcements in a Polylactic Acid (PLA) matrix. It would be expected that variation of the scale of reinforcement may provide a synergistic combination of the benefits of micro and nanofillers and a possibility to tailor the composite's properties. Specifically, silane-treated micro-structured fireclay and basalt fibers were used as a micro-scale reinforcement for PLA, hybridized with nano-silica and layered silicate clays, in order to study their relative effects on the biocomposite's performance. The incorporation of nanofillers was expected to influence the fiber/particle-matrix interface by improving the interfacial shear strength and stiffening the matrix in the interfacial regions. The ultimate goal of this study is the optimization of the stress distribution near the fibre/particle surface by incorporation of nano-reinforcements, which could lead to improvement of the load transferring capability at the fiber/matrix interface, resulting to enhanced mechanical properties.

Self-assembly of organized clay nanotube patterns

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This work describes the preparation of polyvinylbutyral (PVB) nanocomposites reinforced with pristine and oxidized carbon nanotubes (CNT), graphene oxide (GO) and graphene nanoplatelets (GNP), via 'in situ' polymerization, at concentrations varying from 0.1 to 2.5 wt%. It was found that the presence of nanoreinforcements during the synthesis altered the degree of acetalization of PVB, since CNT and GO-reinforced samples had acetalization degree values between 50 and 77 mol%, whereas pure PVB and GNP-reinforced samples had values close to 65 mol%. FTIR, Raman and ¹H NMR results indicated interfacial interactions between oxidized CNT and PVB, while XRD results showed exfoliation of GO in PVB for all concentrations. GNP-reinforced nanocomposites presented exfoliation only for the lower concentrations. DMA analyses showed that the storage modulus increases 38.5, 20.5 and 20% for samples reinforced with 2.5 of GO, 0.5 of 'pristine' CNT and 1.0 wt% of oxidized CNT, respectively. Increases of 10, 12 and 7 °C in T_g were also observed for the same samples, respectively. DMA analyses of samples with higher degrees of acetalization show the presence of two Tan δ peaks, attributed to PVB and to PVA, characterizing a material with two immiscible phases. The entanglement degree, reinforcement efficiency factor ('C' coefficient) and 'A' adhesion factor, calculated from DMA results, evidenced higher degrees of dispersion, adhesion and reinforcement efficiencies for nanocomposites with 2.5 of GO, 0.5 of pristine CNT and 1 wt% oxidized CNT. The results showed that the 'in situ' polymerization method can improve the dispersion and final properties of the nanocomposite only if the nanoparticles are able to form relevant interfacial interactions during the PVB synthesis process. In addition, it was verified that the presence of nanoreinforcements altered the degree of acetalization of PVB, which also contributes to influence the final properties of the nanocomposites.

Engineered Nano Cementitious Composites for Sustainable Concrete Structures

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Ordinary Portland Cement (OPC) production is one of main contributors to CO₂ emissions and counts for about 8% of global CO₂ emissions. The production of OPC is expected to increase in the next 30 years due to limited cost-effective binders that can replace it. This will result in more CO₂ emissions. There is a growing need for new OPC-based materials that have smaller ecological footprint and exhibit improved mechanical and durability characteristics. This paper represents newly developed high performance cementitious composites with properties superior than the current OPC products. The proposed nano-cementitious composites consist of OPC reinforced with new hybrid and self-assembled nanoparticles composed of nanocrystal cellulose-carbon nanotubes (NCs/CNTs). In this paper, the processing of the hybrid (NCs/CNTs) particles will presented and their effect on the hydration, microstructure and mechanical properties of the cementitious composites will be discussed.

Mechanical, Thermal, and Flammability Behaviour of Low Density Polyethylene - Oil Based Mud Fillers Nanocomposites

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Novel low density polyethylene (LDPE)/Oil based mud fillers (OBMF) nanocomposites were manufactured by a melt compounding process. Fourier Transform Infrared (FTIR) Spectroscopy was used to characterise the structure of the nanocomposites. The results revealed the influence of different clay minerals present in OBMFs in forming chemical bonds within microstructures. Scanning electron microscope (SEM) and Energy Dispersive X-Ray Analysis (EDXA) confirmed the materials were nanocomposites and also provided the elemental composition of the filler and nanocomposites. Thermal properties were investigated by Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). The char yields of nanocomposites increased with OBMFs content. The TD5% (onset degradation temperature at 5 weight% loss) of the LDPE nanocomposite with 10.0 wt% OBMFs was ~4° c higher than that of neat LDPE. Limiting Oxygen Index (L.O.I.) and UL94 tests revealed that the nanocomposites possess excellent flame retardancy which increased with increasing percentage of OBMFs. Tensile and flexural tests were also conducted which showed there was not any significant effect of OBMFs on tensile strength and flexural modulus of the nanocomposites and thereby offering an alternative material choice.

Mechanical Properties of Graphene Oxide / Epoxy- Carbon Fibre Reinforced Composites

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This paper investigate the impact of graphene oxide (GO) reinforcement into epoxy/carbonfibre reinforced composites. The graphene oxide was synthesised using improved Hummers method. This method is a modern enhancement on the pioneering synthesising method first introduced by Hummers. It was then dispersed into epoxy matrix using methanol as a solvent and a sonication routine followed by drying sessions. The composites samples were manufactured by hand lay-up using vacuum infusion technique. Universal testing equipment were then used for mechanical properties evaluation correlating neat samples with 0.1%, 0.3% and 0.5% GO/epoxy carbon fibre-reinforced s specimens. Visual, optical and scanning electron microscopy was employed for damage characterisation. The early stage results shows minor improvements below 10% on both tensile and flexural strength on application of GO in the epoxy resins. However major benefits seems to indicate improved toughness for impact resilience in compression after-impact-strength test results.

Mechanical and swelling properties of hydroxyl-terminated polybutadiene polyurethane elastomers and nanoclay composite

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We investigated the polyurethane system composed of PBHT: MRG: IPDI with the addition of different mineral charges (nano clay, TiO₂, Carbon Black, ZrO and ZnO) and the effect of not using chain extender. The swelling character of the polyurethanes was investigated with the aid of the gel fraction, the degree of crosslinking and the average molecular weight between crosslinks, in addition to characterizing them by FTIR to study the character of the CO stretching signal in urethane. It was found that the crosslink densities for the HTPB-MRG-IPDI polyurethane system were minimal for a nanoclay polyurethane nanocomposite. This could be attributed to the blocking effect of the nanoclay. The sample without chain extender showed a slightly higher value in the crosslink density. No significant relationship was found between the hydrogen bonding index (HBI) values and the crosslink density.

Mechanical properties were also studied, looking for correlations with the crosslink density data and it was found that with TiO₂ and nanoclay there is a correlation between this density and elongation at break, the greater one, the greater the other. In the case of other charges (Carbon Black, ZrO and ZnO) the same effect does not occur, this may be due to the fact that they significantly decrease the elongation at break.

Synergistic action of micro and nanofillers on Polylactic Acid mechanical properties

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PLA-based materials are attractive for the manufacture of medical devices, rigid packaging solutions and, more recently, electronic devices and automotive parts. Their renewable bio-based nature, biodegradability and recyclability, are attractive features for their application and potential establishment in various industries. Ongoing research on PLA is mostly targeted on resolving specific drawbacks, such as its low heat-distortion temperature and low toughness. It is well-known that both micro and nanoparticles can potentially improve the mechanical, electrical, thermal, optical, fire-retardant etc. properties of polymeric composites. This study presents and evaluates the synergistic effects of micro and nano-sized reinforcements in a Polylactic Acid (PLA) matrix. It would be expected that variation of the scale of reinforcement may provide a synergistic combination of the benefits of micro and nanofillers and a possibility to tailor the composite's properties. Specifically, silane-treated micro-structured fireclay and basalt fibers were used as a micro-scale reinforcement for PLA, hybridized with nano-silica and layered silicate clays, in order to study their relative effects on the biocomposite's performance. The incorporation of nanofillers was expected to influence the fiber/particle-matrix interface by improving the interfacial shear strength and stiffening the matrix in the interfacial regions. The ultimate goal of this study is the optimization of the stress distribution near the fibre/particle surface by incorporation of nano-reinforcements, which could lead to improvement of the load transferring capability at the fiber/matrix interface, resulting to enhanced mechanical properties.

Prediction of cure mechanism of Polyester based composites across Die during Pultrusion process

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Thermal conductivity of uncured mass plays crucial role in curing of reinforced thermosets composites. The rheological and kinetic changes take place during the curing of resin are also crucial in understanding the pultrusion process for producing reinforced composites. In this study, the kinetics, thermal conductivity and rheological parameters of the resin and the composites have been determined through model fitting of experimental results from differential scanning calorimeter (DSC) and rheological Measurements. Thermal conductivity from the TGA is fitted in mathematical model to predict the thermal conductivity of uncured mass in the die during processing. These parameters are then used in another mathematical Model representing a pultrusion die. This model can be used to predict the influence of operating conditions, such as heating rate and fibre volume fraction on curing in the die.

Session 2.3 –Biomaterials & Biomedical Devices – Chair Radhakrishna Prabhu

3D arranged reduced graphene oxide – polyethylene glycol – amine based biosensor platform for super-sensitive detection of procalcitonin

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The antibiotic crisis is a major problem in international healthcare. A poor infection prevention and control coupled with the misuse and overuse of antibiotics are identified as main reasons of this crisis [1]. Therefore the US Center of Disease Control and Prevention (CDC) advises to improve the antibiotic prescribing using extra diagnostics during the general medical examinations [2]. Existing diagnostic systems are expensive, bulky and can only be operated by special trained staff, which extremely reduces their applicability. On the other hand, low-cost quick tests are less sensitive and only have qualitative outputs. There is a high demand for high sensitive, low-cost, reliable, easy-to-use and fast biosensors.

In this paper we present a fast, high-sensitive and cheap biosensor platform utilizing the superb electrical properties, the tremendous surface area and biocompatibility of novel 3D arranged Graphene flakes, merged with the selective antigen affinity of antibodies. The biosensor platform is a label-free concept and an Electrochemical Impedance Spectroscopy (EIS) read-out is used leading to quantitative biomarker detection. All fabrication processes are standard scalable MEMS processes.

PCT is used as biomarker as PCT allows diagnose between bacterial and virus related infections, which dramatically helps to make the right decisions during antibiotic prescribing [3]. The PCT levels are ranging from 0 to 10 ng/ml (see figure 1). Within the 3D Graphene biosensor approach a fast detection speed of < 10 minutes is observed and a Limit of Detection (LOD) of < 0.2 ng/ml PCT is identified. These finding indicates a much better sensitivity of our device compared to commercial PCT quick-tests [4].

To fabricate the novel 3D arranged Graphene biosensor, the reduced Graphene Oxide - Polyethylene Glycol - Amine (rGO-PEG-NH₂) was suspended in Isopropyl alcohol. The ζ -potential of the in-solution Graphene flakes was optimized adding MgCl₂ · 6H₂O and enhanced to +46mV. A high performance ultrasonic mixer where used to crumple and disperse the rGO-PEG-NH₂ flakes within the solvent. Subsequently the Graphene was deposited from solution onto 5 μ m line and space interdigitated gold electrodes, utilizing Electrophoretic Deposition (EPD) technique. In order to control the deposition quality, Electron Microscope (SEM) was used to identify the successful deposited 3D arranged Graphene structures (see figure 2). 1-Ethyl-3-(3-Dimethylaminopropyl) Carbodiimide (EDC) and N-hydroxysuccinimide (NHS) were used to covalently couple monoclonal procalcitonin (PCT) antibodies to the deposited Graphene. Dry milk protein was used to block the surface and prevent unspecific bindings. To validate the successful Graphene antibody coupling, and to prove the antibody viability after functionalization, a sandwich fluorescence assay based on Alex Fluo 488 was performed (see figure 3). The detection behavior of the developed biosensor was characterized by Electrochemical Impedance Spectroscopy (EIS). The sensor signal can be seen in figure 1. It shows the excellent potential of the new sensor platform.

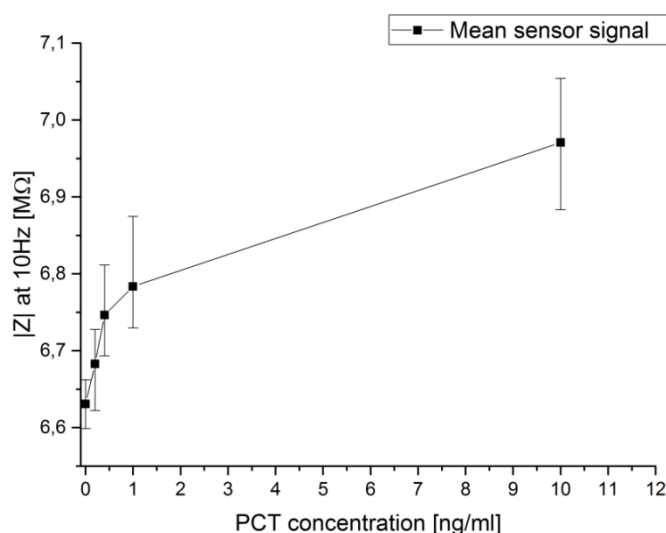


Figure 1: Mean sensor impedance of five label-free 3D arranged Graphene based biosensors detecting PCT levels from 0 to 10ng/ml at 10Hz.

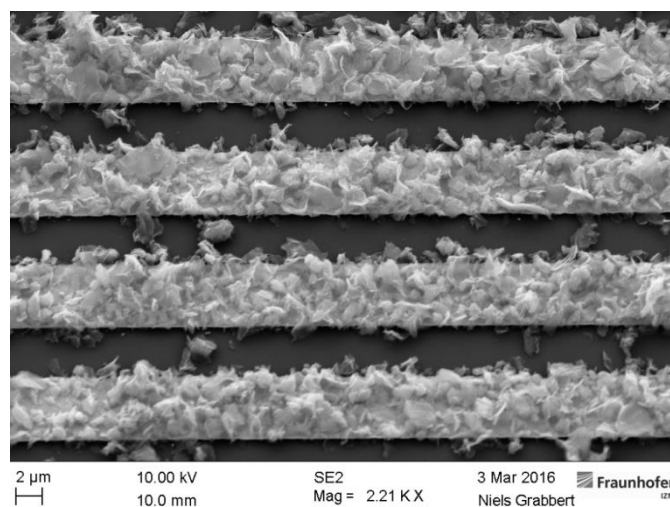


Figure 2: SEM image of electrophoretic deposited 3D arranged Graphene flakes on top of 5μm line and space interdigital gold structure.

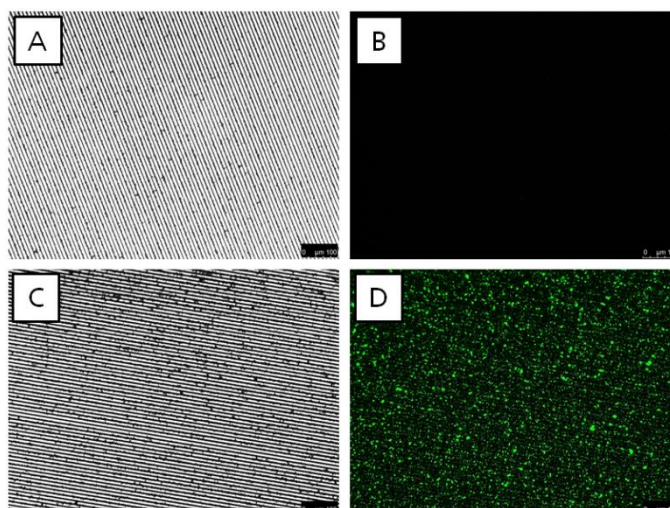


Figure 3: Fluorescence microscopic prove of successful binding between PCT antibodies and Graphene flakes, negative control: (A) transmission light and (B) fluorescence light, positive control: (C) transmission light and fluorescence light (D).

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Investigations on sensitivity enhancement of SPR biosensor using tunable wavelength and graphene layers

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Surface plasmon resonance (SPR) is a well-known, rapid and sensitive technique used for probing the biomolecular interactions in real-time. Typical conventional SPR biosensors include a thin metal film coated on a prism isolating the sensing medium from the prism. Most commonly, a thin gold film is used in SPR sensors because of the stable optical and chemical properties. However, adsorption of biomolecules on the gold surface is very poor which limits the sensitivity of the SPR biosensors. Several new approaches have been suggested to improve the sensitivity of SPR sensors over the last two decades. Most of them are based on creating nanostructures on the metal surface to enhance the localized E-field and therefore, it is quite challenging to have control over their optical properties.

Graphene, a single layer of carbon atoms arranged in the honeycomb structure, is emerging as the most popular material of the decade which is under intense research. Recently, there have been few reports on using graphene on a metal film based SPR sensor to improve the sensitivity. Graphene offers several advantages over the conventional SPR sensing due to its unique structural and optical properties. However, the role of incident light wavelength and graphene layers in sensitivity enhancement is unclear. This paper reports computational investigations on sensitivity enhancement of SPR biosensor using tunable wavelength and graphene layers. The reflectivity of p-polarized incident light has been calculated using the N-layer model for the most common Kretschmann configuration. Sensitivity enhancements over a conventional SPR sensor have been calculated. Computational results show that tuning the wavelength from 1600-600 nm, sensitivity of the graphene-based SPR biosensor can be increased under angular interrogation method. Also, irrespective of the incident light wavelength, up to ten layers of graphene, a sensitivity of the SPR biosensor increases linearly with a number of graphene layers.

Mechanical structural design of a MEMS-based piezoresistive accelerometer for head injuries monitoring: A computational analysis by increments of the sensor mass moment of inertia

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This work focuses on the proof-mass mechanical structural design improvement of a tri-axial piezoresistive accelerometer specifically designed for head injuries monitoring where medium-G impacts are common; for example, in sports such as racing cars or American Football. The device requires the highest sensitivity achievable with a single proof-mass approach, and a very low error (<1%) as the accuracy for these types of applications is paramount. The optimization method differs from previous work as it is based on the progressive increment of the sensor proof-mass mass moment of inertia (MMI) in all three axes. Three different designs are presented in this study, where at each step of design evolution, the MMI of the sensor proof-mass gradually increases in all axes.

The work numerically demonstrates that an increment of MMI determines an increment of device sensitivity with a simultaneous reduction of cross-axis sensitivity in the particular axis under study. This is due to the linkage between the external applied stress and the distribution of mass (of the proof-mass), and therefore of its mass moment of inertia. Progressively concentrating the mass on the axes where the piezoresistors are located (i.e., x- and y-axis) by increasing the MMI in the x- and y-axis, will undoubtedly increase the longitudinal stresses applied in that areas for a given external acceleration, therefore increasing the piezoresistors fractional resistance change and eventually positively affecting the sensor sensitivity. The final device shows a sensitivity increase of about 80% in the z-axis and a reduction of cross-axis sensitivity of 18% respect to state-of-art sensors available in the literature from a previous work of the authors. Sensor design, modelling, and optimization are presented, concluding the work with results, discussion, and conclusion.

Nanoparticle emissions due to automated drilling on epoxy, polyester and polypropylene based nanocomposites

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The use of silicate nanofillers as mechanical reinforcements in polymers is increasingly being well established throughout literature. This has generated an influx into various commercial industries such as the automotive industry. However, there is still an insufficient understanding on how these fillers effect the release of nanoparticles to evaluate and quantify the full risks associated to nanorelease and nanoparticle exposure. In this study, the effect on nanorelease due to drilling on Polypropylene (PP) reinforced with 20% Talc, 5% montmorillonite (MMT) and 5% wollastonite (WO) is investigated. With 5% WO, equivalent tensile properties with a 10 % weight reduction were obtained relative to the reference 20% Talc sample. The materials were fabricated through a twin screw extruder. The nanorelease studies were undertaken using the controlled drilling methodology for nanoparticle exposure assessment developed within the SIRENA life project. Measurements were taken using CPC, SMPS and DMS50 equipment for real-time characterization and measurements. The particle number concentration (of particles <100nm) and particle size distribution (4.87nm – 562.34nm) of the particles emitted during drilling were evaluated to investigate the effect of the silicate fillers on the particles released. The nano-filled samples exhibited a 33% decrease (MMT sample) or a 30% increase (WO sample) on the average particle number concentration released in comparison to the neat polypropylene sample. The size distribution data displayed a substantial percentage of the particles released from the PP, WO and MMT samples to be around 10nm, whereas the Talc sample appeared to emit larger particle diameters. No independent nanoparticles of the fillers were found in the microscopy (SEM) analysis on samples collected within the test chamber.

Acknowledgement

The work is part of EC project named Simulation of the release of nanomaterials from consumer products for environmental exposure assessment (SIRENA, Pr. No. LIFE 11 ENV/ES/596) and QualityNano (Grant Agreement No:INFRA-2010-262163).

Development of a ring cavity-based fibre optic sensor for MR-compatible medical sensing applications

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Advances in robotic systems and rapid developments in minimally invasive surgery (MIS) have made their use possible in the operating room due to many distinct advantages offered by MIS over conventional operations. The constant increase of medical examinations/surgeries using intraoperative guidance with magnetic resonance imaging (MRI) has promoted research on new sensors to be applied in this scenario. However, as the MIS is performed under constrained spaces, there is a need for micro-/nanosensors to monitor localised biophysiological conditions. Optical fibres offer several advantages such as inertness, no electromagnetic interference (ideal for MR compatibility), small size allows miniaturization adequate for most common minimally invasive medical applications and integration of micro-/nanosensors on the fibre tip, remote and real-time in vivo measurement/monitoring capability of multi-parameters.

Optical fibres can be used to excite surface resonance modes (SRM) of a ring cavity design. Specific SRM can be created around the ring cavity which is highly sensitive to the surrounding environmental conditions in nano to micrometer distances from the surface. These resonant surface waves highly depend on the ring cavity design. The phenomena of SRM of the ring cavity was utilised to develop the fibre optic sensor. Herein, we report a preliminary ring cavity-based fibre optic sensor design and development on the tip of the fibre for medical sensing applications. The ring cavity was developed using a PMMA doped with 250 μ M Rhodamine 6G. A 532nm laser was used to excite the fluorescence in the ring cavity and the emitted fluorescence signal was measured using a spectrometer through an optical fibre. Developed sensor was tested for temperature monitoring. Tests for the MRI compatibility were performed on the developed sensor under the 1.5T MRI system. This paper includes investigations on a new sensor design, characterisation and initial experimental test results.

Selective Separation of Lead Ions Using New Nano-Adsorbent GH-92

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One of the main sources of environment pollution is the industrial wastewater which contains heavy metals and can be found in many industries. If these heavy metals enter in the human body, would cause many health problems. On the other hand, different researches around the world show that nanotechnology is an effective way to remove pollutants. In this research, for the first time in the world, a type of natural sponge of Persian Gulf that has Nano holes has been used to remove the lead ion selectively from calcium, magnesium and cobalt ions in aqueous solution. The present study identified a sample belonging to the sponge of Demospongiae class. The aggregation of absorption in the sponge, contact time, particle size and by measuring environment's pH were measured. The results show this type of sponge, GH-92, is able to absorb different amounts of mentioned metal ions. Adsorption amount of calcium, magnesium and cobalt by this type of sponge was very small. The highest adsorption capacity belonged to lead ion in pH= 4.5 to 5 with mesh 230 which was 79.19 mg per gram of adsorbent. This is the highest adsorption capacity of lead comparison with reported articles for selective separation of lead ion.

Magnetoactive microrods: Fabrication, characterization and magnetic hyperthermia effect

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Nowadays, polymeric nano/microstructures attract high attention in the biomedical field for the development of novel therapeutic systems. The present work focuses on the fabrication of magnetoactive, polymer-based fibrous microrods belonging to the broad category of stimuli-responsive materials. The microrods consist of the water soluble and biocompatible poly(ethylene oxide) (PEO), the biocompatible and biodegradable poly(L-lactide) (PLLA) and pre-formed oleic acid coated magnetite nanoparticles (OA.Fe₃O₄). The fabrication protocol involved the initial preparation of electrospun magnetoactive fibers by electrospinning, followed by fiber “cutting” in order to obtain the microrods. The “cutting” process made use of sonication and UV-irradiation processes. Magnetic hyperthermia studies were carried out under an alternating magnetic field in the presence of both, the as-prepared electrospun fibers and the corresponding microrods containing different magnetic loading and conclusions were extracted in regards to the magnetic hyperthermia effect induced by these nanocomposites.

Acknowledgements

This work is based upon work from COST Action TD1402 “Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy (RADIOMAG)”, supported by COST (European Cooperation in Science and Technology, www.cost.eu). The Fe₃O₄.OA sample used in this work was synthesized by Florica Balanean (University Politehnica Timisoara).

Life cycle analysis of products incorporating engineered nanomaterials: a practical example to incorporate specific human health and environmental effects on PEG-CdTe added printing ink

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Life Cycle Assessment (LCA) is a standardized methodology for determining and assessing the environmental impacts of products across their whole life cycle, for comparing different options/products with respect to their potential impacts on the environment and for identifying the critical points within the product life cycle that contribute most to these impacts. Within the Life Cycle Impact Assessment (LCIA) phase, characterization factors (CF) are applied in order to quantitatively characterize the impacts of a certain substance to the different impact categories. Such factors are substance-specific and are based on models of cause-effect chains that describe the behaviour of a substance in the environment.

Different research studies have addressed the LCA for products incorporating engineered nanomaterials (ENMs), however, most of these studies do not incorporate specific CFs for ENMs and publications are being released describing the process to generate them. Within the present study a LCA has been performed considering as functional unit one DINA4 paper printed with polyethylene glycol cadmium telluride quantum dots (PEG CdTe QDs) additivated ink.

The main goal of performing this LCA has been twofold, on the one hand, to compile a life-cycle inventory (LCI) to quantify the total materials, energy and emissions flow related to (i) the production of a water based printing ink containing PEG-CdTe QDs, (ii) a particular application of the manufactured ink, namely the printing process of a DinA4-paper sheet with a household ink-jet printer; and (iii) the end-of-life scenario (EOL) of the printed paper in a landfill. On the other hand, to evaluate the environmental performance in freshwater ecosystems and the effect on the human health of the nanoadditivated ink along its whole life. The present LCA represents the ideal scenario where all substance data gaps are covered including CFs specifically developed for EMNs and their released forms throughout products' life cycle.

Fluorescent conjugates with halloysite - prospective biomarkers

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Halloysite – aluminosilicate nanotubes with different chemistry of inner and outer surface – can be conjugated with quantum dots and fluorescent dyes. Halloysite plays a role of solid support preventing quantum dots from agglomerating. The obtained conjugates demonstrate fluorescent properties and are resistant to photobleaching. Halloysite – quantum dots composites can be employed as biomarkers for imaging of living human cells. Furthermore, the lumen of halloysite nanotubes can be loaded with functional additives (e.g., anticancer drugs), thus opening the way for combined imaging/therapy approach. The improved resistance of brightly colored halloysite-based composites to photobleaching also promises their applicability in fluorescent paints and coatings.

On the uses of predictive toxicology for engineered nanomaterials approval to be used as biocidal active substances under the Biocidal Products Regulation

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To date only two engineered nanomaterials (ENMs) have been approved to be used as biocidal active substances in the formulation of biocidal products under product type 18 (insecticides, acaricides and products to control other arthropods). Such materials are silicon dioxide (as a nanomaterial formed by aggregates and agglomerates) and synthetic amorphous silicon dioxide (nano). The use of non-animal alternative test methods has been foreseen in the Biocides Product Regulation, Regulation (EU) 258/2012 (BPR). Further, the BPR is one of the existing regulations that includes a specific definition of nanomaterials. On the present article, a review is made on the potential uses of Quantitative Structure-Activity Relationship approach (Nano-QSARs) to be used as a non-testing method for the generation of ecotoxicological data required for the approval of new active substances in the nanometric scale. Relevant challenges are to be faced in the application of computational chemistry but it could meet the needs imposed by the BPR in relation to the use of non-testing methods. However nanospecific adaptations need to be implemented further on ecotoxicological testing so that obtained results are considered a suitable input for models' building. The BPR, thus, sets the framework for innovative approaches in the regulatory approval of new chemicals that integrate special considerations derived from the chemical nature of ENMs and the application of non-testing methods but, to date, the implementation of such actions is not feasible in practical terms.

Session 2.4 – Functional Nanocomposites – Chairs: Krzysztof Pielichowski & Alina Adriana Minea

A correlation between nano and micro-hardness properties of TiN nanoparticles strengthened SAF 2205

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Plastics are ubiquitous in everyday life and offer increasing technological and medical advances to improve/extend quality of life. However, with current global production of 311 m tonnes per annum, and forecast increase to 1,124 m tonnes by 2050, reflecting an 8% to 20% of oil demand exceeding that used by the aviation industry. Use of fossil fuel as raw materials combined with the high energy demand for their production (accounting for 15% total carbon budget by 2050) is not sustainable.

Petrochemical based plastics are non-biodegradable resulting in severe global pollution (an estimated 10-20 million tonnes per annum entering the world's oceans) causing damage to marine ecosystems, associated industries and public health. Consequently, plastic pollutants will continue to accumulate from over 150 million tonnes in the oceans today, rising to potentially 250 million tonnes by 2025 with the suggestion that there will be a greater mass of plastic than fish in the sea by 2050, unless action is taken. In addition to the polymers themselves, most plastics contain additives such as the lead in PVC, posing further hazards to the environment and human health.

The combination of decreasing fossil fuel reserves, environmental pollution coupled to increase in demand for plastics has led to the need for a shift to exploiting bio-based, biodegradable plastics for long term sustainability, and protection of the environment.

A range of microbes produce monomers and polymers suitable for plastic production, but as a consequence of the high price of production, and the controversial use of food crops for this purpose, the current market share of bioplastics is limited to 0.2%. This paper presents strategies for exploiting microbes grown on waste substrates for production of polyhydroxalkanoates (PHAs), a group of polyesters produced mainly as storage compounds in bacteria where biosynthesis is triggered by nutrient limitation and stress.

Erbium Modified Titania Decorated MWCNT Nanocomposite: A visible light driven photocatalyst for the decolourisation of Reactive Red 120

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Photoactive Erbium modified titanium dioxide (Er:TiO₂) nanoparticles decorated onto multi-walled carbon nanotubes were synthesised by sol-gel technique. TiO₂ was grafted onto MWCNT and were used as starting materials. Er³⁺ cations were adsorbed onto the TiO₂@MWCNT. In order to obtain the target photoactive nanocomposites, the solids obtained from the sol-gel suspensions were subjected to high-temperature thermal treatment. The surface morphology, crystalline structure, chemical composition and optical properties of the nanocomposites were characterized by scanning electron microscopy, transmission electron microscopy and X-Ray diffraction, FT-IR and UV-Vis spectroscopy. Inclusion of Erbium and MWCNT induced a shift of the TiO₂ bandgap with respect to the neat TiO₂. The photocatalytic activity of the Er:TiO₂@MWCNT system was evaluated based on the photooxidation of Reactive Red 120, an azo dye. Complete decolourisation of RR120 was achieved in 90 minutes compared to neat TiO₂, which had not decolourised the dye solutions after 3 hours. This study demonstrates that inclusion of erbium and MWCNT can induce a marked improvement in the performance of TiO₂ in visible light.

Effect of graphite addition on the tribological properties of pure titanium carbonitride (TiCN) prepared by spark plasma sintering

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Titanium carbonitride (TiCN) based cermet has received extensive attention as important components substantially utilized in cutting tools, milling operations and in sliding bearings. Recently, conventional WC-Co based hard alloys are being replaced with TiCN based cermets accompanied with the trend of high speed machining. These materials are considered potential candidate for a variety of tribological applications. In this study, the effects of graphite additions on titanium carbonitride (TiCN) based cermet were investigated. This involved consolidation of TiC_{0.7}TiN_{0.3} composition of pure TiCN based cermet and with 0.5, 1.0 and 1.5 wt % graphite using spark plasma sintering (SPS). The comparative studies on the tribological behaviours of the TiCN based cermets with graphite additions were performed using ball on disc set up at ambient temperature. Results show that the presence of different composition of graphite influences the microstructures of TiCN. In addition, a change in wear response of the sintered compacts was observed.

Temperature effect on the mechanical characteristics of niobium nitride thin films

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The mechanical, physical, chemical and tribological properties of niobium nitride thin films are making them suitable for a wide range of applications such as protective coatings, microelectronics and so on. The paper has two main goals: (a) the deposition of niobium nitride thin films by direct current magnetron sputtering on silicon Si (100) substrates and (b) the highlighting of temperature influence on their mechanical properties. The films were deposited at different nitrogen flow rates ranged between $0 \text{ cm}^3 \cdot \text{min}^{-1}$ and $2.2 \text{ cm}^3 \cdot \text{min}^{-1}$, while the deposition time and temperature, argon flow rate, discharge current, pressure and the distance between the substrate and the target were kept constant. The so-obtained coatings were further investigated by atomic force microscopy analyses to determine their topographical and mechanical properties namely the hardness and the modulus of elasticity. The tests were performed at temperatures between $20 \text{ }^\circ\text{C}$ and $100 \text{ }^\circ\text{C}$ while the relative humidity was kept constant. The results pointed out that both the modulus of elasticity and the nanohardness of the films decreased with the increase in testing temperature. The increase in nitrogen flow rate up to $1.65 \text{ cm}^3 \cdot \text{min}^{-1}$ went hand in hand with the increase in both mechanical properties.

Analysis of humidity influence on adhesion and tribological properties of niobium nitride thin films

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This paper is focused on characterizing several samples of niobium nitride thin films using an atomic force microscope at different humidity levels. The samples were deposited by direct current reactive magnetron sputtering on silicon substrates by varying the deposition temperature from room temperature up to 400 °C. The main objective of this paper is to investigate the influence of the humidity level on the adhesion force and on the tribological properties for this type of thin films. Hence, the relative humidity was ranged between 30 % and 80 % and the adhesion force between the AFM tip and each sample was experimentally determined using the spectroscopy in point mode of the AFM. Also, the friction force was determined, and then, based on its experimental values as well as on the values obtained for the adhesion force, the friction coefficient between the AFM tip and the sample was computed. The results obtained from the conducted experimental investigations allow establishing the niobium nitride thin films which have superior properties with respect to adhesion and tribology.

Highly efficient planar perovskite solar cells based on a D35 organic dye modified titanium dioxide electron transport layer

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Based on the panchromatic response of the perovskites [1], the mesoscopic solution processed solar cells have rapidly evolved in one of the most pioneering fields of nanomaterials-based renewable energy applications. The efficiency of such devices has already exceeded 20%, although stability issues are still under severe considerations [2].

In our group, the latest efforts aim at improving the performance of perovskite-based photovoltaics focusing on the synthesis of new perovskite [3,4] and device engineering, that consists of optimizing the absorber/compact layer interface. For this purpose, the compact layer was sensitized using the D35 D-p-A organic dye [5]. As a result, the energy levels at the corresponding interface were suitably aligned, and the electron transport process via the modified compact layer was facilitated. The obtained results imply a significant 12% improvement, leading to a 16.77% power conversion efficiency (PCE) champion device. In addition, the influence of the dye on charge carriers' transportation was investigated by electrochemical impedance spectroscopy and Raman analyses, providing further insight and confirmation on the role of the dye interlayer. The present work opens new perspectives in the field, as new developments in terms of improved photovoltaic efficiency and enhanced stability are expected via this ingenious approach.

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Synthesis and characterization of *N*-halamine-functionalized poly (fluorinated acrylate)/silica nanocomposite coating

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This paper is focused on characterizing several samples of niobium nitride thin films using an atomic force microscope at different humidity levels. The samples were deposited by direct current reactive magnetron sputtering on silicon substrates by varying the deposition temperature from room temperature up to 400 °C. The main objective of this paper is to investigate the influence of the humidity level on the adhesion force and on the tribological properties for this type of thin films. Hence, the relative humidity was ranged between 30 % and 80 % and the adhesion force between the AFM tip and each sample was experimentally determined using the spectroscopy in point mode of the AFM. Also, the friction force was determined, and then, based on its experimental values as well as on the values obtained for the adhesion force, the friction coefficient between the AFM tip and the sample was computed. The results obtained from the conducted experimental investigations allow establishing the niobium nitride thin films which have superior properties with respect to adhesion and tribology.

Polymer Nanocomposites for waste water remediation*Ajay Kumar Mishra**Nanotechnology and Water Sustainability Research Unit, College of Engineering, Science and Technology, University of South Africa, Johannesburg, South Africa***Corresponding Author: mishrak@unisa.ac.za*

Nano size materials have been extensively studied due to their size, high surface area and affinity for the adsorption. Polymer nanocomposites, have diversified applications in different areas such as biological sciences and wastewater treatment. Nanocomposites usually used to be incorporated within different functionalized materials such as multiwalled carbon nanotubes, activated carbon, reduced graphene oxide, and different polymeric matrices. Water pollution is mainly caused by the pollutants that result in severe environmental problems. Adsorption of different pollutants such as heavy metal ions and dyes from the contaminated water using nanocomposites has attracted significant attraction due to their characteristic properties. Polymer nanocomposites have better adsorption capacity, selectivity, and stability than nanoparticles. Magnetic polymer nanocomposites are also a very efficient class of nanocomposites in which magnetic nanoparticles have been used as the reinforcing material. They have the advantages of both magnetic separation techniques and nano-sized materials, which can be easily recovered or manipulated with an external magnetic field. The current research will be focused on the present and future status of effective for the removal of both organic and inorganic pollutants using polymer nanocomposites..

Experimental and Numerical studying on the Mechanical Behaviour of Epoxy Resin based two types of functionalization MWCNTs

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This paper is focused on characterizing several samples of niobium nitride thin films using an atomic force microscope at different humidity levels. The samples were deposited by direct current reactive magnetron sputtering on silicon substrates by varying the deposition temperature from room temperature up to 400 °C. The main objective of this paper is to investigate the influence of the humidity level on the adhesion force and on the tribological properties for this type of thin films. Hence, the relative humidity was ranged between 30 % and 80 % and the adhesion force between the AFM tip and each sample was experimentally determined using the spectroscopy in point mode of the AFM. Also, the friction force was determined, and then, based on its experimental values as well as on the values obtained for the adhesion force, the friction coefficient between the AFM tip and the sample was computed. The results obtained from the conducted experimental investigations allow establishing the niobium nitride thin films which have superior properties with respect to adhesion and tribology.

Synthesis and characterization of functionalized nanocomposite coatings based on epoxy resin, montmorillonite and (3-glycidyloxypropyl)trimethoxysilane

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This paper is focused on characterizing several samples of niobium nitride thin films using an atomic force microscope at different humidity levels. The samples were deposited by direct current reactive magnetron sputtering on silicon substrates by varying the deposition temperature from room temperature up to 400 °C. The main objective of this paper is to investigate the influence of the humidity level on the adhesion force and on the tribological properties for this type of thin films. Hence, the relative humidity was ranged between 30 % and 80 % and the adhesion force between the AFM tip and each sample was experimentally determined using the spectroscopy in point mode of the AFM. Also, the friction force was determined, and then, based on its experimental values as well as on the values obtained for the adhesion force, the friction coefficient between the AFM tip and the sample was computed. The results obtained from the conducted experimental investigations allow establishing the niobium nitride thin films which have superior properties with respect to adhesion and tribology.

Surface-Functionalization of novel poly (Acrylonitrile -co- Styrene/ Pyrrole) copolymer electrospun nanofibers for using as high-performance carrier for laccase immobilization

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In this work, poly (Acrylonitrile -co- Styrene/ Pyrrole) (poly (AN-co-ST/Py)) copolymer nanofibers was successfully synthesized using microwave preparation technique and used as carriers for immobilized Laccase enzymes. Nanofibers support surface were used for the covalent attachment and modifications using poly ethylenediamine (PEI) a spacer arm, and using glutaraldehyde (GA) as coupling agent. A novel colorimetric assay for the determination of the amount of coupled PEI binding with the poly (AN-co-ST/Py) nanofiber changes of the relative activity of immobilized enzyme. The reaction of complex formation is formed by the binding of copper (II) ions with long chains of PEI molecules on the surface of nanofibers by chelation. The main factor effects on the binding and treatment performance of copper (II) (Cu^{2+}) ions with PEI molecules such as PEI concentration, contact time, contact temperature, and pH are presented. The amine groups capacity as high as $650 \mu\text{l}/\text{cm}^2$ at concentration of PEI up to 2% were obtained. The optimum reaction temperature and pH for the immobilized enzyme were 70°C and 6.0, respectively. The effects of the different factors of PEI on the morphology of the resultant nanofibers were studied. The scanning electron microscopy (SEM) images showed that, the modified nanofibers with PEI has retained its nanofiber structure and uniform morphology with an average diameter of approximately 559.2 nm. The presence of PEI on the nanofiber surface was verified by FTIR and TGA analyses. Therefore, the prepared copolymer nanofiber proposed in this work showed promising potential for applications to enzyme immobilization.

Under potential deposition as a sensitive method for in situ characterization of Au nanoparticles deposited onto TiO₂ nanotubes

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The design of composite systems including noble metal nanoparticles (NPs) deposited on oxide supports is an important issue due to a variety of applications. The performance of these systems is strongly dependent on nature, amount and structural peculiarities of NPs. The main methods for examining of NPs are optical spectroscopy, SEM and TEM. However, these methods are not suitable for determination of total surface area and facet ratio of NPs. Recently, the method of underpotential deposition (UPD) has attracted interest for studying of Au NPs due to providing unique information about fingerprints of the surface. Here, we applied the UPD of Pb for probing the surface of Au NPs deposited onto TiO₂ nanotubes (TNT). TNT were produced by anodization and annealed at 350 °C, 450 °C and 550 °C. Au NPs were loaded onto the annealed TNT by photocatalytical reduction of Au(III) ions using different techniques: direct UV-irradiation of the TNT emerged into Au(III) solution (TNT-Au1) and initial Au(III) ions adsorption onto the TNT followed by UV-irradiation (TNT-Au2). According to the performed TEM and SEM measurements the size of Au NPs depends on the deposition technique and annealing temperature of TNT support. Au NPs in the TNT-Au1 system are larger than those in the TNT-Au2. The increase of annealing temperature of TNT also results in the deposition of larger Au NPs. Lead UPD on Au NPs occurs in the potential range from 0.1 to -0.4 V. The position of the observed peaks is close to the respective peaks of lead UPD on Au bulk electrodes, but their relative intensities point on the predominant [111] crystallographic orientation for TNT-Au1 and [100] for TNT-Au2. The apparent surface

area of the deposited Au NPs varied within 0.14–0.97 cm² per 1 cm² of the electrode geometric surface suggesting a monolayer deposition of lead ad-atoms.

PMMA based nano-composite polymer gel electrolytes for Lithium ion batteries

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Nano-composite polymer gel electrolytes containing poly-(methylmethacrylate) (PMMA), dimethyl carbonate (DMC), lithium perchlorate (LiClO₄), and fumed silica (SiO₂) have been prepared and characterized for ionic conductivity, viscosity and thermal studies. The ionic conductivity of polymer gel electrolytes has been found to be an increase with an increase in concentration of PMMA (at lower polymer content). The addition of nano sized fumed silica to gel electrolytes shows a maximum conductivity at 5wt.% concentration of SiO₂ along-with an increase in mechanical strength. The peak in the conductivity variation with the addition of SiO₂ nano-filler has been explained by percolation threshold model. The decrease in conductivity at higher concentrations of polymer and nano-filler has been correlated with the increase in viscosity of the electrolytes. Thermal stability of nano-composite polymer gel electrolytes has been checked by differential scanning calorimetry (DSC) studies and it has been found that the nano-composite polymer gel electrolytes are thermally stable in the 0–90°C temperature range. The activation energy of the electrolytes has been calculated and correlated with the thermal stability.

Synthesis and characterization of an epoxy/silica/nanoclay hybrid nanocomposite and its application as anticorrosive coating

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In the present work, functionalized nanocomposite based on epoxy resin DER 331, organoclay montmorillonite modified with methyl-tallow-bis-2-hydroxyethyl quaternary ammonium salt (OMMT) and (3-glycidyloxypropyl)trimethoxysilane were obtained at loadings 0%, 0.5%, 1%, 3%, 5% and 10 wt% OMMT. The functionalized nanocomposites were deposited on carbon steel substrates, after were cured at controlled temperature. The functionalized nanocomposite coatings were characterized using physical techniques such as Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR-ATR), Thermogravimetric Analysis (TGA), X-Ray Diffraction (XRD). Anticorrosive properties of the functionalized nanocomposite coatings were evaluated using electrochemical impedance spectroscopy (EIS) methods. The SEM analysis showed that the OMMT was uniformly dispersed in the epoxy matrix and the coatings were uniform, the X-ray analysis showed that exfoliation occurred for the OMMT in the organic matrix. The FTIR analysis showed the characteristic bands of epoxy resin and OMMT in the functionalized nanocomposites. The evolution of the electrochemical impedance spectroscopy parameters studied as a function of time showed that the anticorrosive performance of nanocomposite coatings increased when the coatings were functionalized with (3-glycidyloxypropyl) trimethoxysilane. On the other hand, the adhesion of the coatings to the metallic substrate also was increased.

Influence of aluminium doping on the structural, optical and electrical properties of RF sputtered zinc oxide films

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Zinc oxide is an n-type II-VI oxide semiconductor with wide direct band gap energy of 3.37 eV and large exciton binding energy (~ 60 meV) at room temperature and is highly transparent in the visible region. ZnO can be used as a potential candidate in fabrication of short wavelength optoelectronic devices such as laser diodes, blue and ultraviolet light emitters, photo detectors, gas sensors etc. ZnO powder is mixed with Al₂O₃ powder at different doping concentrations viz., 0, 2, 3 and 5 wt %. The powders are annealed at a temperature of 1200 °C for 6hrs and the pressed pellets of these Al doped ZnO powders are used as sputtering targets. Al doped ZnO films are fabricated by RF magnetron sputtering technique using RF power of 150 W, argon pressure of 0.015 mbar on glass substrate kept at a distance 4 cm from the target for a duration of 45 minutes. The structural, morphological, optical properties and electrical properties of the as-prepared films are studied using XRD, micro-Raman AFM, FESEM, EDS, UV-Vis spectroscopy, PL and Hall Effect measurement system.

The XRD patterns of all the films present a single, sharp and intense peak corresponding to (002) lattice reflection plane of hexagonal wurtzite phase of ZnO. Raman analysis supports the formation of wurtzite structure. The morphological study using AFM and FESEM images show uniform dense distribution of grains. All the films except 5 wt% Al doped ZnO film exhibit high transmittance up to 90%. PL spectra show intense luminescence peaks corresponding to UV and yellow emission for an excitation wavelength of 325 nm. The electrical study shows that high mobility is exhibited by pure ZnO film and 3wt% Al doped ZnO film shows highest value of carrier concentration ($0.8304 \times 10^{20}/\text{cm}^3$) and lowest value of electrical resistivity (0.18 Ωcm).

Optical properties of nanocomposite film with oriented ellipsoidal inclusions

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Nanocomposite films with the inclusion of ellipsoidal form are considered in the article. The influence of such parameters as the particle orientation in the film and the characteristics of the inclusions were studied. The theory of effective susceptibility was used for this calculation in case of a one-oscillator model of light absorption by particles. This gives an opportunity to calculate the optical absorption spectra taking into account the interaction of particles with the surface and with each other.

For ellipsoidal particles with oblate and prolate form, the absorption spectrum varies greatly with the angle of rotation. The appearance of an additional peak, which changes its intensity with an angle increasing is observed.

For such a model, the influence of the distribution of particle orientation in the film was calculated, since such a model is closer to the experimental data. The Gaussian and step-like distribution of the orientation angle are considered. The transition values of the normal distribution dispersion for an ellipsoidal particle are determined, which is equally elongated along two axes and is twice flattened on the third axis. Namely, the appearance of a new peak occurs when the dispersion value exceeds 0.3 for the simulated film

It is shown that when the form of ellipsoidal particles changes, absorption spectra depending on the angle also changes. For oblate ellipsoids, spectra shifts to the short-wave region, and for prolate ellipsoids spectra shifts to the long-wave, at the same angle of rotation. It is also shown that the absorption spectrum of ellipsoids of various shapes changes non-linear.

Laser ablated molybdenum oxide thin films

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Molybdenum oxide is a wide band gap n-type semiconductor material. It can exist in three crystalline polymorphs: a stable orthorhombic phase (α -MoO₃), a metastable monoclinic phase (β -MoO₃), and an open hexagonal structure. Molybdenum oxide finds variety of applications in numerous optical and electronics devices including organic light emitting diodes, photodectors, gas sensors, photovoltaics, batteries and multichromic coatings. Molybdenum oxide thin films were prepared by Pulsed Laser Deposition (PLD) technique using a frequency tripled laser radiation of wavelength 355 nm from a Q- switched Nd: YAG laser (Spectra Physics, Quanta Ray-INDI- series) having a pulse width of 7 ns and repetition frequency of 10 Hz. The deposition chamber was pre- evacuated to a base pressure of $\sim 10^{-6}$ mbar using a turbo molecular pump and a rotary pump. The films were deposited on quartz substrate kept at a distance of 4.5 cm from the MoO₃ target and the deposition was done with a laser energy of 70 mJ for a duration of 30 minutes. The films were post-annealed in air at different temperatures in the range 300-6000 C. XRD analysis reveals that as-deposited and films annealed at 300 0 C are amorphous in nature and the films annealed at temperatures 400 and 500 0 C show the presence of monoclinic MoO₃ phase. The film annealed at a temperature of 6000 C exhibit orthorhombic phase. The optical spectral analysis shows the film annealed at 6000 C shows good transmittance in the visible range. The films show intense PL emissions at 345, 396, 411, 452, and 470 nm. The emission at 345 nm can be attributed to near band edge emission due to free exciton recombination. The emissions at 3 96, 411, 452, and 470 nm may be attributed to Mo⁵⁺ d–d band transition of a heavily distorted polyhedron.

Silver incorporated indium oxide films - structural, optical and morphological studies

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Indium oxide, an n-type semiconductor finds vast variety of applications in the optoelectronic industry mainly because of its high optical transparency in the visible and near infra-red region, wide band gap energy (3.5 to 3.75eV) and high adhesion to the substrate surface. Noble metal nanoparticles absorb visible light due to surface plasmon resonance and the absorption range varies in accordance to particle size, shape etc. Silver incorporated In_2O_3 films are prepared using RF magnetron sputtering technique using RF power of 150W and an argon pressure of 0.015mbar. Silver powder in desired proportions namely 0,1,2,5 and 10 wt% is mixed with In_2O_3 powder and the well ground mixture is used as sputtering target. The films are sputtered on to clean glass plates for a duration of 45 minutes. The effect of silver incorporation on the structural, morphological, and optical properties are analysed using techniques such as XRD, micro Raman spectroscopy, AFM, FESEM and UV-visible spectroscopy. XRD patterns of pure and silver incorporated films reveal polycrystalline nature of the films and the XRD peaks can be indexed to cubic bixbyite crystalline phase of In_2O_3 . Average particle size of pure film estimated using Scherrer equation is 48nm. The particle size decreases with Ag incorporation. The morphological studies using AFM and FESEM analysis show dense distribution of small grains with grain boundaries. Ag incorporated films possess higher values of rms surface roughness. UV-visible spectral analysis shows that the transmittance of films decreases from 91 to 21% when Ag concentration increases from 0 to 10%. Absorbance of films also shows a systematic increase in the 390-500nm wavelength region and this may be due to surface plasmon resonance of Ag nanoparticles. Band gap energy calculated from the transmittance data is in the range 3.5-3.68eV which matches well with reported values of In_2O_3 .

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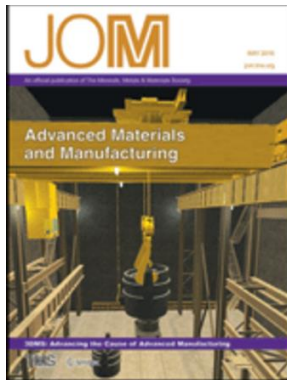
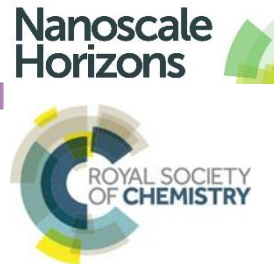
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