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GLOBAL SUMMIT ON ADVANCED MATERIALS SCIENCE AND NANOTECHNOLOGY

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Polylactic Acid-based materials: a journey over the potential versatility of biobased polymers

Abstract: Biobased and biodegradable polymers keep on being extremely promising in almost every technological field, given their potential as possible alternatives to traditional oil-based and non biodegradable plastics. Albeit the promising context, the industrial development of the so-called bioplastics strives to significantly increase its market share, being in 2023 at about 2.18 Mton (52.1% biodegradable, 47.9% biobased non biodegradable) over about 400 Mton of global plastics production, thus representing only about 0.5% of the total plastic market. Polylactic Acid (PLA), commonly syntesised via Ring Opening Polymerization starting from the cyclic dimer of lactic acid (L-lactide) is by far the most important industrial bioplastic, representing 31.0% of the market because it combines relatively good thermal features, i.e. Tg and Tm, with interesting mechanical properties, that make it suitable for different kind of industrial processing such as melt extrusion, filament production, thermoforming etc. Nevertheless, PLA suffers several drawbacks that prevent its use in even more fields: the most important ones are that it is relatively brittle, permeable to gases and the thermal stability at processing temperatures is low. Moreover, given its chemistry, it offers little or even no possibilities for chemical functionalizations, that would broaden the spectrum of its properties thus making it more versatile. The presentation will focus on the synthesis of many different PLA-based materials: the synthesis of PLA-based nanocomposites containing cellulose will be discussed together with an innovative approach using 1,3 Dioxolan-4-ones (DOXs) as functional lactide-equivalent comonomers in polylactic acid bulk polymerization having the aim of introducing many different functional moieties alongside the PLA backbone dramatically increasing the versatily of this polymer

Keywords: Polylactic Acid, PLA, bioplastic, nanocomposite, characterization, Ring Opening Polymerization

Biography: Marco A. Ortenzi is graduated in Industrial Chemistry and is currently (from Oct. 2024) Associate Professor in the Department of Chemistry of University of Milan. He started his career in 2001 and, since then, has been working on polymer synthesis and characterization, mainly polyesters and polyamides, with a strong focus on the potential industrial application of its researches. He cooperates with several companies for the development of innovative polymer-based materials: he is author in about 90 papers and inventor in 10 patents, all in the field of polymer science, most of them coming from joint researches between University and Companies.

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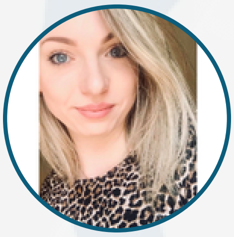

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Influence of Tool Geometry on Material Flow, Temperature Evolution, and Mechanical Properties in the Friction Stir Welding of AA6082

Abstract: The friction stir welding (FSW) process for joining AA6082 aluminum alloy was simulated utilizing computational fluid dynamics (CFD) to examine the effects of tool geometry on the resulting joints. Two distinct tool geometries were employed: a tapered cylindrical pin (simple pin) and a hexagonal pin with grooves (complex pin). The simulations were analyzed in terms of temperature evolution, total heat input, residual stresses, and material flow dynamics. The simulation results indicated that the use of the complex pin resulted in a miximum temperature of 406 °C, which is 5% higher compared to the simple pin. This increased temperature, coupled with higher shear stresses during the welding process with the complex pin, resulted in elevated residual stresses within the weld. Subsequent experimental evaluations of the produced welds included microstructural observations, hardness testing across cross-sections, and tensile strength assessments. The increased temperature during welding with the complex pin facilitated a more effective recrystallization process, leading to enhanced grain refinement in the stir zone (SZ). Specifically, the average grain size in the SZ was measured at 11 ± 1 µm for welds produced with the complex pin, in contrast to 14 ± 1 µm for those produced with the simple pin. Hardness profiles demonstrated that the welds fabricated with the complex pin exhibited higher hardness in the stir zone, recorded at 89.5 ± 1.3 HV, in accordance with the Hall-Petch relationship. The ultimate tensile strength (UTS) values corresponded to joint efficiencies of 72.5 ± 4.9% for the complex pin welds and 55.8 ± 8.6% for the simple pin welds. The findings underscore the significant influence of tool geometry on the thermal and mechanical properties of FSW joints.

Keywords: aluminum alloys, computational fluid dynamics, COMSOL, friction stir welding, mechanical properties, microstructure

Biography: Aleksandra Mirowska PhD, Eng, is an assistant professor at the Faculty of Mechanical Engineering and Ship Technology, Gdańsk University of Technology, Poland. The scientific disciplines she represents are mechanical engineering and materials engineering. Her research interests are related to metals science broadly, with a particular focus on aluminium alloys. She has completed numerous internships in scientific centres in Iran, Taiwan, Italy, Germany, Belarus and Slovakia. She defended her doctoral thesis entitled "Influence of friction stir welding technological parameters on the properties of the joints of selected aluminium alloys" with distinction in the mechanical engineering discipline. She is a reviewer for journals such as Journal of Materials Engineering and Performance, Steel Research International, Scientific Reports and more.

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Understanding and optimizing alternant and non-alternant nanographenes for spintronic and optoelectronic applications

Abstract: Motivated by the recent synthesis of non-alternant isomers of small peri acenes (seen as short armchair nanoribbons, AGNRs, with Z=3, 4 zigzag rings, and A=2 armchair rings) through the introduction of Stone-Wales (SW) and "SW-like" (azulene) moieties, on their alternant isomers (AGNRs), we set here to examine the roots, and profound characteristics of such nanographenes (NGRs or SW-AGNRs) to systematically optimize and functionalize their spintronic and optoelectronic properties. Although decreasing antiaromaticity determines the spin state for a given geometry, increasing aromaticity is the decisive factor for selecting the ground state geometry. Yet, it is not necessarily associated with larger negative values or negligible positive numbers of nucleus-independent chemical shifts (NICS). Actually, "higher aromaticity" may be accompanied by highly antiaromatic rings with positive NICS numbers. It is demonstrated that "increasing aromaticity" in fact describes the topological capability of the non-alternant system to accommodate the full (or the largest part of the) aromaticity pattern of the corresponding alternant NGR, meaning that "defects" should be concentrated as much as possible around the empty rings. The aromaticity pattern is fully determined by the number Z of zigzag rings at the two ends. We suggest that the optimum NGRs are the SW3x4 which is optimum for spintronic applications (but not for optoelectronic applications) and the SW4x4 which is suitable for both. These results and conclusions are in accord with earlier predictions of the present author about the "topological/aromatic" role of "empty" rings. Furthermore, they are also validated by the already synthesized non-alternant NGRs

Keywords: Carbon Nanostructures, Graphene, Magnetic Materials, Materials-Chemistry, Non-alternant nanographenes.

Biography: Aristides D. Zdetsis, Professor Emeritus department of Physics University of Patras, director Molecular engineering Laboratory. The focus of my work for the last ten years is on graphene, graphene-like graphene structures, 2D-materials and non-benzenoid materials with applications in spintronics (molecular magnetism), and optoelectronics. I am an IAAM and a VEBLEO fellow. I have written more than 150 research papers, and I have made more than 300 verified reviews (web of science) in major scientific journals, funding agencies and faculty promotions. I am listed in the top 2% of scientists worldwide in Stanford List, or 0.5% in Scholar GPS, with h=31.

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Cagri Yilmaz

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Mathieu-type nonlinear responses of the resonantly excited micro-cantilever to viscous loads for varying elastic stiffness and quality factors

Abstract: The sensitivity of the micro-cantilevers to target external forces in different environments can be improved by resonating them in monomodal and multimodal operations. Different types of external forces can simultaneously act the resonantly driven micro-cantilevers which interact with the biological samples or function with microelectromechanical devices. Correspondingly, determining the proper properties of the micro-cantilevers for different flexural eigenmodes is quite crucial to achieve the desired micro-cantilever sensitivity. In rheological applications, nonlinear models can be used to predict micro-cantilever behaviors in different fluids. Dynamic responses at the first two flexural eigenmodes considerably change in response to varying excitation amplitudes in the Mathieu function. Out-of-plane displacements of the micro-cantilevers are strongly responsive to varying elastic stiffness and quality factors. It is worth mentioning that the equilibrium position is higher for the smallest elastic stiffness of 0.9 N/m at the first flexural eigenmode. Furthermore, hydrodynamic loads determined using Sader's functions induce non-periodic oscillations. Hydrodynamic peak forces mostly ascend with increasing dynamic viscosity and density as expected. More deterministic hydrodynamic force patterns are also obtained for different quality factors at the first flexural eigenmode when compared with the higher flexural eigenmode. Observable sensitivity to viscous loads can be enhanced by selecting proper quality factors of the micro-cantilever, especially at the fundamental eigenmode. Therefore, nonlinear models can be robustly utilized to reflect the hydrodynamics of resonating micro-cantilevers with different mechanical properties.

Keywords: hydrodynamic sensitivity, micro-cantilever, elastic stiffness, quality factor, Mathieu function, higher flexural eigenmode

Biography: Cagri Yilmaz received his undergraduate degree in mechanical engineering from Middle East Technical University (METU) in 2007. He went on to complete his master's degree in mechanical engineering at Duisburg-Essen University in Germany in 2010. He worked as an intern in the manufacturing department at ThyssenKrupp MillServices & Systems in Duisburg. In 2010, he successfully completed his master's thesis at Trützchler Spinning firm in Mönchengladbach, Germany, as part of the T-Data project. Subsequently, he worked as a research assistant in the Distributed Artificial Intelligence Laboratory (Dai-Labor) at the Technical University of Berlin from 2011 to 2014, focusing on robot systems and smart grids. He completed his doctoral studies in the field of acoustics and vibration at Akdeniz University's mechanical engineering department in may 2022. Currently, he is engaged in theoretical studies on the sensitivities of micro-cantilevers to external forces under multi-frequency operations.

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Daniel BALSALOBRE LORENTE

University of Castilla-La Mancha (Spain)

The Influece Of Ict Over Sustainable Development: A Fresh Approach

Abstract: In the era of development, the world is facing severe challenges, and environmental degradation is one of them. However, the globe has tried to introduce several initiatives to fight for environmental sustainability, such as the Sustainable Development Goals. The leading role of the proposed goals is to balance development and environmental anxiety. Therefore, to these issues, artificial intelligence and technological advancements play a vital role in the natural resource economy in the digital age. Policy analysts are always looking for solutions and have come up with several viable remedies to this problem. Consequently, information & communication technology (ICT) plays a significant role in sustainability in the digital era. However, under the theme of natural resource sustainability, the effectiveness of ICT has a significant impact on sustainability. Accordingly, the current study investigates the long-run effect of income per capita, tourism, natural resources rents, urbanization, and ICT on environmental sustainability in 36 OECD economies from 2000 to 2018. The current research employs an Augmented Mean Group (AMG) and two-step GMM to investigate the study's objectives. Results show the positive contribution of urbanization, natural resources, and tourism to CO2 emissions, while ICT reduces emissions. An inverted EKC curve is also validated for selected economies. In addition, the moderate effect of ICT on urbanization, natural resources, and tourism shows a significant decline in CO2 emissions. In light of the findings, this study recommends several crucial measures for environmental sustainability.

Keywords: Augmented Mean Group (AMG);two-step GMM; urbanization; natural resources; tourism; CO2 emissions; ICT

Biography: Daniel Balsalobre- Lorente (Daniel.Balsalobre@uclm.es) is PhD in Economics and Full Professor (Tenure) in the Department of Applied Economics I, at the University of Castilla-La Mancha, Spain.

At the academic and research level, Daniel Balsalobre is an expert in public finance, energy economics, economic growth and environment, tourism, and innovation and globalization. In recent years I have published more than 100 studies in journals and book chapters of reputed prestige and international scientific impact, including Energy Economics, Energy Policy, Resources Policy, Technological Forecasting and Social Change, Journal of Cleaner Production, Sustainability, Environmental Science and Pollution Research, Energies, and Journal of Public Affairs, among others. Prof Balsalobre currently serves as editor-in-chief of Evaluation Review (SAGE) and associate editor at Heliyon (Elsevier) and Environment, Development and Sustainability (Springer). I am also a guest editor for Renewable Energy (Elsevier), Utilities Policy (Elsevier), Energy Sources Part B (Taylor), Sustainability (MDPI), Energies (MDPI), among others; also being an expert reviewer of more than 300 articles for highly indexed journals and handbooks. As a result of his academic career, he currently accumulates around 11000 citations in google scholar and h-index 45 and has entered the International Ranking elaborated by Stanford University for those top2% Researchers and 2022 Clarivate Highly cited authors. Ive received some Awards as Regional Best Researcher in Social Sciences in Castilla La Mancha

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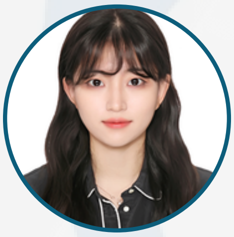

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Tunable pseudocapacitance of electrospun carbon/iron–vanadium oxide nanofibers for high-energy-density flexible supercapacitors

Abstract: Highly flexible and conductive carbon nanofibers (CNFs) embedded with pseudocapacitive iron–vanadium oxide (FVO) were fabricated via electrospinning followed by high-temperature annealing (900 °C). CNFs have a graphitic structure with minimal defects, which could hinder the access of electrolytic ions to multivalent FVO. Therefore, a sacrificial polymer, such as poly(methyl methacrylate) (PMMA), was introduced to enhance the electrolytic ion pathways by altering the internal structure of nanofiber. In addition, terephthalic acid was added to a polyacrylonitrile–PMMA solution to facilitate flexibility by increasing the cross-linking of the electrospun fibers. The fabricated flexible FVO/CNFs exhibited significantly enhanced electrochemical performance. The optimal sample had a high areal capacitance of 1058 mF·cm−2 at a current density of 2.5 mA·cm-2 and showed 100% capacitance retention during long-term cycling (10,000 cycles). The capacitance retention decreased to 81.3% when the current density was increased to 25 mA·cm-2. The wider potential window of 0–1.6 V increased the energy density to 389 µW·h·cm-2. The optimal FVO/CNF sample maintained 90% capacitance retention after 200 bending cycles.

Keywords: Electrospinning, Multivalent FeVO4, Sacrificial polymer, Flexible supercapacitor, Electrochemical sites

Biography: Jiwon Jang is a Master's student in Mechanical Engineering at Korea University, specializing in energy materials. She is presenting her research on pseudo capacitance in carbon/iron–vanadium oxide nanofibers for supercapacitors.

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Jungwoo Huh, Woojin Lim, Jiwon Jang

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Enhancing the piezoelectric coefficient of SrTiO3 nanocubes and PVDF film deposited by supersonic spraying for energy-harvesting nanogenerators

Abstract: Many perovskites and their piezoelectric composites have been investigated for harvesting ambient mechanical energy over the past two decades; however, the prospects for their commercialization appear remote because of several practical challenges. Therefore, highly scalable supersonic cold-spraying technology was used to fabricate flexible piezoelectric films of poly(vinylidene fluoride) (PVDF) and a novel perovskite SrTiO3 (ST). Substantial shear stress was exerted on PVDF during cold spraying owing to the hydrothermally synthesized SrTiO3 nanocubes and supersonic velocity, and the resulting film delivered an effective piezoelectric coefficient (69.6 pm·V-1) as confirmed by piezo-response force microscopy. As a result, the piezoelectric nanogenerator yields a maximum power of 130 µW at a load resistance of 0.9 MΩ. The composite film exhibited durability for 21,000 tapping cycles with 20 N applied force and 7 Hz frequency. The flexibility endurance was confirmed from 3000 bending cycles, and bending PENG attached to knee delivered 1 and 2.3 V on bending to 45 and 90°, respectively. After electrical poling, the PENG was subjected to a 20 N tapping force that yielded a piezopotential of 31 V. To the best of our knowledge, this is the first time piezoelectricity was obtained using an ST/PVDF composite via mechanical energy harvesting. The flexible PENG film deposited by cold-spraying shows good potential for wearable self-powered devices.

Keywords: SrTiO3, PVDF, Piezocomposite, Nanogenerator

Biography: Jungwoo Huh is a Mechanical Engineering student at Korea University, specializing in heat transfer, fluid dynamics, and energy storage. Over six semesters, he has focused on advanced research in supercapacitors, lithium-ion batteries, and piezoelectric materials. His work involves developing micro/nano fibers and coatings using innovative techniques like electrospinning, electroplating, and supersonic flow coating. The primary goal of his research is to improve the efficiency of energy storage devices beyond current standards.

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Osman Adiguzel

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Thermomechanical Transformations Governing Reversibility in Shape Memory Alloys

Abstract: Shape memory alloys take place in a class of advanced smart materials by exhibiting a peculiar property called shape memory effect. This phenomenon is initiated with thermomechanical treatments on cooling and deformation and performed thermally on heating and cooling, with which shape of the material cycles between original and deformed shapes in reversible way. Therefore, this behavior can be called thermal memory or thermoelasticity. Deformation in low temperature condition is plastic deformation, with which strain energy is stored in the materials and released on heating by recovering the original shape. This phenomenon is governed by the thermomechanical transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformations occur on cooling with cooperative movement of atoms in <110 > -type directions on a {110} - type plane of austenite matrix, along with lattice twinning reaction, and ordered parent phase structures turn into the twinned martensite structures. The twinned structures turn into detwinned martensite structures by means of stress induced martensitic transformations with deformation.

These alloys exhibit another property, called superelasticity, which is performed with mechanically stressing and releasing the material at a constant temperature at the parent phase region, and material recovers the original shape upon releasing, by exhibiting elastic material behavior. Superelasticity is performed in non-linear way, unlike normal elastic materials behavior, loading and releasing paths are different, and cycling loop refers to the energy dissipation. Superelasticity is also result of stress induced martensitic transformation, and the ordered parent phase structures turn into the detwinned martensite structures by stressing. However, lattice twinning and detwinning reactions play important role at martensitic transformations, and these reactions are driven by inhomogeneous lattice invariant shear.

Copper based alloys exhibit this property in metastable beta-phase region. Lattice twinning is not uniform in these alloys and cause the formation of complex layered structures. The layered structures can be described by different unit cells as 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. The unit cell and periodicity are completed through 18 layers in direction z, in case of 18R martensite, and unit cells are not periodic in short range in direction z.

In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on copper based CuAlMn and CuZnAl alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging duration at room temperature.This result refers to the rearrangement of atoms in diffusive manner.

Keywords: Shape memory effect, martensitic transformation, thermoelasticity, superelasticity, lattice twinning, detwinning.

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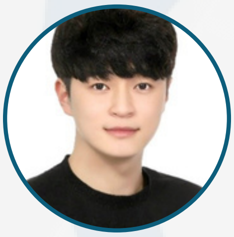

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Flexible high-power piezoelectric nanogenerator fabrication: Augmenting electroactive β- and γ- phases of PVDF with supersonically sprayed Sr2SnO4 nanorods

Abstract: The presence of electroactive β- and γ-phases in poly(vinylidene fluoride) (PVDF) increased by more than two folds upon supersonically spraying Sr2SnO4 nanorods (SSO-NRs). Shear stress between the PVDF and SSO-NRs, induced by supersonic blowing and catastrophic impact against the substrate, amplified the β- and γ-phases, which enhanced the energy-harvesting performance of a flexible piezoelectric nanogenerator (PENG). The high-aspect-ratio SSO-NRs magnified the influence of shear stress by intensifying the turbulence induced by their swirling. The supersonically driven shear stress caused multidirectional stretching, elongation, and twisting of the PVDF and transformed a large amount of the α-phase into electroactive β- and γ-phases, as evidenced by X-ray diffractometry and infrared spectroscopy. The composite film with a minimal filler content of 2.5 wt% exhibited a piezopotential of 40 V without additional poling. The optimal SSO/PVDF-based PENG delivered a high power density of 87 μW·cm−2, when it was subjected to a tapping force. Furthermore, the practical applicability of the PENG was illustrated using air pressure, vibration, and human body movements. The fabricated PENG device was integrated with a supercapacitor electrode to demonstrate its wide range of applications in wearable and portable electronics.

Keywords: Strontium stannate, nanorod, piezoelectric nanogenerator

Biography: Woojin Lim is a Ph.D. candidate in the School of Mechanical Engineering at Korea University, Seoul, South Korea, since 2022. He received his B.S. degree from Dongguk University in 2022. His research primarily focuses on the fabrication of multifunctional films for energy harvesting and energy storage applications using supersonic cold-spraying techniques.

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GLOBAL SUMMIT ON ADVANCED MATERIALS SCIENCE AND NANOTECHNOLOGY

Yasuhiro Yamada

Graduate School of Engineering, Chiba University, Chiba, Japan

Structural control and structural analysis of carbon materials

Abstract: Controlling structures of carbon materials is essential to attain superior properties for various applications. However, controlling structures in carbon materials is challenging because varieties of the reactions proceed during heat treatment to form carbonization and the structures of carbon materials are extremely complicated. Our group has synthesized carbon materials with an exceptionally high percentage of pyrrolic nitrogen at 873 K (94%), pyridinic nitrogen at 973 K (92%), tertiary nitrogen at 973 K (92–98%), pentagons at 773 K (96% retained from the precursor), pentagons-heptagons at 873–973 K (90%), edges with one sp2C–H on one benzene ring (SOLO) at 823 K (100%), and zigzag/armchair edges at 775 K (100% retained from the precursor) by the simple heating of the precursors in glass or quartz ampoules. Since catalysts were not used for the synthesis, mass production is possible and the carbon materials can be applied to many applications. In order to analyze the complicated structures of the carbon materials precisely, a combined analysis using X-ray photoelectron, Raman, and infrared spectroscopy, combustion elemental analysis, density functional theory calculation, and molecular dynamics simulations with a reactive force field was conducted. The origin of the ambiguous assignments of the spectral analyses of carbon materials was revealed.

Keywords: Carbon material, nitrogen, structural control, XPS, IR, Raman spectroscopy

Biography: Dr. Yamada received his Ph.D. from University at Buffalo, The State University of New York in 2008. He worked at National Institute of Advanced Industrial Science and Technology and Nippon Chemi-Con Corp. in 2009. He became an assistant professor in 2009 and an associate professor in 2019 at Chiba University in Japan.

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