10TH YEARS ANNIVERSARY CELEBRATION AMC® Advanced Materials Congress

"Celebrating 10 years Anniversary"

European ADVANCED MATERIALS CONGRESS with Hybrid Setups

Onsite - Online / Live-On Demand

23 - 25 August 2021 | Stockholm, Sweden

SCIENTIFIC PROGRAM & PROCEEDINGS

The multi-inter-trans-disciplinary
Research, Innovations & Technology

JOIN THE LARGEST Advanced Materials Community

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IAA Since 2010 ADVANCEMENT OF MATERIALS TO SUSTAINABLE & GREEN WORLD

AMC®
Advanced Materials Congress
– ESTABLISHED 2011 –

European Advanced Materials Congress

with Hybrid Setups

25 June - 02 July 2022
Genoa, Italy

Onsite - Online/Live - On Demand

www.advancedmaterialscongress.org/europe

Subject area

- Nanomaterials & Nanotechnology
- Biomaterials & Biodevices
- Electronic, Magnetic & Optical Materials
- Structural & Engineering Materials
- Thin Films, Materials Surface & Interfaces
- Computational Materials & Modelling
- Functional Materials
- Energy Materials
- Polymer Science and Technology
- Composite & Ceramic Materials
- Environmental & Green Materials
- Sustainable Construction and Building Materials
- Organic and Composite Thermoelectric Materials
- Nanomaterials and Nano Fibers
- Lighting Materials Research and Technology
- Graphene Innovations and Technology
- Metamaterials
- Nuclear Energy, Minings & Engineering Materials
- Electronic Materials
- Advanced Polymer Nanocomposites
- Fire Safety and Fire Protection Technology
- Battery Materials and Technology
- Ceramics and Dielectric Materials
- Biological and Biocompatible Materials
- Smart Materials
- Micro and Nanostructured Materials
- Analytical Methods and Spectroscopy
- Tissue Engineering and Regenerative Medicine
- Biosensors, Bioelectronics and Biodevices
- Carbon Materials and Technology
- Water Technology
- Epoxy & Resins Technology
- Plastics & Rubber Technology
- Pulp & Paper Technology
- Wood Technology
- COVID Science & Technology

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CALL FOR

Abstracts & Symposium Proposal

Advanced Materials Congress

Advanced Materials Congress
– ESTABLISHED 2011 –

UPCOMING EVENTS 2022

HYBRID SETUPS
Onsite - Online/
Live - On Demand

05 - 12 March	**Composite Materials Congress**	Place: Dubai, UAE www.advancedmaterialscongress.org/composites
10 - 14 April	**American Advanced Materials Congress**	Place: Orlando, USA www.advancedmaterialscongress.org/america
28 May - 04 June	**Baltic Conference Series-Spring**	Place: Kiel, Germany www.advancedmaterialscongress.org/baltic-spring
06 - 10 June	**European Climate Neutrality Congress**	Place: Ulrika, Sweden www.advancedmaterialscongress.org/climate
25 June - 02 July	**European Advanced Materials Congress**	Place: Genoa, Italy www.advancedmaterialscongress.org/europe
17 - 24 September	**Advanced Functional Materials Congress**	Place: Barcelona, Spain www.advancedmaterialscongress.org/functional
02 - 09 October	**Advanced Materials World Congress**	Place: Venice, Italy www.advancedmaterialscongress.org/world

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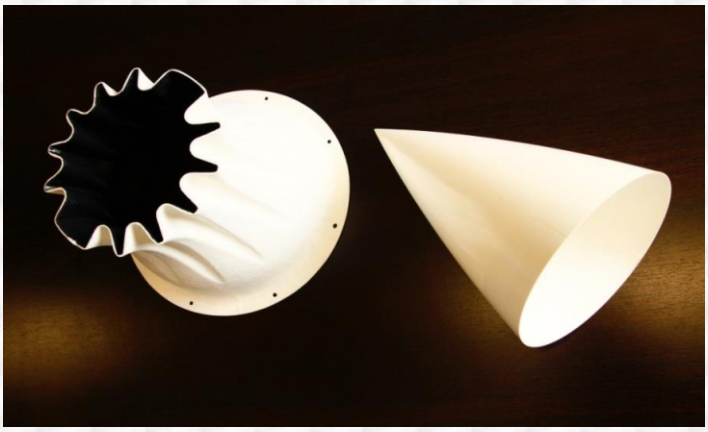

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Organizer's Desk

Greetings of the day!

International Association of Advanced Materials (IAAM, www.iaamonline.org) takes immense pride in welcoming all of you to the *European Advanced Materials Congress,* www.advancedmaterialscongress.org/eamc during 23 - 25 August 2021, Sweden. This is the 41st assembly of the Advanced Materials Congress (AMC, www.advancedmaterialscongress.org) running with Onsite (at venue)-Online LIVE-On-demand Hybrid conference setups.

We deem it an honor to have the wonderful chance to host esteemed delegates like you in the hybrid conference format of Onsite, Online LIVE and On-Demand setups for the next three days from 23 to 25 August 2021. We hope that these days will prove to be true conclusion of information, research, and understanding. IAAM is a premier non-profit research organization in the sphere of advanced materials that works to bring together students, researchers, professionals, and business giants to form truly global and collaborative networks for the betterment of scientific community and society.

The *European Advanced Materials Congress* is called with the IAAM Fellow Summit dedicated to exploring the knowledge in the field of advanced materials, next generation technologies and innovation supporting new research in the study, development, and exploitation of materials tools. The 41st assembly of AMC assembly is going to be a presentation of 17 thematic sessions from more than 25 countries including 45 keynote/invited lectures, a series of oral and poster presentation with welcome ceremony.

The organization works in this direction with the vision of *"Advancement of materials to global excellence"*. AMC assemblies stand out in the academia and industry not just in terms of quality but also the dual format. The representatives of esteemed research organizations and educational institutes shares their research on a global platform and gain valuable benefits. The congress will also give the companies a chance to share their ideas and will get the chance to take a toll of their competitors. The 41st assembly of AMC is going to serve as a platform where the delegates get a chance to celebrate the world of advanced materials and science like nowhere else. To add to this celebration, the congress will also witness the *Open Round Table Discussion* among all delegates in the *Onsite Session 4* as below:

- *Advanced materials innovations and knowledge transfer and Consortium on Education, Research and Innovation,* Institute of Advanced Materials, IAAM, Sweden

The congress assembly is going to witnessed following advanced materials professionals to confer the title *Fellow of IAAM,* www.iaamonline.org/fellow-of-iaam, which is a notable distinction to

recognize researchers and scientists for their important contribution and efforts towards the advancement of materials for global excellence. Key features of EAMC 2021, lies in *Poster Sessions devoted to IAAM Young researchers and women researchers* who were ready to demonstrate their idea and research in front of worldwide experts to get direct comments and encouragement.

The sessions will give the young budding researchers a platform of unparalleled prestige and allow them a chance to get in touch with esteemed scientific elites. It will also provide opportunities for researchers, engineers, students, professionals, and business giants to present their research results, breakthrough innovations, product display, and new products launch at a global platform. The 41st assembly of AMC is going to be an amalgamation of several important research fields of health, energy and environment for research, innovation, and technology with a special focus on materials knowledge and discoveries.

Furthermore, this 41st AMC assembly will also witness the release of the August 2021 issue of IAAM's prestigious journal, "Advanced Materials Letters". The August issue of Advanced Materials Letters exemplify the evolution of advance functionality in the materials via nanotechnology-based concept along with elicited towards sustainable climate. The editorial of the journal issue contains in detail and highlights 2030 agenda of the International Association of Advanced Materials on "Advancement of Materials to Sustainable and Green World" for climate neutrality. IAAM working in line with the United Nations' Sustainable Development Goals and also synchronizes its agenda with the action plans of European Green Deal which is aimed to making the Europe as climate neutral by 2050 for which they have taken a set of policy initiatives.

With a rich legacy of having hosted more than 16000 delegates and over 7000 speakers from more than 100 countries in multiple congresses, IAAM is widely recognized as the organizer of the highest quality of conferences. With consortiums and symposiums like these, IAAM also facilitates global forums to support translational research and new-age-technology. IAAM also believes in recognizing outstanding contributions made by scientific elites and potential researchers. Therefore, in the AMC assemblies, IAAM honors individuals and organizations to promote inspiring research and facilitate the advancement of materials for sustainable and green world.

We take this opportunity to express our regard for all the scientific committee members who have gathered here to share their experience, research, and results. Also, we thank all session chairs, poster jury, Institute of Advanced Materials (www.iaam.se), and the cruise staff members who have agreed to provide their excellent support to smoothly organize this event. With hope that this European AMC assembly makes the best of the next three days and delve into an ocean of quality research and interdisciplinary ideas; association welcome again and wish you good luck.

Sincerely,

International Association of Advanced Materials
Gammalkilsvägen 18, 590 53 Ulrika, Sweden
www.iaamonline.org

Scientific Program

Online LIVE Sessions

Joining Details

Time zone: Central European Summer Time (CEST)

Joining Link:

https://us06web.zoom.us/j/89773575057?pwd=UXVYOEhndVpDRWtlSHNtZDlKcW9GQT09

Passcode: 707830

Webinar ID: 897 7357 5057

Guidelines for Online LIVE Delegates

Hardwire your internet connection: This will help you avoid any issues with an unstable WiFi or wire connection, which can affect your audio quality and the overall attendee experience.

Test the audio before your webinar begins: This will ensure your speakers and mic are working properly before the live event begins. Here's how to test your device audio.

Minimize background noise: Try to host your webinar in a quiet place. If you must be in a loud environment, using a headset with a mic often reduces background noise compared with your computer's built-in microphone. In fact, a headset is a general best practice for higher-quality audio than other built-in options.

Dress for webinar: You'll be on video, so be sure to wear business attire. We recommend solid colours as opposed to garments with patterns.

- All the speakers should join the meeting 15 minutes in advance.
- The presentation time will be different for lecture categories:
  - ❖ Keynote Talk: 30 min (25 min for presentation + 5 min for discussion).
  - ❖ Invited Talk: 20 min (17 min for presentation + 3 min for discussion).
  - ❖ Oral Presentation: 15 min (12 min for presentation + 3 min for discussion).

Please visit for guidelines and info to speakers, session chairs, etc.
https://www.advancedmaterialscongress.org/eamc/pages/guidelines-information

- Keep your device charged and ensure your internet connection is stable.
- Please download the **Zoom meeting application** before the meeting.
- Click on the zoom meeting link or copy and paste the URL to a browser.
- Once you join, you will be directed to download/open the Zoom Meeting App.
- There will be a "Share screen" option in the Zoom platform to share your ppt.
- After the lecture, there will be a discussion session with the chair & panel members.
- To ask question(s) during/after the lecture, click on Q&A icon and type your query.
- The organization reserves the right to use photos/videos for the promotion of advanced materials on international platforms.

The organizer reserves the right to make any changes, alter or modify the program at any time without prior notice.

Important Information-EAMC-2021

Speakers

- **All the lectures will be recorded and may be published** in the open access video journal of IAAM, "Video Proceedings of Advanced Materials" after the peer-review. After the proofread by the presenting author, the lecture may be published online as an audio video article.
- Kindly ensure your focused face towards camera and effective sound quality for better recording.
- IAAM office circulates the open access video article to leading researchers and members of association.
- As the lecture may be published for open science under **"Live knowledge at Web",** you are advised to not use any confidential information in the presentation.

Session Chairs

- Session chair should join the respective session at least 15 min prior to the starting to avoid any technical issues.
- Session chairs will be responsible for the course of the session.
- In the attendees' minds, you are an extension of the congress and should be knowledgeable of the basics relating to the online event.
- Session chairs should gather some brief about the respective speakers of the session

23 - 25 August 2021

Scientific Program: Online LIVE Sessions

Day - 1: Monday, 23 August 2021
Central European Summer Time (CEST)

23 August 2021

09.00 - 09.10 **Welcome Message from Organizer: Ashutosh Tiwari**, Secretary General, International Association of Advanced Materials; and Director, Institute of Advanced Materials, IAAM, Sweden

09.10-12.00 **Session 01: Materials Horizons for New Edge Technology**

Session Chair(s): Jurgen Eckert, Austrian Academy of Sciences, Austria, **Shigehiro Hashimoto,** Kogakuin University, Japan and **Yuan Chen,** The University of Sydney, Australia

09.10-09.40 **Keynote Lecture: Werner Mueller, Bio-artificial intelligence of morphogenetically active polyphosphate nanoparticles for regenerative medicine and a prophylactic drug against SARS-CoV-2 infection,** University Medical Center of the Johannes Gutenberg, University Mainz, Germany

09.40-10.10 **Keynote Lecture: Lixin Xiao, Long-lived electron-transporting materials for OLEDs,** Peking University, China

10.10-10.40 **Keynote Lecture: Shigehiro Hashimoto, Is micromachined back-markers on thin film of scaffold effective to measure repetitive contraction of myotubes?,** Kogakuin University, Japan

10.40-11.00 **Invited Lecture: Jiun-Haw Lee, Benzotrifluoride derivatives with different hole transporting moieties for efficient exciplex-OLEDs,** National Taiwan University, Taiwan

11.00-11.20 **Invited Lecture: Josep Nogues, Magnetoplasmonic nanodomes as a novel structure for biomedical applications,** Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain

11.20-11.40 **Invited Lecture: Chol-Jun Yu, Advances in design of new energy materials for sustainable and clean energy supply,** Faculty of Materials Science, Kim Il Sung University, Democratic People's Republic of Korea

11.40-12.00 **Invited Lecture: Chunxiao Cong, Synthesis and optical properties of two-dimensional materials and heterostructures,** Fudan University, China

12.00-12.20 **Invited Lecture: Yuan Chen, Computational design for 3D printing of continuous carbon fibre composites with negative poisson™ ratios,** The University of Sydney, Australia

12.20-13.00 **Break**

23 August 2021

13.00-16.10 **Session 02: Composite Engineering and Materials**

Session Chair(s): Rudiger Ballas, Wilhelm Buchner Hochschule, Mobile University of Technology, Germany, **Josep Nogues,** Catalan Institute of Nanoscience and Nanotechnology (ICN2), Spain and **Kok Wai Cheah,** Hong Kong Baptist University, Hong Kong

13.00-13.30 **Advanced Materials Award Lecture: Jurgen Eckert, Design and processing of biocompatible Ti alloys for bone implant applications,** Austrian Academy of Sciences, Austria

13.30-14.00 **Sponshorship Plus Lecture: Guillaume Jandin, The alternative of oxide-oxide composites using the chemistry of geopolymers,** Pyromeral Systems S.A., France

14.00-14.20 **Invited Lecture: Yannick Willemin, Seamless solution for industrial-grade continuous carbon fibre 3D-printed composites,** 9T Labs AG, Switzerland

14.20-14.40 **Invited Lecture: Arkadii Arinstein, Nano vs macro: small size does matter,** Technion-Israel Institute of Technology, Israel

14.40-15.00 **Invited Lecture: Jesus Prado-Gonjal, Microwave Chemistry: Rapid and sustainable routes for the preparation of energy materials,** Universidad Complutense de Madrid, Spain

15.00-15.20 **Invited Lecture: Rudiger Ballas, A versatile modeling method in electromechanics-The canonical equivalent circuit representation of a clamped-free piezoceramic multilayered bending transducer,** Wilhelm Buchner Hochschule, Mobile University of Technology, Germany

15.20-15.40 **Invited Lecture: Pradeep Rohatgi, Metal and Polymer Matrix composites including composites incorporating waste by products and plant based materials for sustainability,** University of Wisconsin-Milwaukee, USA

15.40-15.55 **Oral: Kamil Janeczek, Thermal endurance of swelling anti-fire composites equipped with RFID technology,** Łukasiewicz Research Network, Tele and Radio Research Institute, Poland

15.55-16.10 **Oral: Thomas Hoyer, Development and production of organic-inorganic nanocomposite coating materials,** Fraunhofer IKTS Hermsdorf, Germany

16.10-17.00 **Break**

23 August 2021

17.00-20.00 **Session 03: Biomedical Materials and Technology**

Session Chair(s): Michael Thompson, University of Toronto, Canada, **Werner Mueller,** University Mainz, Germany and **Menahem Rotenberg,** Technion - Israel Institute of Technology, Israel

17.00-17.30 **Keynote Lecture: AC Matin, A side-effect free chemotherapy for treating cancer by directed gene delivery and a prodrug using exosomes,** Stanford University, USA

17.30-18.00 **Keynote Fellow Lecture: Thomas Webster, 25 years of commercializing nanomedicine: Lessons learned and necessary future directions,** Northeastern University, USA

18.00-18.30 **Keynote Lecture: Michael Thompson, Surface linker chemistry with minimization of non-specific adsorption on sensor materials,** University of Toronto, Canada

18.30-19.00 **Keynote Fellow Lecture: Debora Rodrigues, Enrofloxacin entrapped in polymer based nanocarriers for gut infection prevention,** University of Houston, USA

19.00-19.20 **Invited Lecture: Juan Vivero-Escoto, Recent advances on multifunctional hybrid silica-based nanoparticles for cancer treatment,** University of North Carolina Charlotte, USA

19.20-19.40 **Invited Lecture: Celso de Melo, Use of conducting polymer composites in biomedical protocols,** Universidade Federal de Pernambuco, Brazil

19.40-20.00 **Invited Lecture: Menahem Rotenberg, Cell-Silicon hybrids for bioelectrical interrogation with sub-cellular resolution in 3D tissues,** Faculty of Biomedical Engineering, Technion - Israel Institute of Technology, Israel

Day - 2: Tuesday, 24 August 2021
Central European Summer Time (CEST)

24 August 2021

09.00-12.55 **Session 04: Materials Interface and Energy Harvesting**

Session Chair(s): Shuji Ogata, Nagoya Institute of Technology, Japan,
Albert Chin, Natl Yang Ming Chiao Tung University, Taiwan and
Arkadii Arinstein, Technion-Israel Institute of Technology, Israel

09.00-09.30 **Keynote Lecture: Shuji Ogata, DFT-based simulations about stability and adhesion of metal-organic interfaces,** Nagoya Institute of Technology, Japan

09.30-10.00 **Keynote Fellow Lecture: Albert Chin, Three-dimensional brain-mimicking device structure for computing energy crisis,** Natl Yang Ming Chiao Tung University, Taiwan

10.00-10.20 **Invited Lecture: Olaf Karthaus, Transparent flower petals and their biomimetic polymer films for optic applications,** Chitose Institute of Science and Technology, Japan

10.20-10.40 **Invited Lecture: Fengxian Xin, Tunable acoustic impedance of Helmholtz resonators for perfect sound absorption via roughened embedded necks,** Xi'an Jiaotong University, China

10.40-11.00 **Invited Lecture: Hsien-Yeh Chen, Vapor deposition to construct particles and scaffolding materials for regenerative medicine,** National Taiwan University, Taiwan

11.00-11.20 **Invited Lecture: Junzhong Wang, Graphene Materials: prepared and used through electrochemical routes,** Anhui University, China

11.20-11.40 **Invited Lecture: Ikuo Yanase, Reversible CO_2 capture/release of sodium manganate,** Saitama University, Japan

11.40-12.00 **Invited Lecture: Chao Gao, Main-chain twisted non-fullerene acceptors for efficient organic solar cells,** Xi'an Modern Chemistry Research Institute, China

12.00-12.20 **Invited Lecture: Santi Tofani, Electron spin as a key factor for improving the treatment of genetically-based diseases like cancer,** Scientific Advisor, Italy

12.20-12.40 **Invited Lecture: Anne Julbe, Perovskite coatings on ceria foams and membranes for solar fuel production,** University of Montpellier, France

12.40-12.55 **Oral: Jiayue Geng, Ammonium citrate carbon dots naturally have a high selectivity to helicobacter pylori,** Ocean University of China, China

12.55-15.00 **Break**

24 August 2021

15.00-16.55 **Session 05: Energy Materials and Composites**

Session Chair(s): Pradeep Rohatgi, University of Wisconsin-Milwaukee, USA and
Mei Cai, General Motors, USA

15.00-15.30 **Keynote Fellow Lecture: Mei Cai, Cathode design for high energy lithium metal batteries,** General Motors, USA

15.30-15.50 **Invited Lecture: Carsten Strobel, A novel graphene base heterojunction transistor with saturated output current,** TU-Dresden - Institut fur Halbleiter-und Mikrosystemtechnik, Germany

15.50-16.10 **Invited Lecture: Giovanni Piazza, Innovative usage and application-oriented simulation of veneer based hybrid materials in vehicle structures,** German Aerospace Center - Institute of Vehicle Concepts, Germany

16.10-16.25 **Oral: Hassan Yassine, Study of the aging of Lithium-ion coin cells with impedance and noise measurements,** ULCO UDSMM, France

16.25-16.40 **Oral: Devika Chauhan, Carbon nanotube hybrid fabric-manufacturing and applications,** University of Cincinnati, USA

16.40-16.55 **Oral: Prasad Venkatesan, New titanium-composite bipolar plate material for electrolyzer,** Hochschule Nordhausen, Germany

16.55-17.00 **Break**

17.00-19.05 **Session 06: Nanomaterials and Nanotechnology**

Session Chair (s): AC Matin, Stanford University, USA, **Debora Rodrigues,** University of Houston, USA and **Xijia Wu,** National Research Council Canada, Canada

17.00-17.30 **Keynote Fellow Lecture: Jun Kameoka, A low cost paper sensor with molecularly imprinted conductive polymer electrodes,** Texas A&M University, USA

17.30-17.50 **Invited Lecture: Gregory Light, On spin-polarization and anti-particle asymmetry,** Providence College, USA

17.50-18.10 **Invited Lecture: Stanislav Moshkalev, New piezoresistive composite material based on nanographite in glassy matrix,** UNICAMP, Brazil

18.10-18.30 **Invited Lecture: Jason R. Stagno, Ordered phase transitions triggered by synchronous conformational changes in riboswitch crystals,** Center for Cancer Research, National Cancer Institute, Frederick, USA

18.30-18.50 **Invited Lecture: David Heyner, Innovative usage and application-oriented simulation of veneer based hybrid materials in vehicle structures,** German Aerospace Center - Institute of Vehicle Concepts, Germany

18.55-19.05 **Oral: Dana C Toncu, IAAM commitment to high quality colloberative R & I,** Institute of Advanced Materials, IAAM, Sweden

25 August 2021

Day - 3: Wednesday, 25 August 2021
Central European Summer Time (CEST)

09.00-12.25 **Session 07: Electronic, Magnetic Materials and Nanotechnology**

Session Chair(s): Bing-Huei Chen, Fu Jen Catholic University, Taiwan, **Jeffrey Zheng,** Yunnan University, China and **Carsten Strobel,** TU-Dresden - Institut fur Halbleiter-und Mikrosystemtechnik, Germany

09.00-09.30 **Keynote Fellow Lecture: Chih Chen, Highly (111)-oriented nanotwinned Cu and its applications in microelectronic devices,** National Yang Ming Chiao Tung University, Taiwan

09.30-10.00 **Keynote Fellow Lecture: Shang-Lien Lo, Microwave-induced titanate nanotubes for visible-light-driven hydrogen production,** National Taiwan University, Taiwan

10.00-10.20 **Invited Lecture: Liming Wang, Electrospun nanofiber fabric: An efficient moist-electric generator,** College of Textiles, Donghua University, China

10.20-10.40 **Invited Lecture: Jiangyi Zhang, High-amplitude sound propagation in acoustic transmission-line metamaterial, Faculty of Civil Engineering and Geosciences,** Delft University of Technology, Netherlands

10.40-11.00 **Invited Lecture: Bing-Huei Chen, Effects of black garlic extract and nanoemulsion on the deoxy corticosterone acetate-salt induced hypertension and its associated mild cognitive impairment in rats,** Fu Jen Catholic University, Taiwan

11.00-11.20 **Invited Lecture: Jeffrey Zheng, Equivalence relations among phylogenetic trees and genomic index maps,** Yunnan University, China

11.20-11.40 **Invited Lecture: Kok Wai Cheah, Continuous Tunable Lasing Characteristics of Blended Polymer System,** Institute of Advanced Materials, Hong Kong Baptist University, China

11.40-11.55 **Oral: Carmen Vladu, Electrospun core-shell nanofibers for protection against corrosion,** CEST Centre of Electrochemical Surface Technology, Austria

11.55-12.10 **Oral: Tien Quach, Interface characterisation for the next generation of multi-materials additive manufacturing,** University of Nottingham, UK and Ho Chi Minh City University of Technology, Viet Nam

25 August 2021

12.10-12.25 **Oral: Jeong Hoon Rhee, Measurement of material levels inside a silo using a hotspot detector and artificial neural network and optimization of measurement points using genetic algorithm,** Yonsei University, Republic of Korea

12.25-13.25 **Session 08: Poster Session - Materials Engineering and Technology**

Poster Jury: **Chunxiao Cong,** Fudan University, China and **Yannick Willemin,** 9T Labs AG, Switzerland

The online poster presentation: The attendee / delegates can write questions in the chat box / Q&A and poster jury will discuss their questions with the poster presenters.

12.25-12.30 **K Z M Abdul Motaleb, Effect of gamma radiation on mechanical properties of natural fabric reinforced polyester composites,** Faculty of Mechanical Engineering and Design, Kaunas University of Technology, Kaunas, Lithuania

12.30-12.35 **Santanu Patra, Removal and recycling of gadolinium from wastewater samples using imprinted magnetic graphene oxide,** VBRI Innovation, New Delhi, India

12.35-12.40 **Chang Che, Microstructural evolution for Super304H austenite steel used in China plants,** China Special Equipment Inspection and Research Institute, China

12.40-12.45 **Dharmesh Kumar, Switchable photoelectrocatalytic water splitting based on optically and electrically active molecule,** VBRI Innovation, New Delhi, India

12.45-12.50 **Katarzyna Jankowska, Electrospun fibers made of polyacrylonitrile and polyethersulfone with laccase immobilized for biodegradation of estrogen,** Institute of Chemical Technology and Engineering, Poznan University of Technology, Poland

12.50-12.55 **Oral: Genesis Opazo, Nanopapers based on lignocellulose nanofibers and their potential use in water treatment contaminated with metal cations,** Universidad de Chile, Chile

12.55-13.25 **Poster discussion**

13.25-17.00 **Break**

25 August 2021

17.00-20.00 **Session 09: Computational Materials, Modeling and Nanotechnology**

Session Chair(s): Ramesh Agarwal, Washington University in St. Louis, USA, **Gregory Light,** Providence College, USA and **Pablo Martin,** Universidad de Antofagasta, Chile

17.00-17.30 **Keynote Fellow Lecture: Ramesh Agarwal, Design of metamaterials for thermal, acoustic and hydrodynamic cloaking,** Washington University in St. Louis, USA

17.30-18.00 **Keynote Fellow Lecture: Thomas Wong, Polarization coupling in an asymmetrical semiconductor nanodimer,** Illinois Institute of Technology, USA

18.00-18.30 **Keynote Fellow Lecture: Xijia Wu, Modelling fatigue of additively manufactured materials,** National Research Council Canada, Canada

18.30-18.50 **Invited Lecture: Pablo Martin, Accurate analytic approximation for the bessel functions Jv(x),** Universidad de Antofagasta, Chile

18.50-19.05 **Oral: Vianessa Ng, One step synthesis of high-quality carbon nanofabric,** University of Cincinnati, USA

19.05-19.20 **Oral: Katarzyna Jankowska, Electrospun fibers as a support for oxidoreductase immobilization: Improving stability of the produced biocatalysts,** Institute of Chemical Technology and Engineering, Poznan University of Technology, Poland

19.20-19.35 **Oral: Nazih Assaad Al Ayoubi, Multi-scale computational modeling of flow of hybrid composites,** High Performance Computing Institute, France

19.35-20.00 **Announcements of Best Oral & Poster Presentations and Congress Closing Remarks**

Thank you for your participation.
Welcoming you to upcoming AMC Assemblies..

Scientific Program

Onsite Sessions

Venue:
Conference Auditorium, Deck 10, M/S Gabriella,
Viking Line Terminal, Stadsgården, 11630
Stockholm, Sweden

Guidelines For Onsite Delegates

1. The onsite conference will run as per the **Current Location Time** as given below:
    - **24th August 2021**, conference will run as per **Swedish Time**
    - **25th August 2021**, conference will run as per **Finish Time**
    - **26th August 2021**, conference will run as per **Swedish Time**
    - **There is one hour deference** between Swedish and Finish time zone.
2. **Internet will be available during the conference**; however, organizer will not guarantee to provide a high-speed internet. For the internet facility on board, please contact the cruise information desk at Deck 7.
3. You will get **Congress Name Batch, Cruise Ticket** (Cabin Access Key) together with the conference materials from registration desk at the harbor, Viking Line Terminal, Stockholm, Sweden on 24th August 2021 and Time: 09.00 - 10.00.
4. The delegates must wear their **Name Batch** (which you will get during the congress registration) and **Face Mask** all the time during the conference. It is note that delegates will be identify on the Cruise by their Name Batch even to get access for Breakfast, Lunch and Dinner during the conference in the Viking Buffet, Deck 8.
5. Please read **COVID guidelines and instructions** at https://www.sales.vikingline.com/find-trip/timetable/traffic-bulletin/information-regarding-the-coronavirus-situation
6. **Please drop your luggage** on 24th August 2021, just after check-in to cruise at Conference Auditorium (Deck 10).
7. The cabin access will be available after lunch on 24th August 2021 (Check-in time of cabin: 15:00 – 16:00).
8. **Please make sure that all presenter's/speakers don't forget to upload their presentation** (power point or PDF) in the computer present in respective session, 30 minutes prior to session starts and conference staff will help speakers to upload their presentations.
9. **Notepad and pen** will also be provided in session during the conference.
10. The organizer reserves the **right to make a change, alter or modify the program** at any time without prior notice.
11. **Poster sticks** will be available at **conference helpdesk, conference center, Deck 10**. If you need any assistance to hang your poster-on-poster board, you can ask conference staff available at helpdesk.
12. **Presentation/participation certificate** will be sent to your registered email ID after the conference.
13. **Accompanying persons can enjoy health club, tax-free shopping,** etc. available on board.
14. The **children's club** will be accessible for your kids.
15. We have also exclusive **cultural activities** during first and second days of the event. Both days in the evening at the club mar nightclub, Deck 8.
16. Please get together at the Cruise Information Desk, Deck 7 for Group Photo, Sightseeing in Helsinki and Stockholm.
17. Sightseeing in Helsinki on 25th August 2021 assembling at the Cruise Information Desk, Deck 7, time 14:00 and Stockholm on 26th August 2021 assembling at the Cruise Information Desk, Deck 7, time 09:30 with your luggage.
18. After sightseeing in Stockholm on 26th August 2021, bus will drop to Stockholm train station at 12.30.

Scientific Program - Onsite at Venue

Day - 1: Tuesday, 24 August 2021, Port of Stockholm | Time Zone: GMT+2 (Swedish Time)

24 - 26 August 2021

09.00-10.00 **Registration and Cruise Check-in** at Viking Line Terminal, Stadsgården, 11630 Stockholm, Sweden

10.30-11.00 **Boarding to M/S Gabriella,** Viking Line Cruise and Drop Luggage at Conference Auditorium, Deck 10, Conference Centre

11.00-11.10 **Welcome Message and Instructions** for the Onsite, European Advanced Materials Congress (EAMC- 2021)

24 August 2021

11.10-12.00 **Session X: Functional Materials Engineering and Technology**

Conference Audiorium, Deck 10, Conference Centre, M/S Gabriella

Chair(s): Ashutosh Tiwari, International Association of Advanced Materials, Sweden and **Jaroslav Jerz,** Slovak Academy of Sciences, Slovakia

11.10-11.40 **Keynote Fellow Lecture: Guenter Schmid, Renewable synthesis of chemical feedstock and specialties employing low temperature electrochemical reduction of CO_2,** Siemens Energy Global GmbH & Co.KG, Germany

11.40-12.00 **Invited Lecture: Miroslaw Maczka, Synthesis, phase transitions, lattice dynamics, dielectric properties and photoluminescence of two-dimensional methylhydrazinium lead halides with strongly reduced dielectric confinement,** Polish Academy of Sciences, Poland

12.00-13.00 **Lunch Break, Deck 08**

13.00-15.00 **Session XI: Advanced Materials and Devices**

Conference Audiorium, Deck 10, Conference Centre, M/S Gabriella

Chair(s): Miroslaw Maczka, Polish Academy of Sciences, Poland and **Ermelinda Falletta,** Department of Chemistry, University of Milan, Italy

13.00-13.30 **Keynote Fellow Lecture: Paddy French, Silicon based devices for in-vivo applications,** Delft University of Technology, Netherlands

13.30-14.00 **Keynote Lecture: Wouter Maijenburg, Metal oxide nanowires and nanofibers for solar water splitting,** Martin-Luther-University Halle-Wittenberg, Germany

14.00-14.20 **Invited Lecture: Jaroslav Jerz, Morphology and heat transfer performance of high-density aluminium foam,** Institute of Materials & Machine Mechanics, Slovak Academy of Sciences, Slovakia

14.20-14.40 **Invited Lecture: Alessio Bucciarelli, A new approach to the production of a high-performance silk based bioplastic,** University of Trento, Italy

14.40-15.00 **Invited Lecture: Maurizio Sansotera, PFPE peroxide decomposition as universal approach for PFPE chain grafting to carbon nanostructured materials,** Politecnico di Milano, Italy

15.00-16.00 **Coffee Break, Cabin Access and Poster Setup** for the Session on Multi-Inter-Trans-Disciplinary Research and Technology

24 August 2021

16.00-16.50 **Session XII: Functional Materials and Nanotechnology**

Conference Room, Deck 10, Conference Centre, M/S Gabriella

Chair(s): Alessio Bucciarelli, University of Trento, Italy and
Wouter Maijenburg, Martin-Luther-University, Halle-Wittenberg, Germany

16.00-16.20 **Invited Lecture: Jaroslav Filip, Low-requirement nanomaterials for electrochemical sensors,** Tomas Bata University in Zlin, Czech Republic

16.20-16.35 **Oral: Rana Choumane, Extraction of polyoxotantalate in basic medium by layered double hydroxide: Capacity and mechanism studies,** PSLA Universite, Chimie ParisTech, France

16.35-16.50 **Oral: Marc Chavalle, Chloride-Sulfate exchange mechanisms in $(LiCl)Al_2(OH)_6$ type layered double hydroxides,** Chimie Paristech, France

16.50-17.30 **Session XIII: Symposium on Innovations and Knowledge Transfer**

Discussion on the "Future utilization of research and innovation: Knowledge transfer", Mikael Syväjärvi, Institute of Advanced Materials, IAAM, Sweden

About Symposium: The symposium stimulates commercialization research avenues and their translational potentials towards climate crisis, energy needs, health, etc. Discussions, exchanges of experiences, R&D practices and forming research consortium for national, international and EU calls will take place during the session.

Consortium on Education, Research and Innovation, Ashutosh Tiwari, Institute of Advanced Materials, IAAM, Sweden

17.30-18.00 **Session XIV: Poster Presentation**

Conference Room, Deck 10, Conference Centre, M/S Gabriella

The conference will have a poster support desk. Any information regarding individual poster can only be collected from the Registration Desk. Poster session is open for all and Jury will discuss the topics, relevence and importance.

Poster Jury: **Wouter Maijenburg,** Martin-Luther-University Halle-Wittenberg, Germany and **Maurizio Sansotera,** Politecnico di Milano, Italy

12.40-13.00 **Poster Setup: Multi-Inter-Trans-Disciplinary Research and Technology**

P-1 **Angelika Zaszczynska**, **Smart piezoelectric scaffold for nerve regeneration,** Institute of Fundamental Technological Research, Polish Academy of Sciences, Poland

P-2 **Beata Niemczyk-Soczynska, Fragmentation of bioactive electrospun PLLA fibers,** Institute of Fundamental Technological Research, Polish Academy of Sciences, Poland

P-3 **Celia Moreno Gonzalez, Developing acoustical absorbers made from used cigarette butts,** Universidad de Extremadura, Spain

P-4 **Madhusmita Dash, Biomass utilization, energy and sustainable environment,** Institute of Advanced Materials, IAAM, Sweden

P-5 **Ayushi Tiwari, Sustainable healthcare management in pandemic,** Institute of Advanced Materials, IAAM, Sweden

P-6 **Robert Pilemalm, Development of Advanced Composite Pressure Vessels for Hydrogen Storage,** ALMINICA AB, Ulrika, Sweden

P-7 **Mikael Syväjärvi, Future research and innovation in energy materials concepts of today: The utilisation motivation in European and International context,** Institute of Advanced Materials, IAAM, Sweden

19.00-20.00 **Dinner at Viking Buffet, Deck 8**

20.00-22.00 **Cultural Programme, Deck 8**

25 August 2021

Day - 2: Wednesday, 25 August 2021, Port of Helsinki | Time Zone: GMT+3 (Finland)

07.30-08.30 **Breakfast at Viking Buffet, Deck 8**

09.00-10.45 **Session XV: Composite Materials and Applications**

Conference Room, Deck 10, Conference Centre, M/S Gabriella

Chair(s): Paddy French, Delft University of Technology, Netherlands and **Mikael Syväjärvi,** Institute of Advanced Materials, IAAM, Sweden

09.00-09.30 **Keynote Lecture: Zdenek Drozd, Mechanical and thermal properties of an AZ31 alloy subjected to rotary swaging,** Charles University, Czech Republic

09.30-10.00 **Keynote Lecture: Ermelinda Falletta, Photoactive floating conducting polymers for water remediation,** Department of Chemistry, University of Milan, Italy

10.00-10.15 **Oral: Achraf Ben Fekih, Effect of processing parameters on the porosity generation of Out-of-Autoclave manufactured laminated thermoplastic composites,** ONERA - The French Aerospace Lab, France

10.15-10.30 **Oral: Pietro Ballarin, Experimental and numerical identification of frictional effects in mode II delamination of composites,** Politecnico di Milano, Italy

10.30-10.45 **Oral: Madiha Rashid, Thermal characterization of fire-retardant coated green biocomposite,** INSA Centre Val de Loire, France

10.45-11.00 **Coffee Break at Conference Center, Deck-10**

25 August 2021

11.00-12.50 **Session XVI: Materials Engineering and Applications**

Conference Audiorium, Deck 10

Chair(s): Guenter Schmid, Siemens Energy Global GmbH & Co.KG, Germany and **Paddy French,** Delft University of Technology, Netherlands

11.00-11.30 **Keynote Fellow Lecture: Deb Jaisi, Altering chemistry to enhance the solubility of a slow-release nanofertilizer,** University of Delaware, United States of America, USA

11.30-11.50 **Invited Lecture: Milos Beran, Antimicrobial polyhydroxyburtyrate submicrone fiber mat loaded with extract of hypericum perforatum,** Food Research Institute Prague, Czech Republic

11.50-12.05 **Oral: Jihane Mzoughi, Controlled drug release kinetics from rolled up biocapsules based on thermally treated gelatin films,** IS2M France, France

12.05-12.20 **Oral: George Vlasceanu, Design and fabrication of highly porous graphene oxide composited biopolymer blends with osteoinductive properties,** Faculty of Medical Engineering, University Politehnica of Bucharest, Romania

12.20-12.35 **Oral: Denys Bondar, Oxime-functionalized nanodiamonds as a platform for treatment of organophosphate poisoning,** Tallinn University of Technology, Estonia

12.35-12.50 **Oral: Ahmad Soltani Nejad, Information of database resources for open access publications,** Institute of Advanced Materials, IAAM, Sweden

13.00-14.00 **Lunch at Viking Buffet, Deck 8**

	14.05-14.15	**Conference Group Photo, Cruise Information Desk at Deck 7**
	14.30-16.30	**Sightseeing in Helsinki**
		Meeting place, Cruise Information Desk at Deck 7 and meeting time at 14.15
		■ Sibelius Monument, Ateneum Art Museum / Central Railway Station, Market Square ■ The Stunningly Designed Rock Church, Botanic Garden ■ Senate Square, Olympic Stadium ■ Helsinki Lutheran and Uspenski Orthodox Cathedrals
25 August 2021	**17.00-17.45**	**Session XVII: Materials Processing, Manufacturing and Coating Technology**
		Conference Room, Deck 10, Conference Centre, M/S Gabriella
		Chair(s): Deb Jaisi, University of Delaware, USA and **Zdenek Drozd,** Charles University, Czech Republic
	17.00-17.15	**Oral: Cyril Oberlin, Elaboration of silica ceramics by indirect additive manufacturing and aqueous gelcasting,** Institut Europeen des Membranes, France
	17.15-17.30	**Oral: Suhad Sbeih, Anti-wettability of chemically and physically modified surfaces,** German Jordanian University, Jordan
	17.30-17.45	**Closing Ceremony: Announcements of Best Oral & Poster Presentations and Congress Closing Remarks, Conference Center, Deck-10**
	19.00-20.00	**Dinner at Viking Buffet, Deck 8**
	20.00-22.00	**Cultural Programme, Deck 8**
26 August 2021		**Day - 3: Thursday, 26 August 2021, Port of Stockholm | Time Zone: GMT+2 (Sweden)**
	07.30-08.30	**Breakfast at Viking Buffet, Deck 7**
	09.30-10.00	**Check-out from the Cabin with Luggage and Disembarkation from the Viking Cruise**
		Meeting place, Cruise Information Desk at Deck 7 and meeting time at 09.30
		Social Activity in Stockholm for registered participents
	10.30-12.00	Stockholm City Hall, The Royal Palace (Östermalm), Gamla Stan (Old Town), Långholmen and The Royal Djurgården, Stockholm's islands and waters, Fjällgatan Stockholm is world famous for being stunningly picturesque and sits on 14 islands. It is surrounded by water and presents parkland, forest and beautiful views. During this tour you will get to know Stockholm and history of the city.
	12.00	**Commencement of Tour at Central Train Station, Stockholm**

Thank you for your participation

Abstracts

Keynote Lectures
Invited Talks
Oral and Poster Presentations

Bio-artificial Intelligence of Morphogenetically Active Polyphosphate Nanoparticles for Regenerative Medicine and A Prophylactic Drug against SARS-CoV-2 Infection

Werner E. G. Müller*, Meik Neufurth, Shunfeng Wang, Heinz C. Schröder, Xiaohong Wang

ERC Advanced Investigator Grant Research Group at the Institute for Physiological Chemistry, University Medical Center of the Johannes Gutenberg University Mainz, Germany

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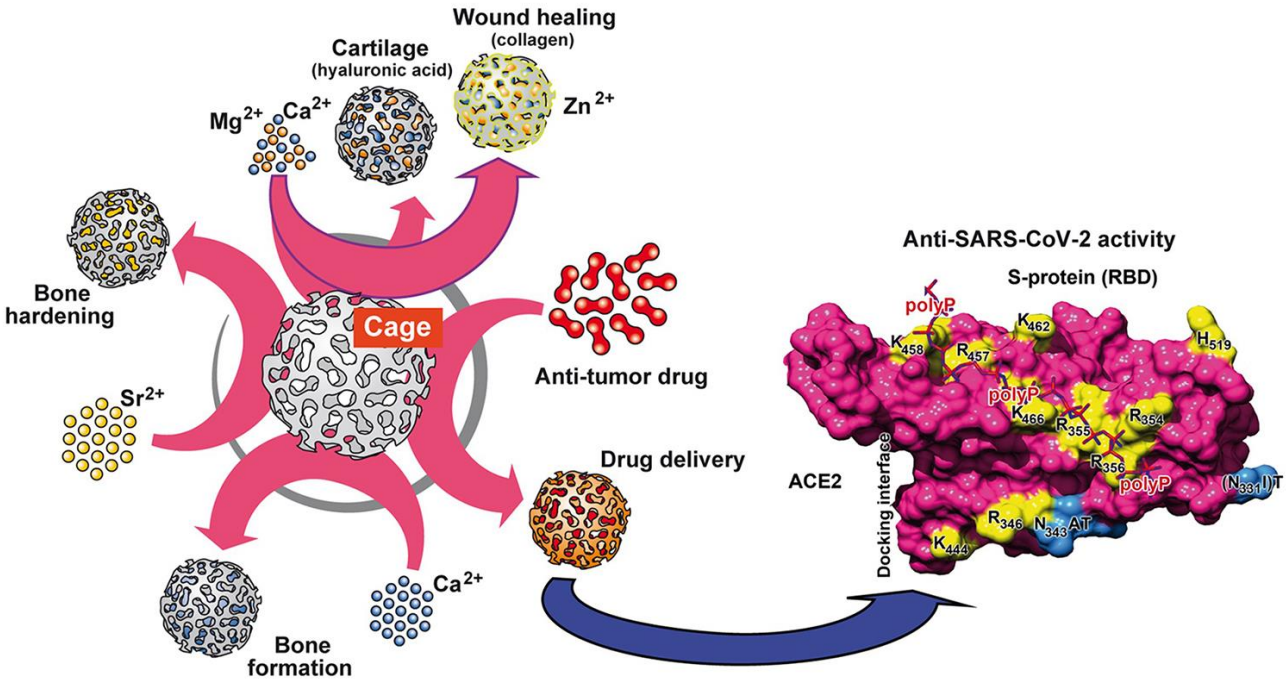
Graphical Abstract



Abstract

Inorganic polyphosphate (polyP) is one of the oldest chemical energy-providing molecules in biological systems. This polymer, containing a much longer sequence of high-energy phosphate units than the universal energy donor adenosine triphosphate (ATP), has attracted increasing attention for potential biomedical applications because of its diverse metabolic and regulatory functions and its ability to form biologically active nano/microparticles.

In its particulate form, polyP is not biologically active but these particles easily transform into a coacervate form in which polyP is biologically active. polyP can be easily combined with other materials used in tissue engineering, e.g., for the production of bioprintable bioinks (even for cell printing) or stable polymers such as polymethacrylate of polycaprolactone. In this way, the material could be applied not only as a filler, but also for the fabrication of larger mechanically more stable implants. In addition, together with other negative polyanions, polyP is able to selforganize the presence of divalent cations to polymer bundles stabilized by Ca^{2+} bridges, or polyP nano/microparticles can be created in situ from polyP incorporated into certain hydrogels.

Through the selection of suitable hydrogel-forming polymers and controlled hardening via calcium ions, hybrid biomaterials of defined porosity and mechanical properties can be fabricated, which are not only morphogenetically active, i.e., capable of promoting cell growth, differentiation and migration via specific gene induction, but also provide the cells with the energy needed for their function, including those processes which proceed in the extracellular space.

With the discovery of polyP and the characterization of the multiple functions of this energy-rich biopolymer, a new physiological molecule has been introduced into the growing group of biomaterials of biomedical interest, which adds a novel principle: metabolic energy-delivery in addition to morphogenetic/regenerative activity. There is no other biomaterial that is provided with this property combination.

Very recently, we investigated the effect of polyP in innate immunity on the binding of the receptor-binding domain (RBD) of the SARS-CoV-2 spike protein to the cellular ACE2 receptor and disclosed a potential therapeutic benefit of polyP against SARS-CoV-2 infection.

Keywords: Poly-phosphate; regenerative medicine; morphogenetically active; SARS-CoV-2.

Acknowledgements

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References

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2. W. E. G. Müller, S. F. Wang, M. Ackermann, T. Gerich, M. Wiens, M. Neufurth, H. C. Schröder, X. H. Wang, *Advanced Functional Materials*, **2019**, *29*, 1905220.
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5. M. Neufurth, X. H. Wang, H. C. Schröder, Q. L. Feng, B. Diehl-Seifert, T. Ziebart, R. Steffen, S. F. Wang, W. E. G. Müller, *Biomaterials*, **2014**, *35*, 8810.

Surface Linker Chemistry with Minimization of Non-Specific Adsorption on Sensor Materials

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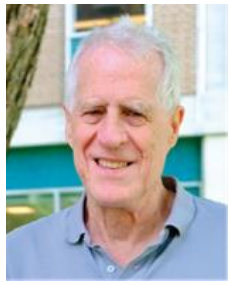
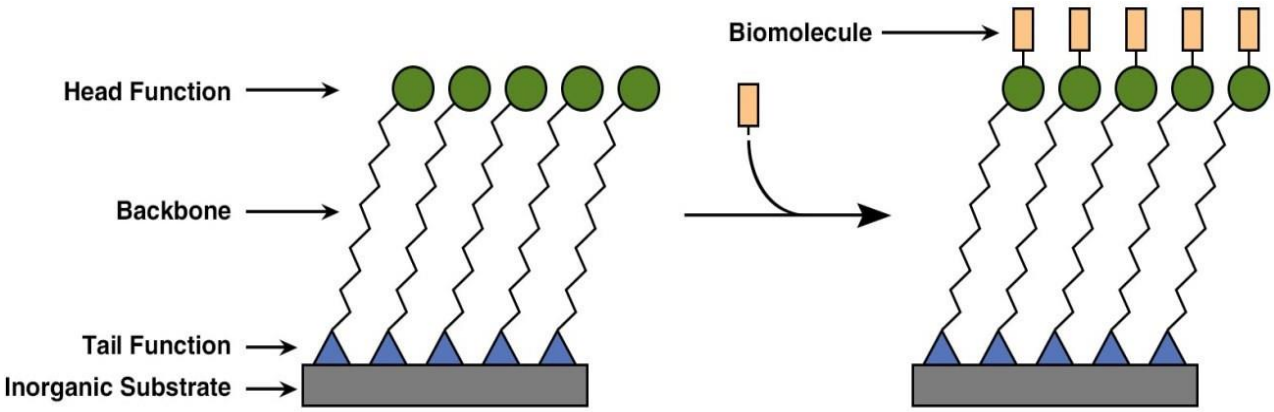


Graphical Abstract



Abstract

The operation of biosensors requires surfaces that are both highly specific towards the target analyte and that are minimally subject to fouling by species present in a biological fluid. This involves the attachment of a probe for the target in tandem with surface modification to avoid fouling. Both of these surface chemistries often involve application of linker molecules for surface-binding purposes. In this work, we further examine a thiosulfonate-based linker in order to construct robust and durable self-assembling monolayers (SAM) onto hydroxylated surfaces such as silica. These SAMs are capable of the chemoselective immobilization of thiol-containing probes (for analytes) under aqueous conditions in a single, straightforward, reliable and coupling-free manner. The efficacy of the method was assessed through implementation as a biosensing interface for an ultra-high frequency acoustic wave device dedicated to the detection of avidin via attached biotin. The device was comprised of quartz disc excited by an AC-powered flat spiral coil which operates at frequencies up to 1 GHz. Fouling was assessed via introduction of interfering bovine serum albumin (BSA), IgG antibody or goat serum. Improvements were investigated systematically through the incorporation of an oligoethylene glycol backbone employed together with a self-assembling diluent without a functional distal group. This work demonstrates that the incorporation of a diluent of relatively short length is crucial for the reduction of fouling. The glycol moiety in the diluent is hydrated with water of limited mobility which appears to provide the antifouling characteristic. Included in this work is a comparison

of the surface attachment of the linker to Si_3N_4 and AlN, both materials used in various types of sensor technology.

Keywords: Biosensor materials; surface linker; antifouling chemistry; acoustic wave detection.

Acknowledgements

Support for this work from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

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DFT-based Simulations about Stability and Adhesion of Metal-Organic Interfaces

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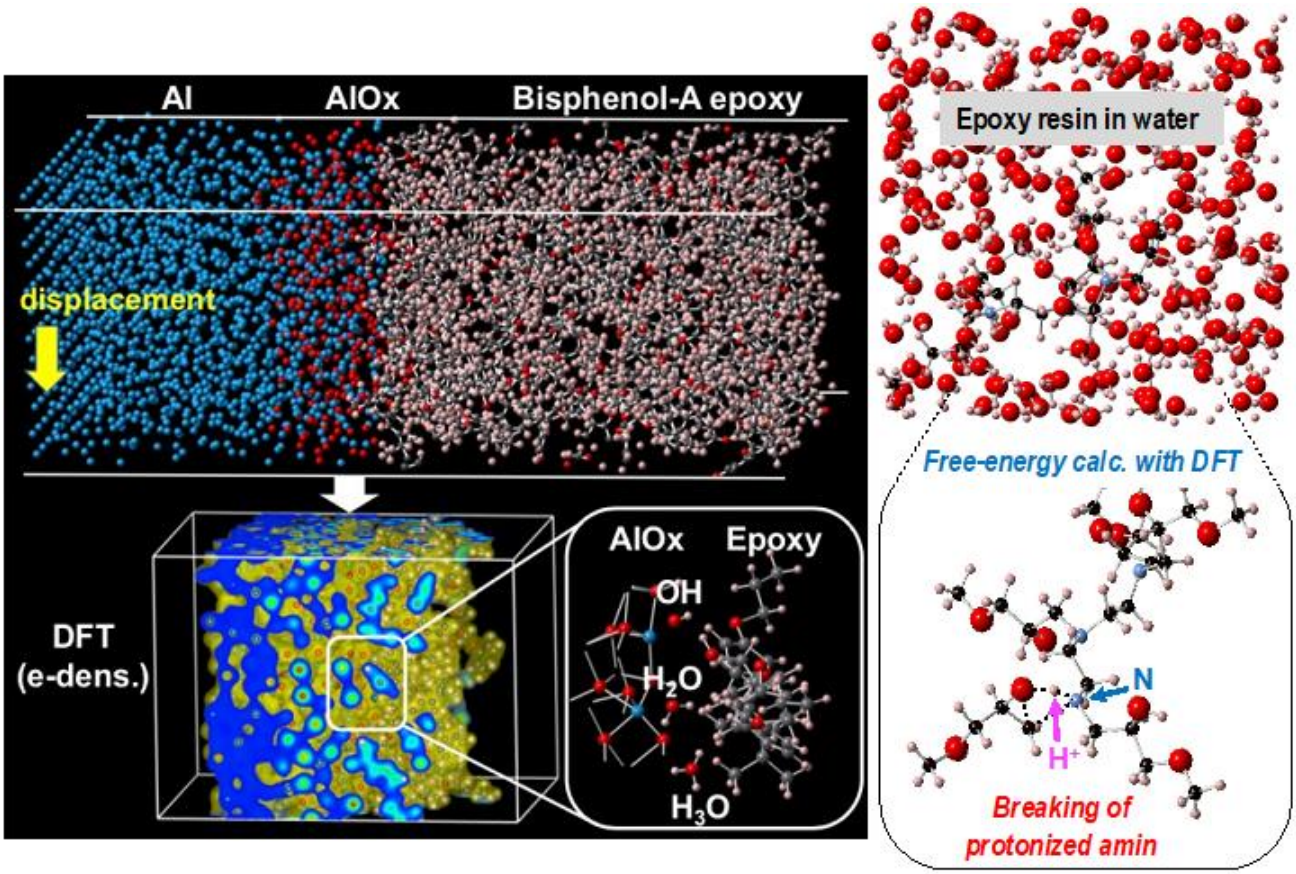
Graphical Abstract



Abstract

The adhesive bonding has become a key technique for automotive manufacturing. The bisphenol-A epoxy resin with curing agent has been used widely as the bonding glue. One of the fundamental open problems in the adhesion between metal and epoxy resin is that the adhesion strength reduces significantly in a moist environment. Microscopic understanding of the phenomena is

essential to propose an innovative method to solve the problem. In this talk I summarize our recent simulations.

(i) To simulate the moisture-induced weakening of the adhesion strength, we perform the hybrid quantum-classical (QM-CL) simulation of various aluminum substrate and epoxy resin interface with water molecules inserted in the contact region. In accordance with experimental conditions, the aluminum layer is surface oxidized while the bisphenol-A type epoxy molecules are either cured or uncured. Calculated adhesion strength is about 50 MPa and decreased by about 50 % when H2O molecules are inserted at the contact region, in agreement with the experimental observation. Three types of novel chemical reactions that involve unsaturated Al atom of the surface-oxide (amorphous alumina) are found.

(ii) Protonation and deprotonation free energies of cured epoxy resin are addressed from the first-principles DFT calculations using the vertical energy-gap method. The amin group located originally at the end of the curing agent is protonated at equilibrium when the epoxy resin is embedded in water under normal conditions. Their effects on the weakening of chemical bonds of the epoxy resin are clarified. Comparing the barrier energies, we predict that the breaking of protonated amin group is the principal process of epoxy resin breaking in wet conditions.

Keywords: Adhesion; protonation; inorganic-organic interface; DFT.

References

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25 Years of Commercializing Nanomedicine: Lessons Learned and Necessary Future Directions

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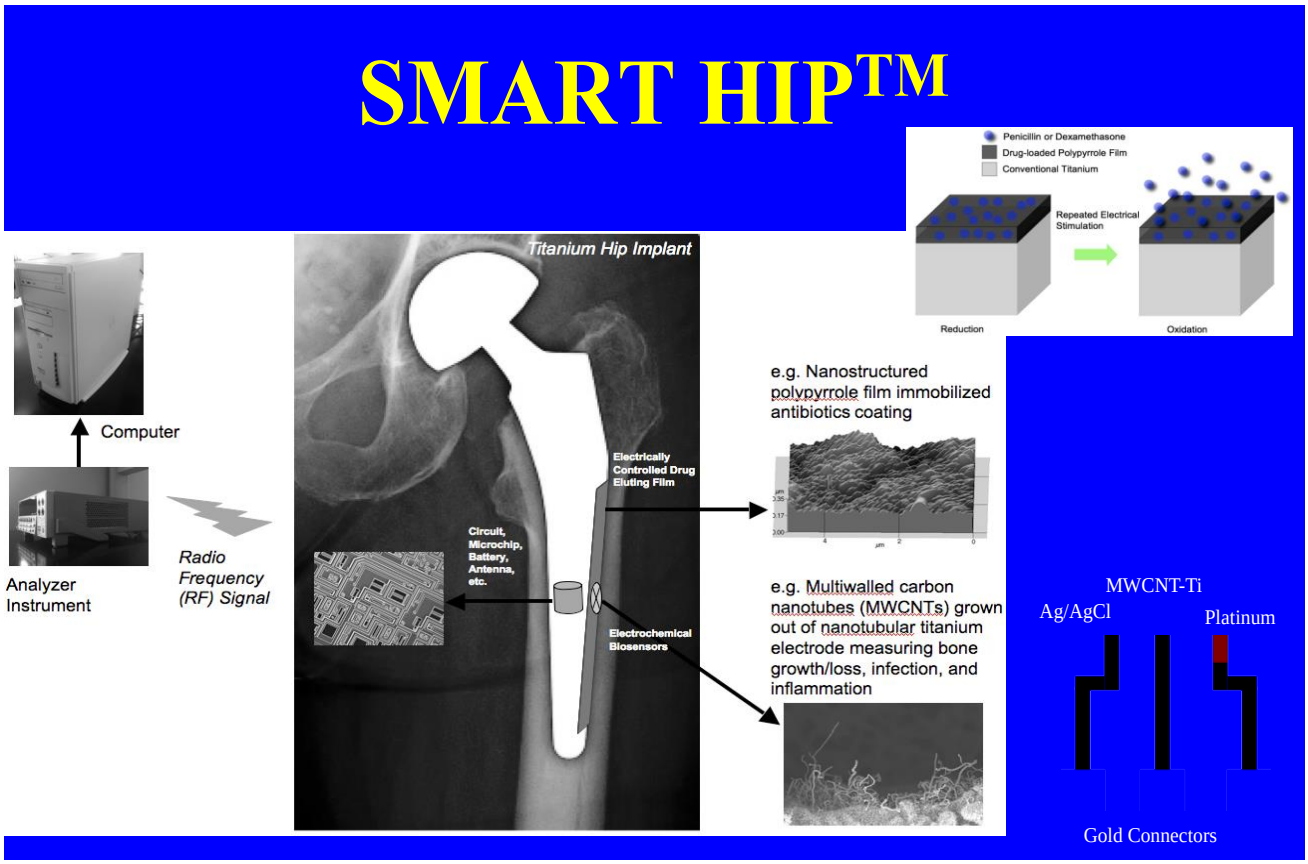
[1]Interstellar Therapeutics, Audax Medical, and Northeastern University, Boston, MA USA 02915

Graphical Abstract

Nanomedicine has made clear and unprecedented improvements in the prevention, diagnosis, and treatment of numerous diseases. While we celebrate that success, as we have learned from the COVID-19 pandemic, it is key to constantly improve medicine. As just one of many examples, below is an implantable nanosensor grown off of a hip implant that can sense what cells attach, what tissue is growing, communicate such information to a hand held device, and respond on-demand to release biomolecules to kill bacteria, inhibit inflammation, or promote tissue growth.



Abstract

25 years ago, I embarked on a journey to determine if nanomaterials (nanoparticles, nanotubes, nanotextured surfaces, self-assembled materials, and so on) could improve the prevention, diagnosis, and treatment of various diseases. The idea was simple. Our body is composed of nanomaterials, such as proteins or in bone calcium phosphate crystals, so nanomaterials would be an obvious solution to improve medicine. 25 years later, nanomedicine is now a mature field providing solutions for treating infections, cancer, neurological diseases, more efficient and effective diagnostic kits, higher resolution medical imaging techniques, and so much more. Just as impressive, in this very short time, regulatory agencies around the world have approved dozens of nanomaterials for implantation, including the recent Moderna and Pfizer-BioNTech COVID-19 vaccines which employ nanoparticles.

However, while it is important to celebrate our success, it is equally as important to continue to push nanomedicine even further to solve our most difficult medical problems. This talk will cover not only past achievements but future nanomedicine promises. Such future directions include implantable nanosensors that can determine in real-time cellular functions, changing the shape of implantable materials once implanted inside the body from outside stimuli, and how predictive equations can be used to estimate the size of nanofeatures on medical devices that can decrease infection or inflammation while promoting tissue growth.

Through such work, it is not only clear that nanomedicine has already revolutionized medicine, but will continue to do so for decades to come.

Keywords: Biomaterials; implantable sensors; nanoparticles; nanotextured surface.

Catalytic Performance of MXenes for HER Predicting by DFT Calculations

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[2]Science and Technology on Advanced Composites in Special Environments Laboratory, Harbin Institute of Technology, Harbin, 150001, PR China

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Developing low cost, stable and high active nonprecious hydrogen evolution reaction (HER) catalysts is one of key factors for hydrogen energy economy. Two-dimensional metal carbide and nitride (MXenes) materials have shown characteristics of promising HER catalysts. Herein, we explored systematic studies on the exfoliation properties of MAX phases to MXene phase, and the HER performances of MXenes to search the universal descriptors for HER performances of MXenes. Results illustrate that the exfoliation ability of MAXs is connected to the binding energy of element A in MAX, the lower binding energy of A element, the higher exfoliation energy of 2D MXenes from MAXs. A critical value of exfoliation energy (0.253 eV/Å^2) was obtained, MAXs with exfoliation energy lower than this value will favor the exfoliation. For the predication of HER performances of MXenes, a new descriptor, the surface terminated O-*p* orbital center ε_p, was proposed to predict the HER performances of MXenes. Applying ε_p to serious MXenes with different surface functional groups shows that the best values of ε_p are in the range of -4.1 to -3.3 eV. Our results indicated that O* terminated $M'_2M''C_2$ are promise HER electrocatalysts for generating hydrogen by water splitting, and transition metal surface modification and carbon vacancy are effective ways for achieving a promising electrocatalysts for HER.

Lixin Xiao*, Ph.D, Professor, FRSC

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Current Researching Interests on organic electronics:

1. OLED

To design highly efficient materials for organic light-emitting devices (OLEDs) especially on blue emission and electron transporting materials as well as enhancement of light output of OLED by using nanotechnology.

2. PV

Lead-free perovskite photovoltaic (PV) materials and enhancement of energy conversion efficiency and stability by introducing nanotechnology.

Has published more than 150 papers and 30 patents, 3 books, SCI cited more than 4000 times. Selected as the "annual influence" list of the world's top 2% scientists in 2020. The first prize of natural science of the Ministry of Education of China (first author, high efficiency organic blue emitters and its meso structure light emitting devices, 2015).

Professional Experience

2015.12-	:	Present Fellow of Royal Society of Chemistry
2011.8-	:	Present Professor, Department of Physics, Peking University (China)
2006.5-2011.7	:	Associate professor, Department of Physics, Peking University (China)
2005.4-2006.5	:	Researcher, Nippon Valqua Industries, Ltd (Japan)
2003.4-2005.3	:	Researcher, Optoelectronic Industry and Technology Development Association (OITDA),1-20-10 Sekiguchi, Bunkyo-ku, Tokyo 112-0014 (Japan)
2001.4-2003.3	:	Professor, Institute of Metallurgical Physicochemistry and Materials Chemsitry, Central South University (China)
2000.4-2001.3	:	Researcher, Department of Applied Chemistry, Tokyo University of Agriculture & Technology (Japan)
1994.7-1996.9	:	Assistant professor and lecturer, Institute of Metallurgical Physicochemistry and Materials Chemistry, Central South University (China)

Education

1997.4-2000.3	:	Department of Applied Chemistry, University of Tokyo (Japan), Ph. D
1991.9-1994.6	:	Chemistry Department, Hunan Normal University (China), M. Sc.
1984.9-1988.7	:	Chemistry Department, Hunan Normal University (China), B. Sc.

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Brief Biodata

Professor Ramesh K. Agarwal is the William Palm Professor of Engineering in the department of Mechanical Engineering and Materials Science at Washington University in St. Louis. From 1994 to 2001, he was the Sam Bloomfield Distinguished Professor and Executive Director of the National Institute for Aviation Research at Wichita State University in Kansas. From 1978 to 1994, he was the Program Director and McDonnell Douglas Fellow at McDonnell Douglas Research Laboratories in St. Louis. Dr. Agarwal received Ph.D in Aeronautical Sciences from Stanford University in 1975, M.S. in Aeronautical Engineering from the University of Minnesota in 1969 and B.S. in Mechanical Engineering from Indian Institute of Technology, Kharagpur, India in 1968. Over a period of 45 years, Professor Agarwal has worked in various areas of Computational Science and Engineering - Computational Fluid Dynamics (CFD), Computational Acoustics and Electromagnetics, Computational Materials Science and Manufacturing and Multidisciplinary Design and Optimization. In materials science, his research interests are in modeling of metamaterials, biodegradable composites, shape memory alloys, polymer-matrix and ceramic matrix nanocomposites. He is the author and coauthor of over 600 publications. He has given many plenary, keynote and invited lectures at various national and international conferences worldwide in over sixty countries. He is a Fellow of 22 professional societies including American Institute of Aeronautics and Astronautics (AIAA), American Society of Mechanical Engineers (ASME), Institute of Electrical and Electronics Engineers (IEEE), Society of Automotive Engineers (SAE), American Association for Advancement of Science (AAAS), American Physical Society (APS) and Institute of Materials, Minerals & Mining (IOM3), U.K. He has received many prestigious honors and national/international awards from various professional societies and organizations for his research contributions including the AIAA Reeds Aeronautics Award, SAE Medal of Honor, ASME Honorary Membership and Honorary Fellowship from Royal Aeronautical Society.

Seamless Solution for Industrial-Grade Continuous Carbon Fibre 3d-Printed Composites

Y. Willemin[1,*], M. Eichenhofer[1]

[1]9T Labs AG, Zurich, Switzerland

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Abstract

Nowadays, the comparably high costs associated with carbon fiber (CF) composite parts to its aluminium or steel contenders remain a constraining factor. A higher degree of freedom to optimize the part geometry and the fiber layup in combination with increased automation in manufacturing will reduce the current constraint. 3D printing, an additive manufacturing technology, is believed to deliver on those demands for manufacturing.

9T Labs' radical all-in-one Red Series technology provides a fully integrated solution, starting from CAD design to final part. Further, it enables 3D printing of performance composites with high fiber volume content (>50%) materials, ensures part quality by introducing appropriate consolidations steps, and scales through parallelization of affordable printing units.

Keywords: Composites, design, digital prototyping, 3d printing, additive manufacturing, serial production

Polarization Coupling in an Asymmetrical Semiconductor Nanodimer

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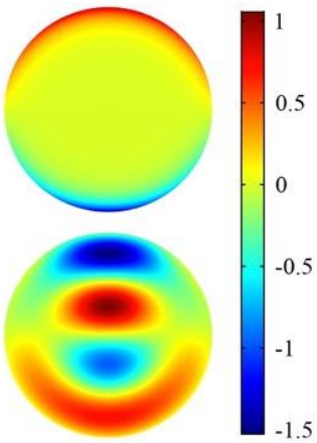
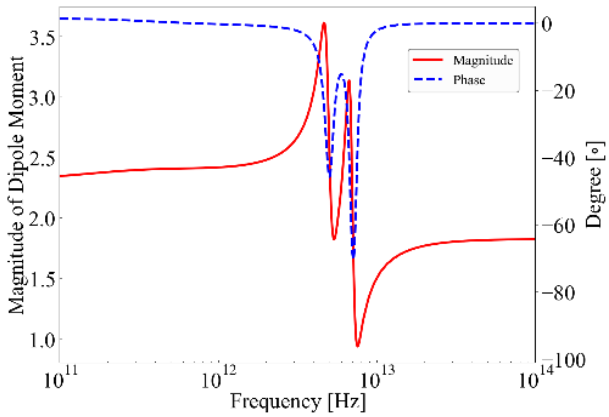
Graphical Abstract



Charge distribution in a semiconductor nanodimer in a terahertz electric field near the surface plasmon resonances



Magnitude and phase of the induced dipole moment on the semiconductor nanodimer

Abstract

A dimer is a simple form of cluster bearing the salient characteristics of polarization interactions between the constituent particles while being amenable to tractable analysis. Semiconductor nanoparticles (SNP) exhibit surface plasmon resonance (SPR) in the terahertz range, for which they are receiving considerable interest as impetus for device and circuitry applications in that part of the electromagnetic spectrum. The provision for variation in charge concentration by doping of semiconductors adds a degree of freedom in the design of semiconductor nanostructures not easily achieved with metals, allowing for applications in wider frequency range and adjustment in polarization spectral response. A semiconductor nanodimer (SND) formed by two SNPs with unequal doping levels exhibits a dipole moment spectrum with unique signature resulting from the interference in the secondary field arising from the polarizations in the constituent SNPs. In this investigation, the response of an asymmetrical SND in a terahertz electric field is studied by

electromagnetic simulation with transport formulation for charge dynamics in the semiconductor. The observed skewed polarization spectrum can be interpreted in terms of the interference among the secondary field arising from the intrinsic surface plasmon resonance (SPR) of the SNPs, each slightly red shifted as a result of coupling interactions. At the SPR at lower frequency, the charge polarizations in both particles are within 90^0 phase delay from the applied field, leading to enhancement in the dipole moment. On the other hand, at the SPR at higher frequency, the particle with lower doping has charge polarization substantially out of phase with the applied field while the particle with higher doping is close in phase with the applied field, leading to a smaller magnitude in the total dipole moment. The intensified electric field in the gap region goes through a process of undulation as the frequency of the applied field is varied over the two SPRs. The phenomenon can be employed to implement field scanning effect in senor applications.

Keywords: Nanodimer, semiconductor, polarization, dipole moment, interference.

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Photoactive Floating Conducting Polymers for Water Remediation

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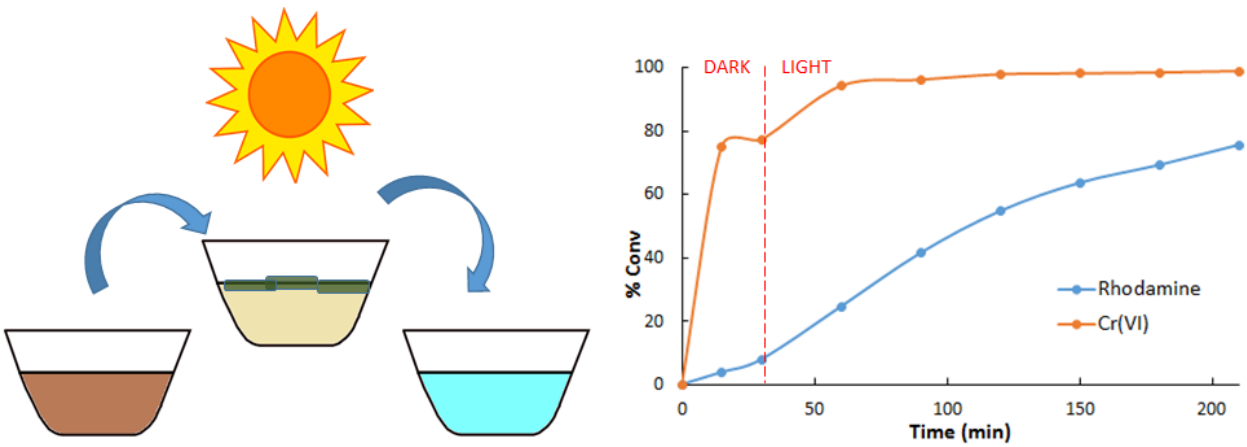
Graphical Abstract



Abstract

The chemical industry of the forthcoming years will be shaped by a number of emerging global megatrends strictly related to the demand of innovative materials able to solve new needs in different fields. Among them. environmental deterioration and the scarcity of fresh water have become imperative global issues to be solved nowadays. In the last three decades many efforts have been addressed to develop photoactive materials which could be suitable for real-world use in the field of water remediation. In this regard, water-floating photocatalysts could represent good alternatives to traditional materials thanks to their characteristics in terms of efficiency and reasonability including a high oxygenation of the photocatalyst surface, a fully irridiation, easy recovery and reuse.

Thanks to its high photocatalytic activity and good stability TiO_2 has been proved to be an excellent photocatalyst [**1**]. However, because of its wide band gap (3.2 eV) its efficiency under solar light is dramatically limited. Hence, much effort has been devoted to improve the utilization of solar light by extending the photoresponse of TiO_2 to the visible region, such as metal ion doping,

non-metal doping, noble metal deposition, narrow band-gap semiconductors coupling and dye sensitization [**2**]. Recently, conducting polymers, such as polyaniline (PANI) and polypyrrole (PPy) have been reported as promising sensitizers to extend the spectral response of TiO_2 to visible light effectively in TiO_2 photocatalysts. The photocatalytic activity of conducting polymers modified TiO_2 under visible light irradiation resulted from the visible light absorption of conducting polymers and effective charge separation of photogenerated carriers owing to the heterojunction built between TiO_2 and the conducting polymers [**3**]. In the present study, PANI/TiO_2 and PPy/TiO_2 modified floating materials were fabricated by inexpensive, ease and innovative environmentally friendly approaches, properly characterized and applied in the photodegradation of rhodamine and in the reduction of CrVI to CrIII under solar light. The role of the conducting polymers in the pollutants abatement on the basis of their chemical-physical characteristics were also investigated. The best materials were subjected to recycle tests in order to demonstrate their stability under the reaction conditions.

Keywords: Decontamination; dyes; heavy metals; conducting polymers, titania.

Acknowledgements

The authors thank Velux Stiftung Foundation for the financial support through the project 1381 “SUNFLOAT – Water decontamination by sunlight-driven floating photocatalytic systems”.

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Morphology and Heat Transfer Performance of High-density Aluminium Foam

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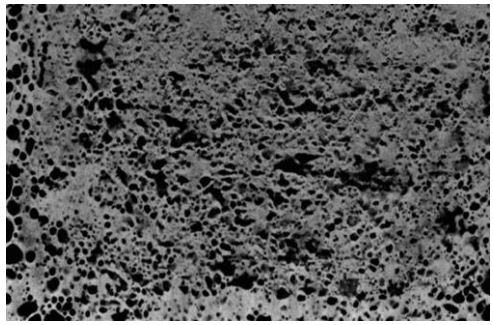
Graphical Abstract

Aluminium foam ceiling heat exchangers



Cross sectional image of Al-foam sample obtained byX-Ray tomography using Phoenix / Nanotom 180.

Abstract

The high-density aluminium foams prepared by powder-metallurgical process have been studied in this contribution. The observed increase in thermal conductivity of Phase Change Material (PCM) which is impregnated in the porous structure of aluminium foam, gives the possibility of applying the porous metallic structures for efficient latent heat storage when the phase phase transition of PCM between liquid and solid state occurs repeatedly. The energy-efficient aluminium foam heat exchangers impregnated with PCM have a huge potential for use in various industrial sectors. Relatively homogenous cloced-cell aluminium foam structure with only 40 % porosity (density of aluminium foam: 1.6 g/cm^3) in which the pores are interconnected by microcracs of pore walls, seems to be the optimum from the point of view heat transfer and heat storage performance.

A thorough investigation of the morphology and technological possibilities of the manufacturing process enabling the industrial production of energy efficient heat exchangers from these foams is the main subject of this study.

Keywords: Aluminium foam; phase change material; heat storage; powder metallurgy; energy efficiency.

Acknowledgements

The financial support by the Slovak Research and Development Agency under the contract APVV-17-0580 (project: Research of roofing with integrated function of heat exchanger, acronym: RoofFoam) is gratefully acknowledged.

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Is Micromachined Back-Markers on Thin Film of Scaffold Effective to Measure Repetitive Contraction of Myotubes?

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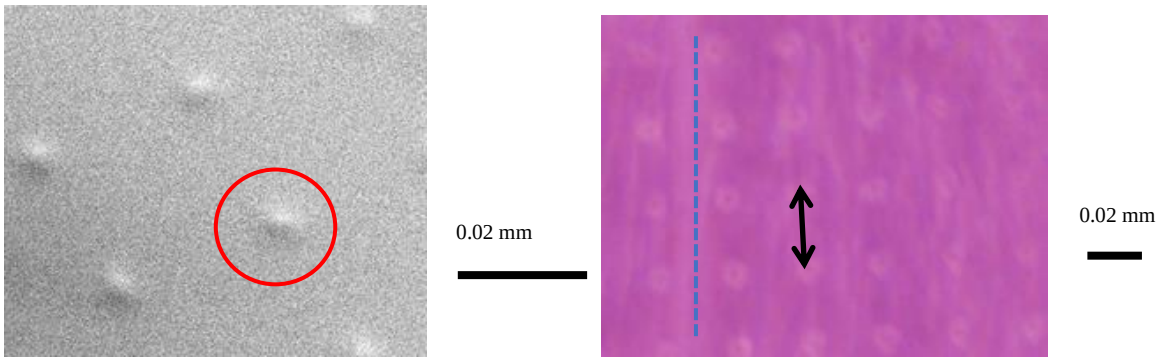
Graphical Abstract



Marker (red circle) on the backside of scaffold film (scanning electron microscope image, left) [1]. Myotubes (longitudinal direction of blue dotted-line) cultured on the scaffold film with back-markers (adjacent markers with arrow) (right) [1].

Abstract

Most of biological cells adsorb on the scaffold, and show activities: migration, deformation, proliferation, and differentiation. These activities depend on properties of the scaffold. The micro topography of the surface of the scaffold, which is close to the cell size, is effective for several applications[2]: the marker to trace each cell, and the tool to control the activity of each cell. The cell aligns along the micro step lower than 1 μm[3]. The micro-striped groove can control the cell orientation in the flow channel. The aspect ratio of the checkered concexo-concave pattern can control the orientation of cells. The taper-striped pattern is effective to observe durotactic migration of cell[4]. C2C12 (mouse myoblast) is used in the present study. The typical diameter of the cell is 20 μm, when it is floating in the medium. The scaffold of the transparent film with micro pattern markers has been designed to measure the contractile force of myotube under electric stimulation *in vitro*. The scaffold is made of a polydimethylsiloxane thin film (thickness 6 μm), of which the back side has arrangement of micro-protrusions (4 μm diameter, 2 μm height, interval 30 μm) made by the photolithography technique[4]. After hydrophilization, cells were seeded on the film at the counter surface to the protrusions at the density of 5×10^4 cells/cm^2. The cells were cultured on the scaffold

for 12 days in the medium containing 10% FBS (fetal bovine serum) and 1% penicillin/ streptomycin at 310 K with 5% of CO^2 content. The electric pulses (amplitude of 30 V (0.06 A); pulse cycle of 1 s; pulse width of 1 ms) were applied between electrodes of titanium wire dipped in the medium. The contraction of myotubes is observed through the transparent scaffold at the microscope. The designed scaffold has a potential for the measurement of the contractile movement of myotube microscopically *in vitro*. The results will contribute to several applications: tissue engineering, and regenerative medicine.

Keywords: Scaffold of cell culture; polydimethylsiloxane; micro-marker; photolithography; surface topography.

Acknowledgements

The experimental work was supported by Mr. Daisuke Watanabe, and Mr. Yuta Saito.

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On Spin Polarization and Anti-Particle Asymmtry

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Abstract

Spin polarization by definition refers to an ambient space of Euclidean 3-D; however, "spin" originated from Dirac's spinor, which is a construct from Clifford algebras, non-Euclidean. This bifurcation impedes material science, as manifested for example by the famed enigma that an electron requires a 720-degree rotation to return to its original state. My talk will show that an electron has four spin states in a 720-degree cycle, down, right, up, and left, by mathematical derivation as well as by physical demonstration, with my publication as reference - - Pauli matrices immersion - ScienceDirect (doi.org); in addition, I will address the production and preservation of anti-particles. The motivation here is to provide mechanical/electrical/nano engineering with a firm Euclidean geometric underpinning.

Keywords: Intrinsic spin; spinor; imaginary *i* as rotation.

Acknowledgements

I am grateful to my colleagues in Providence College for their various forms of support.

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Main-chain Twisted Non-fullerene Acceptors for Efficient Organic Solar Cells

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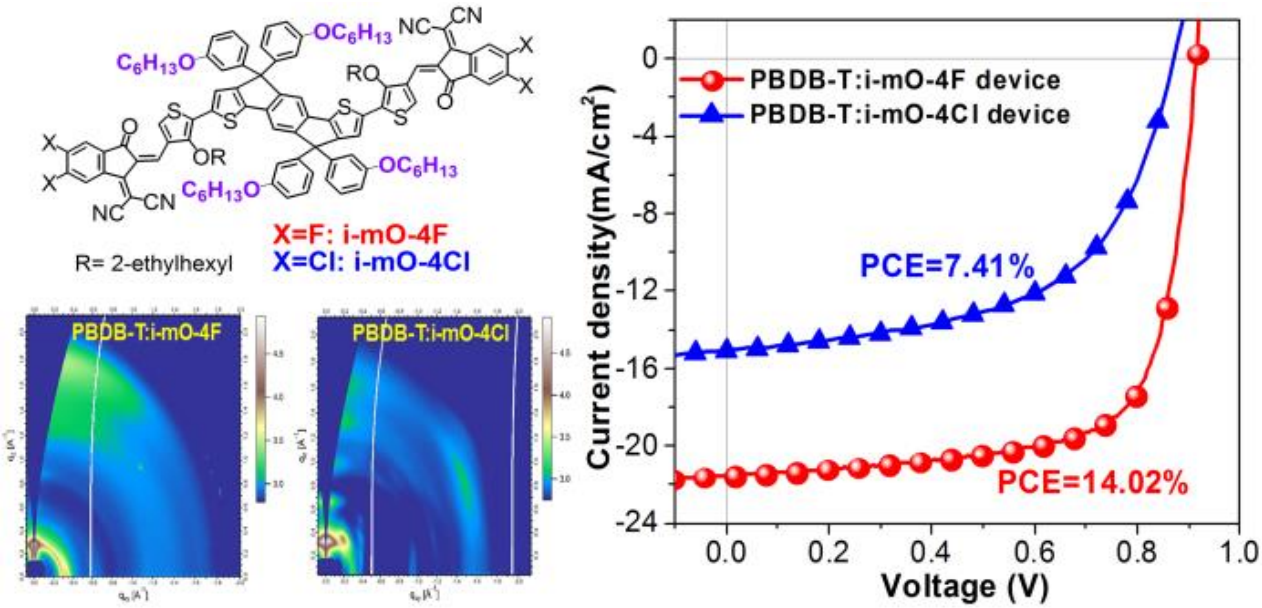
Graphical Abstract



Abstract

Lately, organic photovoltaic cells (OSCs) have been achieved tremendous progress because of the application of non-fullerene small molecule electron-acceptors (NFAs). The planar π-extended structure of NFAs benefits to red-shift the absorption spectra to realize effectively intramolecular charge transfer in the conjugated main-chain. However, it also tends to form aggregation and large domains when blended with polymer electron-donors in the active layer of OSCs, which is detrimental to the performance further improvement of OSCs.

To address this problem, we propose a strategy to properly twist the conjugated main-chain of A-π-D-π-A-type planar NFAs by introducing steric hindrance. The DFT calculation predicted that when changing the ending groups (INCN) of IEICO[1] from 5- to 4-position at the neighboring thiophene π-bridge, because of the steric effect, the dihedral angles of 5.9° and 18.6° were observed

in the molecular backbone, leading to a nonplanar conjugated main-chain. The obtained twisted-NFA i-IEICO[2] showed an exciting performance, including the elevated LUMO energy level, enhanced extinction coefficient. As a result, the device based on J52/i-IEICO achieves a power conversion efficiency (PCE) of 10.48%, while the device of IEICO only shows a low PCE of 5.13%. Combining with the halogenated ending groups, a new di-fluorinated twisted-SMA i-IEICO-4F[3] was also synthesized, which exhibited unique performance superior to its planar analog IEICO-4F, improving the PCE from 8.20% to 13.2%, when blended with a wide-bandgap polymer donor J52 in OSCs.

Based on this main-chain twisted strategy, a series of new A-π-D-π-A-type NFAs have been designed and synthesized in our group. Especially for the *meta*-hexyloxy-phenyl side-chain modified main-chain twisted acceptor i-mO-4F[4], high efficiency of 14.02% was acquired for the PBDB-T: i-mO-4F-based devices. The relationship between the molecular structures and their performances would be revealed.

Keywords: Organic solar cells; non-fullerene electron-acceptors; power conversion efficiency; main-chain twisted molecules.

Acknowledgements

This work was supported by the Natural Science Foundation of China (51903206), Key Research and Development Program of Shaanxi (Program No. 2020GY-288), and Natural Science Basic Research Program of Shaanxi (Program No. 2020JQ-985).

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Accurate Analytic Approximation for the Bessel Functions $J_\nu(x)$

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Abstract

Bessel functions appear in a wide number of applications in Engineering, Material Sciences, Physics, Electrodynamics and others. Those with integer order are usual in systems with cylindrical symmetries and half-integer order in spherical ones. Fractional orders are also very common. Power series for any value of ν are well known, but the convergence is usually slow. For this reason several approximations for particular values of ν have been published [**1-3**]. However, it seems that analytic approximations valid for continuous values of ν have not been found until now. Here a general analytic approximation for $J_\nu(x)$ with good accuracy has been determined, valid for positive values of the variable x and for any positive value of ν, non-larger than two. The structure of the approximate function $\tilde{J}_\nu(x)$ has been elaborated considering the power series and asymptotic expansion. The function is defined through a combination of rational and trigonometric functions, as well as fractional powers. A few parameters are left to be determined in a second step. To do this, the first terms of the power series and the leading terms of the asymptotic expansion are considered. In this way, each parameter becomes a simple elementary function of ν. Given a value of ν, each of the corresponding parameters is obtained immediately by a simple calculation, and the approximation will be valid for any positive value of x. The errors can be determined as a function of x, and the important point is where the maximum error appears. A plot of the maximum errors will be shown as a function of ν. The approximate function is exact for ν=1/2 and ν=3/2. The smallest maximum errors are also for ν near those values. In the method here used, the approximate function is like an extension of the multipoint quasi-rational technique, MPQA [**4**], but now because we have two variables, instead of one, new ideas have been introduced. Furthermore there are additional complications because it was necessary to recover exactly the well-known simple forms of the $J_{1/2}(x)$ and $J_{3/2}(x)$ functions.

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Nano vs Macro: Small Size Does Matter

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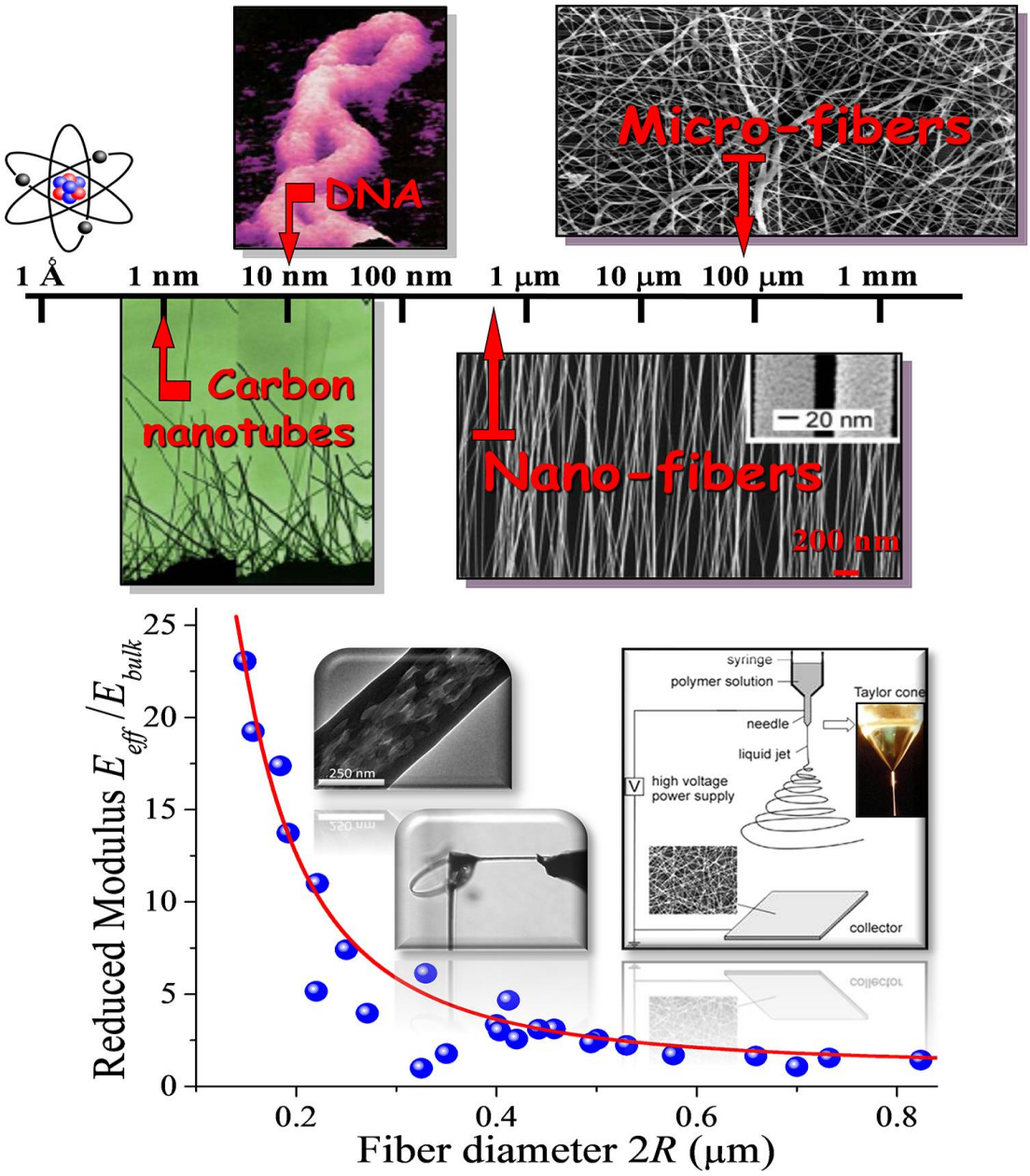
Graphical Abstract



Abstract

Some open problems concerning polymer materials of reduced sizes and dimensions, are discussed. Such objects exhibit exceptional physical properties when compared with their macroscopic counterparts. The lecture will focus on the mechanical and thermodynamic properties of polymer nanofibers fabricated through electrospinning which have attracted much attention recently because of their unique features. More specifically, electrospun polymer nanofibers demonstrate so-called "size-dependent behavior" when thermo-mechanical properties of material start to depend on fibers diameter, if their diameters are enough small. For example, abrupt increases in polymer nanofiber elastic modulus have been observed when diameters drop below a certain value. The thermodynamics properties of polymer nanofibers also demonstrate size-dependent behavior. For example, the temperature dependence of elastic modulus is highly influenced by fiber diameter, a shift in the glass transition and melting temperatures is observed, etc. [**1,2**].

Mechanical (macroscopic) analyses have failed to provide satisfactory explanations for the mechanisms ruling such features, calling for detailed microscopic examination of the systems in question. A hypothesis bridging the current knowledge gaps is presented. The key point of the proposed speculations is based on confinement concept: it is assumed that size-dependent behavior is related to confinement of non-equilibrium supermolecular micro-structure of electrospun polymer nanofibers which is being formed during their fabrication [**3,4**].

Keywords: Nanotechnology; polymer nanofibers; electrospinning; supermolecular structures.

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Renewable Synthesis of Chemical Feedstock and Specialties Employing Low Temperature Electrochemical Reduction of CO_2

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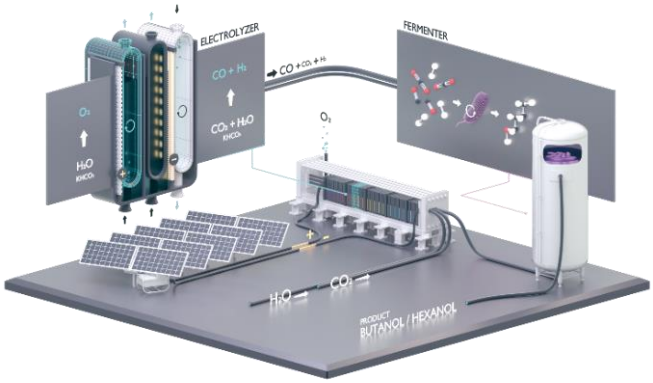
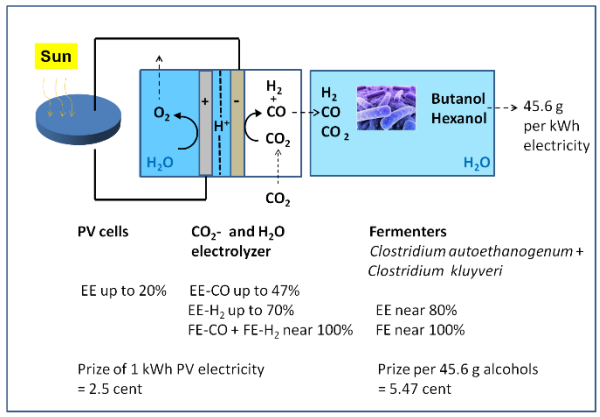
Graphical Abstract

The left artist picture shows a representation of the so-called "Technical photosynthesis". H_2 and CO are produced from H_2O, CO_2 and renewable energy (solar, wind) by electrolyzes, which can be used as molecular feed for an anaerobic bacteria mixture. Final products are butanol and hexanol. A back-of-the envelope calculation on the right shows the potential for economic viability[1].





Abstract

Profitable renewable synthesis of chemicals and fuels is a prerequisite for its implementation into current economics. Boundary conditions for the synthesis sequence are the availability of renewable energy in sufficient quantities and its intermittent character. Profitability is difficult when considering the low fossil energy carrier prices and the physical efficiency limitations of the processes.

In the presentation, two options employing electrochemical reduction of CO_2 are discussed:

The closest to industrial application process consists of two major components: Firstly, electricity from wind or solar is stored by electrolysis into energy carriers like hydrogen (H_2) or carbon monoxide (CO). Current density, Faradaic and electrical efficiency and endurance of this upstream process will be discussed. Secondly downstream, a flexible mixture of CO, CO_2 and H_2 is supplied to a multistep

anaerobic fermentation process, whereas they are initially converted to acetic acid and ethanol with high carbon efficiency and thus almost without any undesired by-products. The todays economic value is obtained by further condensation of the C2 products to C4 and C6 special chemicals (carboxylates and alcohols). Eventually, finally scaled into the hundreds megawatt range the molecules can be used as fuels.

In the talk a potential solution is addressed by using a commercially available silver-based gas diffusion electrode (used in industrial-scale chlorine–alkaline electrolysis) as the cathode in the CO_2 electrolyser. Electric current densities up to 300 mA cm² were demonstrated for more than 1,200 hours with continuous operation. Faradaic efficiency of the anaerobic fermentation processes was almost quantitative [**1**]. Evonik and Siemens have decided to bring the technology toward an industrial scale. The project is named Rheticus [**2**]. Generally, such an approach is called artificial or technical photosynthesis.

Still in research state is the single step direct electrochemical reduction of CO_2 to hydrocarbons, such as ethylene or ethanol. A series of the newly developed electrocatalysts based on the copper mineral paramelaconite will be introduced. The product distribution can be tuned by substituting copper by silver atoms and using the crystallographic arrangement as nano-template [**3**].

Keywords: Technical photosynthesis, direct electrochemical reduction of CO_2, anaerobic fermentation, nano-templated electrocatalyst.

Acknowledgements

The work on the technical photosynthesis was partly funded by the German federal Ministry of Education and Research (BMBF) within the Kopernikus Initiative ‘Power-to-X’ under contract number P2X-03SFK2J0. The funding of the exploration on CO_2 electrocatalysis by the German Federal Ministry of Education and Research (BMBF) within the ‘‘FONA framework program and CO2-WIN funding measure’’ in project PhasKat under contract number 033RC028A is highly appreciated.

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Three-Dimensional Brain-Mimicking Device Structure for Computing Energy Crisis

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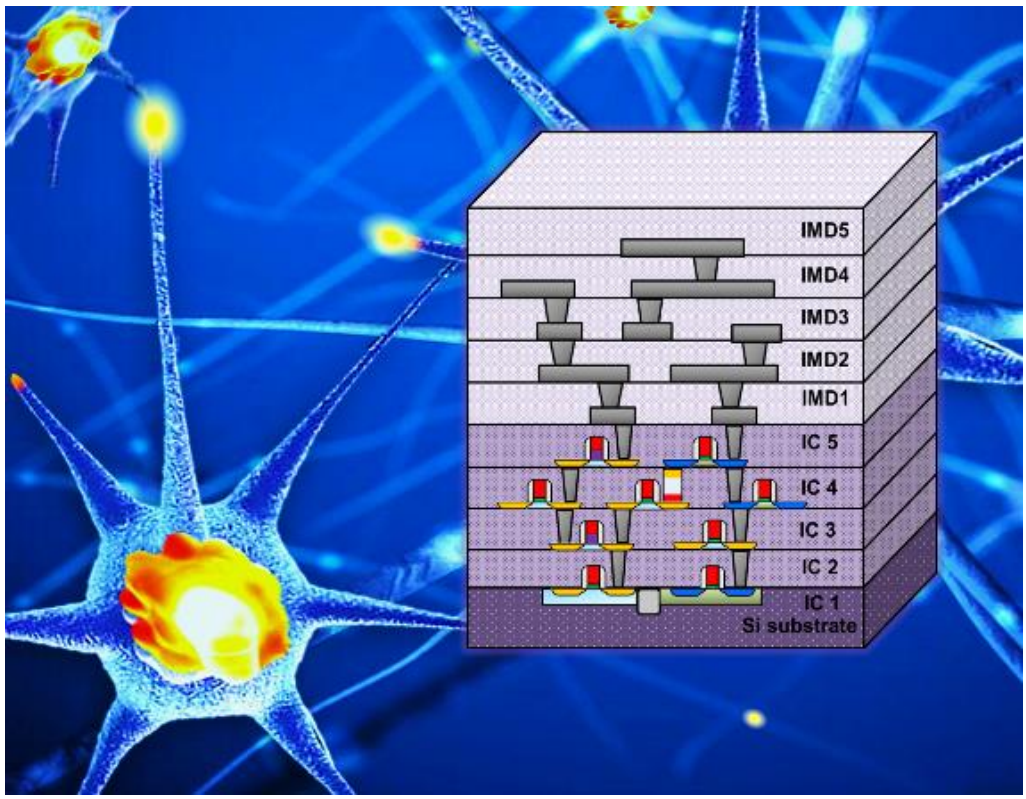
Graphical Abstract



The 3D brain-mimicking IC with high performance n- and p-MOS transistors on the backend amorphous-SiO_x layers of an IC.

Abstract

The forecasted energy consumption by Information and Communication Technology (ICT) at 2030 will reach as high as ~8200 Terawatt-hour (TWh), 30% of world's electricity production at 2020. The electricity consumed by ICT is mainly from the exponential growth of data centres and communication

networks [**1**]. At 2020, the data centres alone used more than 2% of the global electricity, and generated more carbon emissions than the world's airline industry. That is the reason why Stephen Hawking warned that Earth could be burnt by human beings at year 2600. The major energy consumption in ICT is due to the computing in microprocessors. To address the computing energy crisis, we invented the monolithic three-dimensional (3D) integrated circuit (IC) [**2,3**] and brain-mimicking IC [**4**]. The monolithic 3D brain-mimicking IC is formed by using nano-crystalline SnO_2 and SnO materials for n- and p-type MOS transistors respectively, on the amorphous-SiO_x dielectric layers of IC chips [**3,4**]. High field-effect electron and hole mobility of 238 and 7.6 cm^2/V-s were obtained, [**5**] for n- and p-MOS transistors respectively. The monolithic 3D IC offers 1 million times higher interconnect density than the currently used package-level 3D IC, the enabling technology for brain-mimicking IC [**4**].

Keywords: 3D; IC; SnO_2; SnO; CMOS.

Acknowledgements

The authors acknowledge the support from MOST of Taiwan.

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A Low Cost Paper Sensor with Moleculaly Imprinted Conductive Polymer Electrodes

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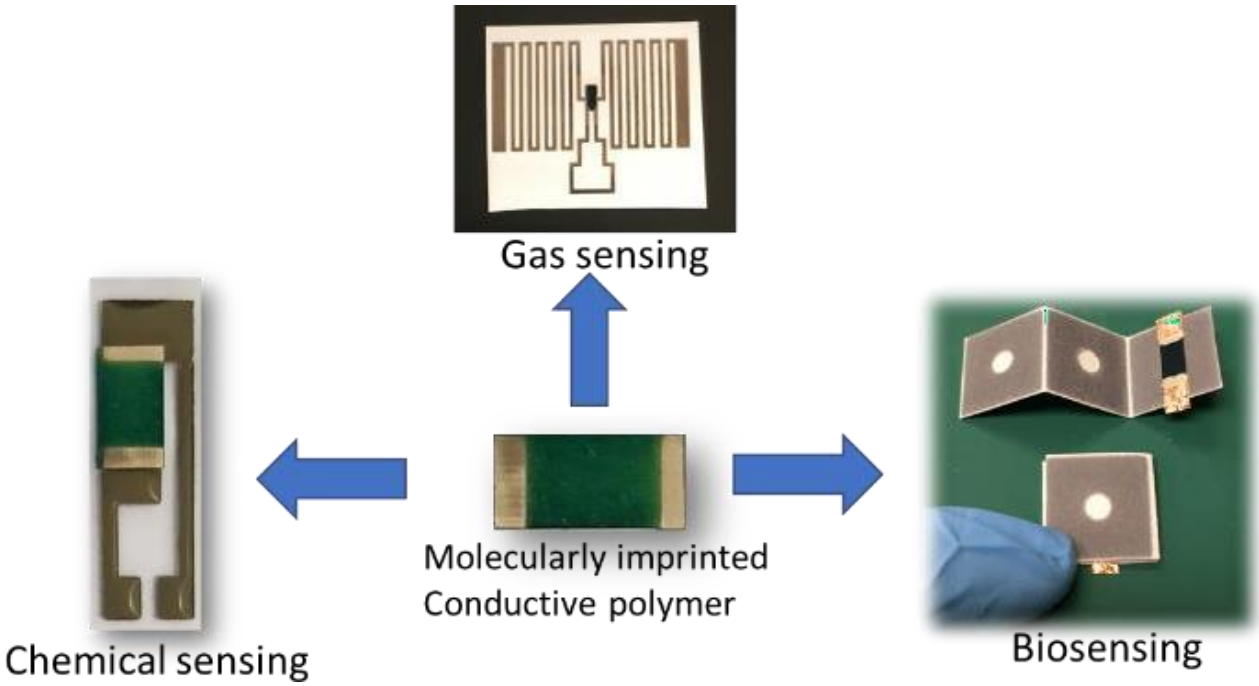
Graphical Abstract



Abstract

A paper sensor has been intensively investigated recently due to its low cost, versatility, portability, multiplexity and disposability for many application areas including clinical diagnostics, food safety and environmental monitoring. For instance, the paper multiplexing sensor that can detect multiple biomarkers has been developed with colorimetric transducers. The colorimetric patterns on the paper sensor are analysed precisely by machine learning process to identify the concentrations of multiple target molecules. Paper has a characteristic to transport and absorb liquid by capillary flow without the needs of external pumping system so that sensing transducers are easily fabricated by an inkjet printer. Target molecules are normally conjugated at the inkjet printer printed optical or electrical

sensing transducers via target recognition molecules such as antibodies or aptamers. The high cost of such bio-reagent impedes the value of low-cost paper sensors. To overcome such weakness, molecular imprinted polymer structure has been integrated with sensing transducers to capture specific target molecules without high-cost bio-reagents. Molecular imprinting (MIP) structures are formed in the polymer structure by templating target molecules during crosslinking process and removing them after the cross-linking process. With this approach, we have demonstrated the integration of MIP structure in conductive polymers for capturing and detecting target molecules. The electrical conduction mechanism in conductive polymer is based on the polaron transmission through polymer structures. Immobilization of target molecules at MIP sites induces the local fluctuation of polaron that reduces or increases the resistance of conductive polymer due to carrier mobility change. Because MIP approach does not require high-cost bio-reagent, it is expected to further leverage the value of paper sensor. In this presentation, I will present the most updated MIP conductive polymer based paper sensing results for medical, agricultural, and environmental monitoring applications. As example, I will present the detection of glucose in blood, methylmalonic acid (MMA), C-reactive protein (CRP), ammonia and Perfluorooctanoic acid (PFOA).

Keywords: Biosensor; paper sensor; conductive polymer.

Acknowledgements

We acknowledge the support from NSF Engineering Research Center (ERC, PATHS-UP) Grant 164841, Melinda and Bill Gates Foundation Grant OPP1199456.

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Equivalence Relations among PhylogeneticTrees and Genomic Index Maps

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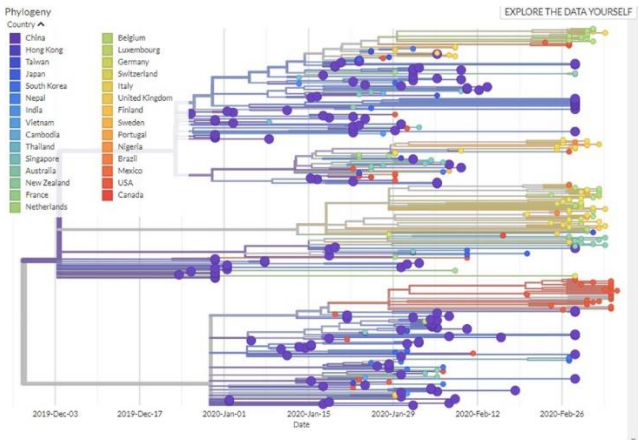
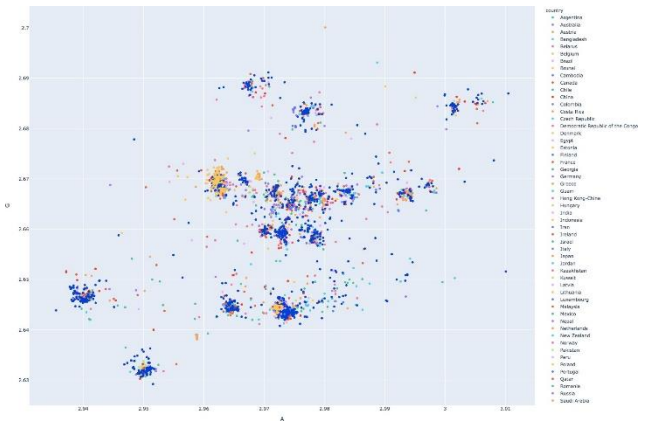
Graphical Abstract

Phylogenetic Tree for SARS-CoV-2 worldwide Countries/Regions.



Genomic Index Map for 72



Abstract

Visual technology of variant construction [**1**] for complicated sequences plays an assistant role in various applications to be useful in both scientific researches and advanced technologies especially for advanced bioinformatics [**2**]. Measuring schemes provide hierarchical tools to analyse complicated sequences as characteristic eigenvalues in wider applications.

In this talk, equivalence relations among phylogenetic trees and genomic index maps are discussed. Using diversity measure to a given set of genomes, equivalent clusters and complementary visual effects are provided between genomic index maps and phylogenetic trees. In this hierarchical framework, it is possible to use a unified framework and a visual tool to represent any selected region for clustering genomes on refined effects. A sample projection is illustrated to analyse three UK variation lineages of SARS-CoV-2 genomes in both BLAST phylogenetic trees and genomic index maps in comparisons. This equivalence relation can be wider applied to any genome and other complex sequences.

Keywords: Equivalence relation; phylogenetic tree; genomic index; SARS-CoV-2; visual maps.

Acknowledgements

This project is supported by the NSFC (62041213).

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Recent Advances on Multifunctional Hybrid Silica-Based Nanoparticles for Cancer Treatment

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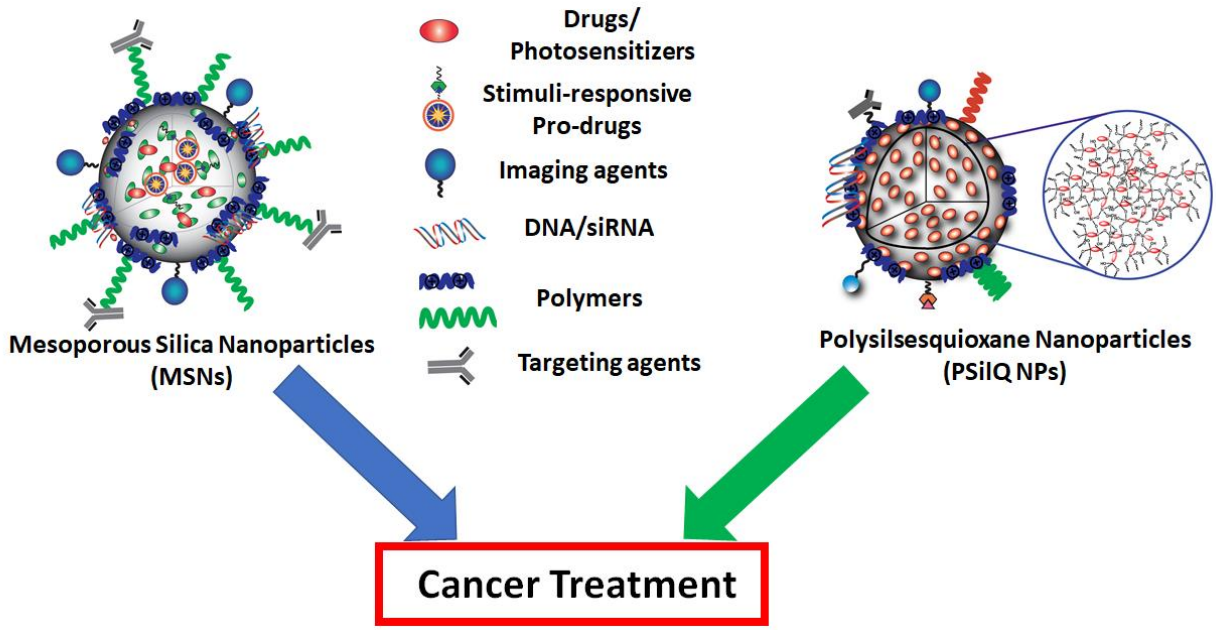
Graphical Abstract



Abstract

Nanoparticles are an innovative platform for cancer treatment that reduces systemic toxicity and allows for active targeting of tumor sites to enhance the therapeutic efficacy. Hybrid silica-based nanoparticles (HSNs) have emerged as an attractive drug delivery system due to their vast functionalization potential, biocompatibility, and high surface area. The surface of HSNs can be modified with targeting agents that allow not only the specific interaction with cancer cells, but also be used to carry nucleic acids. In addition, active molecules such as photosensitizers and/or anticancer drugs can be chemically attached or physically loaded into the interior and/or exterior surface of HSNs. My group has focused its efforts in two HSN platforms, polysilsesquioxane (PSilQ) and mesoporous

silica nanoparticles (MSNs). Herein, I will present our recent results aimed to demonstrate the versatility of HSNs to develop target-specific multifunctional delivery systems for the treatment of cancer. We have developed a target-specific MSN-based delivery system for the effective treatment of pancreatic cancer using combined therapy that includes gemcitabine and cisplatin. Moreover, we have used the same MSN platform to treat triple-negative breast cancer (TNBC) combining chemo and gene therapy. In a similar way, we have fabricated PSilQ nanoparticles for the improved treatment of TNBC using photodynamic therapy as the main therapeutic approach, but also with the combination of chemo and gene therapies. In particular, we have tested doxorubicin and curcumin as chemotherapeutic agents, and siRNA targeting apoptosis regulator gene BCL2. The efficacy of both systems was evaluated in *in vitro* and *in vivo* experiments for the respective type of cancers. Overall, our results demonstrate that both MSN and PSilQ nanoparticle-based platforms can improved the treatment of pancreatic or triple-negative breast cancer. Therefore, we are convinced that MSN and PSilQ nanoparticles may become a new promising approach to efficiently treat cancer and other diseases via the simultaneous targeting of various pathways.

Keywords: Hybrid nanoparticles; mesoporous silica nanoparticles; polysilsesquioxane nanoparticles; cancer treatment; multifunctional nanoparticles.

Acknowledgements

National Science Foundation (EAGER-NSF #1835688), SPRINT UNCC-FAPESP award, Faculty Research Grant award (FRG/UNC Charlotte), National Institute of Cancer under Award Number R15CA192160.

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Enrofloxacin Entrapped in Polymer Based Nanocarriers for Gut Infection Prevention

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Graphical Abstract

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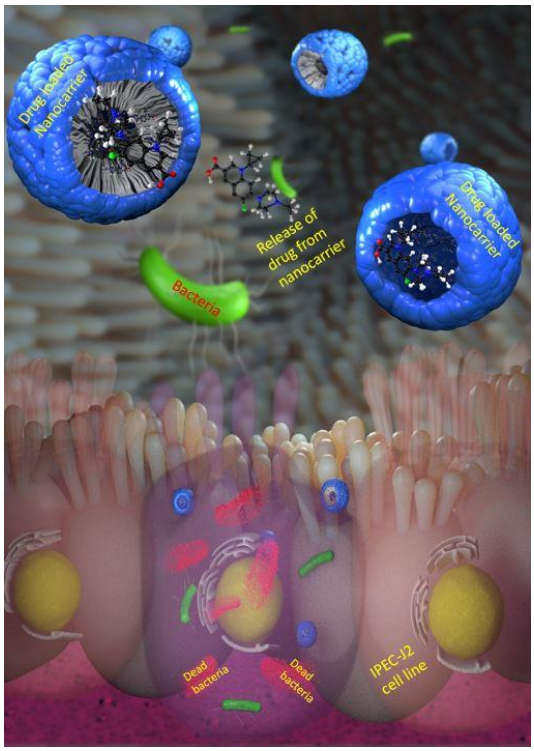

Abstract

Poor bioavailability of free antibiotics, cellular toxicity, and development of antibiotic-resistant bacteria jeopardize the future of antibiotic treatments. To circumvent these issues drug delivery using nanocarriers are highlighted to secure the future of antibiotic treatment. This work investigated the application of nanocarriers to prevent and treat bacterial infection while presenting minimal toxicity to the IPEC-J2 intestinal cell line. To accomplish this, two polymer-based nanoparticles (NPs) of PLGA and lignin-graft-PLGA (LNP) loaded with enrofloxacin (ENFLX) were synthesized, yielding spherical particles with average sizes of 111.8±0.6 nm (PLGA) and 117.4±0.9 nm (LNP). The releases

of ENFLX from PLGA and LNP NPs were modeled by theoretical diffusion model considering two diffusion barriers for drug release. The biocompatible concentrations of free ENFLX, enrofloxacin loaded PLGA(Enflx) and LNP(Enflx) were 0.14, 0.18, and 0.20 μg/mL based on examination of bacterial inhibition, toxicity, and ROS generation. Furthermore, these concentrations were used for treatment of higher and lower multiplicities of infection (MOI of 1:100 and MOI of 1:10) in the IPEC-J2 cells.

Prevention of bacterial infection by LNP(Enflx) was enhanced by more than 50% compared to ENFLX at MOI 1:10. At MOI 1:100, both PLGA(Enflx) and LNP(Enflx) demonstrated 25% higher prevention of bacteria growth compared to ENFLX. The superior treatment achieved by the nano carried drug is accredited to particle uptake by endocytosis and slow release of the drug intracellularly, preventing rapid bacterial growth inside the cells.

Keywords: *E. coli* O157:H7; nanocarrier; drug delivery; intestinal cells.

Acknowledgements

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Graphene Materials: Prepared and used Through Electrochemical Routes

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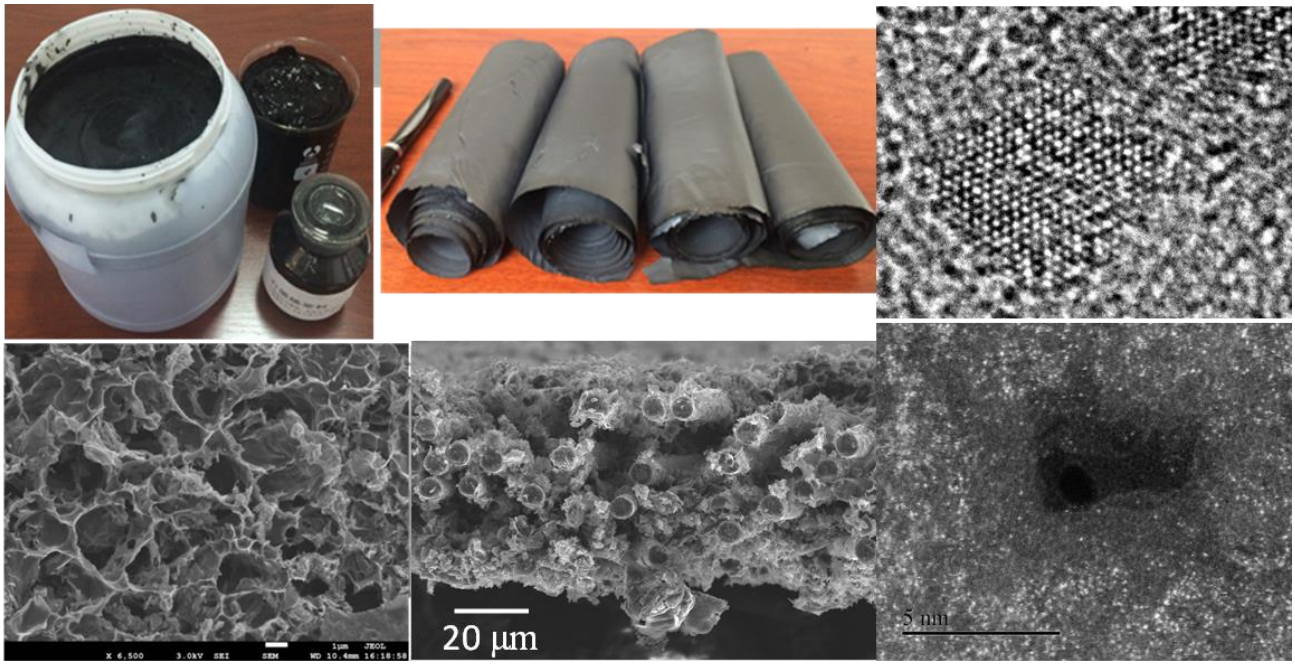
Graphical Abstract

Graphene ink, film, dots, porous graphene composite and supported single-atom catalysts can be prepared through electrochemical routes.



Abstract

In this talk, I will present high-performance graphene materials synthesized through electrochemical approaches for electrochemical application [**1**-**5**]. We could tune the sheet size, layer number, pore size, dopant, and atomic hybridization of graphene. Highly dispersible large literal sheets size of graphene flakes and small graphene microsheets [**5**] were produced at large scale. Porous carbon-graphene composites show high performances on supercapacitor and Li-S batteries. A number of electrochemically exfoliated graphene supported atomic metal electrocatalysts were successfully synthesized by various approaches. I will discuss how well and why we can obtain high electrocatalytic

performances on O_2 [**2,4**] and CO_2 [**1**] reduction reactions using graphene-isolated atomic electrocatalysts.

Keywords: Graphene; energy storage and conversion; single-atom catalyst; electrochemistry.

Acknowledgements

We thank the financial support by grants from Anhui funds (K120662002, S020218017) and Shanxi Major Project (20181102026).

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Cathode Design for High Energy Lithium Metal Batteries

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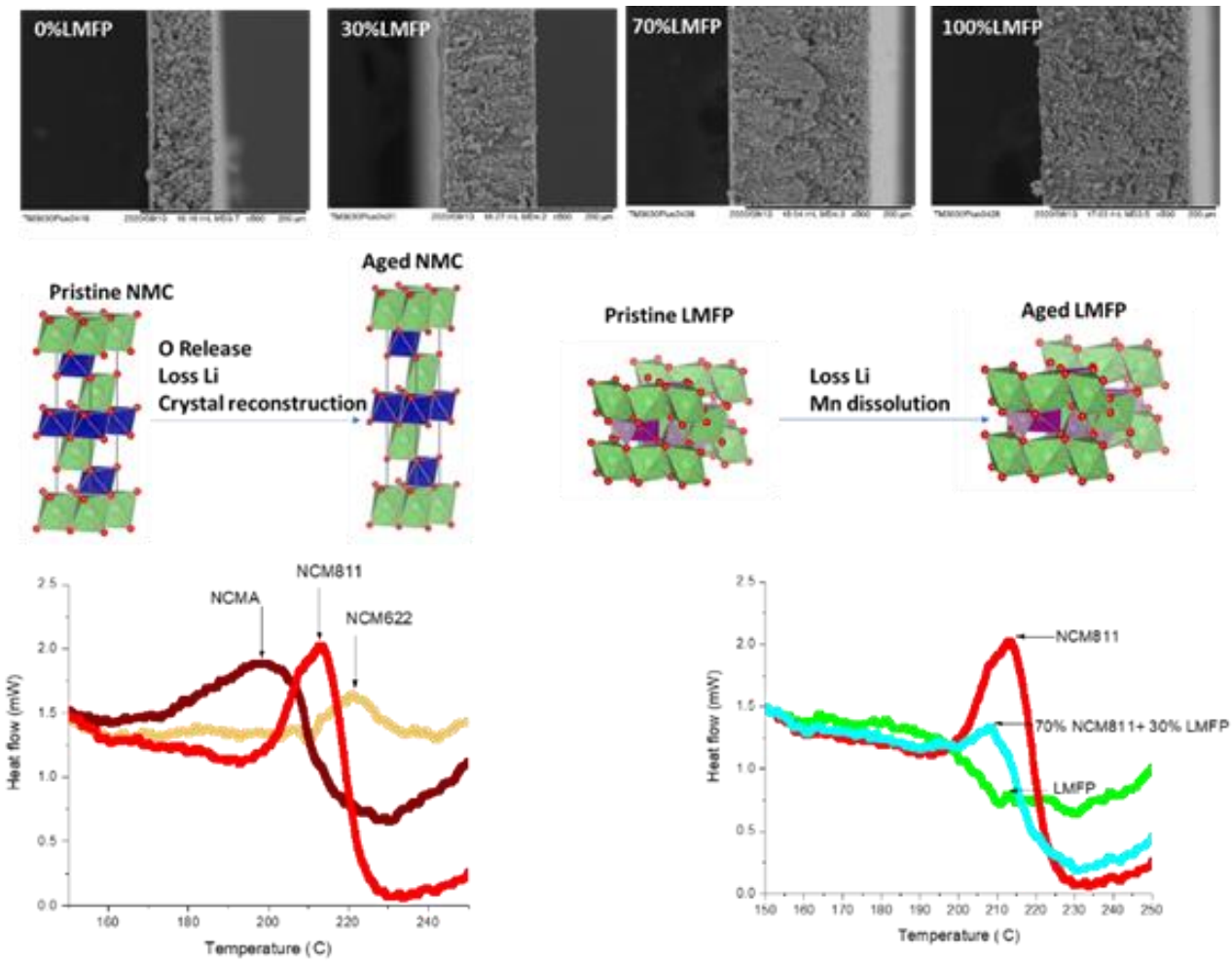
Graphical Abstract

The LMFP/NMC blend cathode design can initiate improved thermostability, crystal structure stability and high energy density of Lithium Metal Batteries.



Abstract

In this study, a complementary cathode design with 70% LiNi0.8Mn0.1Co0.1O2 (NMC811) and 30% LiMnxFeyPO4 (LMFP) as active material facilitates not only stable cycling of high energy density lithium metal batteries (LMBs) with practical loading (< 30 μm lithium anode, cathode loading > 3.5 mAh/cm2), but also better thermostability compared to the cathode comprising solely NMC811 cathode material. Although the use of high Ni NMC material renders cathode electrode with high energy density, the high reactivity of the Ni rich surface results in severe parasitic electrolyte decomposition reactions and undesired cathode structure reconstruction by accelerating the transition metal dissolution, generating gases and forming O vacancies. Furthermore, those side reactions will also consume extra active Li in the system and shorten the cycle life of LMBs. When the high Ni NMC is partially replaced by LMFP, which possesses the Ni and Co free ultra-robust lattice structure, the composite cathode displays much improved thermostability, significantly elongated cycle life, as well as reduced cost.

In this complementary system, 30% LMFP and 70% high Ni NMC was introduced as an advanced cathode design for LMBs. This system not only shows improved electrochemical performance, but also enhanced thermostability compared to the single active material cathode design. The mechanism behind those improvements was also discussed. NMR results comparing the electrolyte decomposition and consumption in LMBs were studied. Differential scanning calorimetry (DSC) experiment confirms the thermodynamics stability of the blended electrode design. The pristine and aged electrode morphology were investigated by Synchrony X-ray diffraction (XRD), which quantified the lattice parameter change, together with other advanced electronic microscopy techniques.

Keywords: High Ni NMC; LMFP; Li metal batteries, high energy cell, complementary cathode design.

Highly (111)-oriented Nanotwinned Cu and its Applications in Microelectronic Devices

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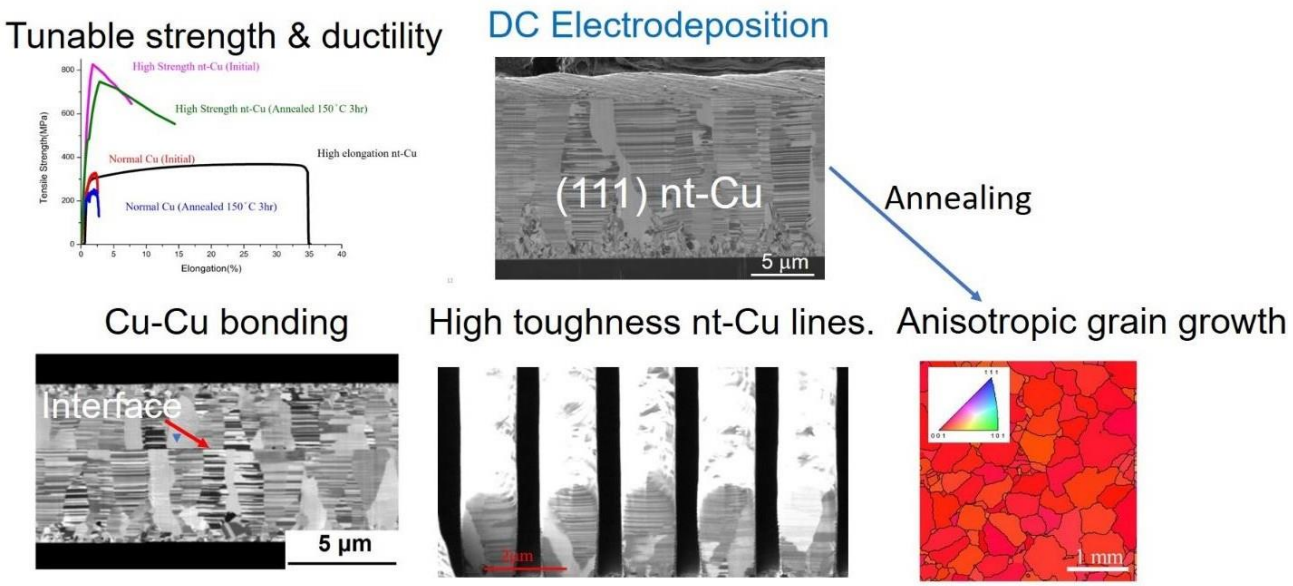
Graphical Abstract



Abstract

Nanotwinned Cu (nt-Cu) has a low resistivity, and it possesses a very high strength and good ductility. We can fabricate highly (111) nt-Cu films by DC electroplating [**1**], which is compatible to the process in microelectronics industry. Columnar (111) Cu grains with densely packed nanotwins can be grown using this approach. Almost very surface grain is (111)-preferred. The regularity of the Cu films is the second best to single crystalline Cu. The nt-Cu film possesses the following properties: high surface diffusivity [**2,3**], low oxidation rates, high electromigration resistance, high thermal stability, high toughness and extremely anisotropic grain growth [**4**]. These properties make it suitable for the interconnects for 3D IC packaging. In this presentation, we will introduce the fabrication and microstructures of the nt-Cu films, unique grain growth behavior, and their applications in microelectronic devices, including Cu-to-Cu direct bonding, high-strength and high-thermal-stability Cu lines for fan-out packaging. For Cu direct bonding, we can accomplish the Cu joints below 200°C in ordinary vacuum and low pressure (~1MPa) by using (111)-oriented nanotwinned Cu, in which almost 100% of the surface area is (111) oriented. We are able to bond two Cu films at 150°C for 1 h.

The bonding time can be reduced to 30 min at 200°C. In addition, two Cu microbumps can be bonded successfully in 10 seconds at 300°C under 31 MPa in N_2 ambient, which is the fastest among the reported literatures. The resistance for a single joint is 4.14 mΩ. The contact resistivity was 3.98×10^{-8} $\Omega \cdot cm^2$. The Cu-Cu bonding may be the core technology in the "fifth generation" of electronic packaging technology, after wire-bonding, TAB, flip chip, and microbump and TSV. For the extremely large grain growth, by annealing the nt-Cu film at 400 to 500 °C up to an hour, we grow a number of extremely large <100> oriented large crystals of Cu of size from 200 to 400 μm. By patterning and annealing the nt-Cu film, we grow an array of <100> oriented single crystals of Cu of size from 25 to 100 μm on Si. These large Cu single crystals may be served a substrate for the growth of 2D materials.

Keywords: Nanotwinned Cu; Cu-to-Cu direct bonding; electrodeposition.

Acknowledgements

This work was financially supported by the "Center for the Semiconductor Technology Research" from The Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education (MOE) in Taiwan. Also supported in part by the Ministry of Science and Technology, Taiwan, under Grant MOST 109-2634-F-009-029. In addition, the authors would like to thank the financial support from TSMC, MediaTek, Lam Research, and Chemleaders Inc.

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Modelling Fatigue of Additively Manufactured Materials

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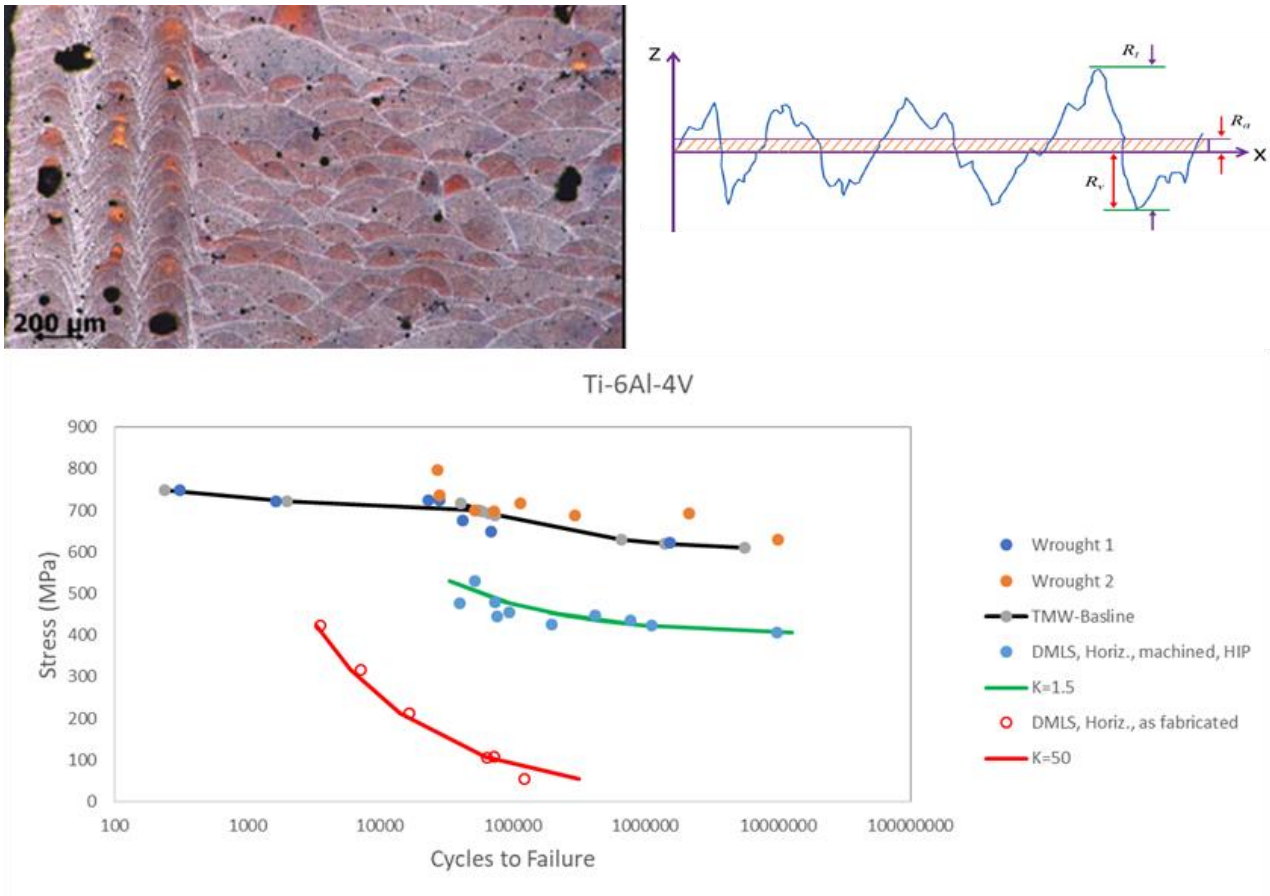
Graphical Abstract



Abstract

Additive manufacturing (AM) has drawn a tremendous interest of engineering application, because it offers almost unlimited possibilities of innovative structural design to save weight and optimize performance [**1**]. However, fatigue properties are one of the limiting factors for structural applications of AM materials. Characterization of fatigue behaviours by conventional means requires extensive testing, which hinders the development of advanced AM materials, as it is impossible to fully explore

and optimize manufacturing parameter-property relationships through testing. The recently modified Tanaka-Mura-Wu (TMW) model has been shown to be capable of predicting the fatigue curves of metallic materials as functions of stress or plastic strain, based on the material's elastic modulus, surface energy and Burgers vector [**2**]. AM materials contain manufacturing defects such as Lack of Fusion (LOF) defects, porosities, and un-melted particles, which may act as stress concentration sites. As-built AM materials also have high surface roughness, which may promote surface crack nucleation. With consideration of these physical attributes of AM materials, the TMW model is extended to describe fatigue life behaviours of AM materials. The model is found in favourable agreement with the available test data on some popular AM alloys produced by selective laser melting (SLM), direct metal laser sintering (DMLS) and power-bed fusion (PBF) methods, as well as their conventional (wrought) forms. Establishing physics-based fatigue life prediction model can be very useful in assessment of fatigue performance and durability of safety critical components, as well as process optimization in manufacturing, saving the testing cost and shortening the design cycle.

Keywords: Fatigue; AM materials; TMW model.

Acknowledgements

The work was conducted as a study assignment in the graduate course MECH 5602 at Carleton University, Ottawa, ON, Canada. The participating students did the data curation under the instructions of the author.

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Advances in Design of New Energy Materials for Sustainable and Clean Energy Supply

Chol-Jun Yu[1,*], Un-Gi Jong[1,2], Song-Hyok Choe[1,2], Kum-Chol Ri[1], Jin-Song Kim[1], Yun-Hyok Kye[1,2], Song-Nam Hong[1], Yong-Guk Choe[1]

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Graphical Abstract

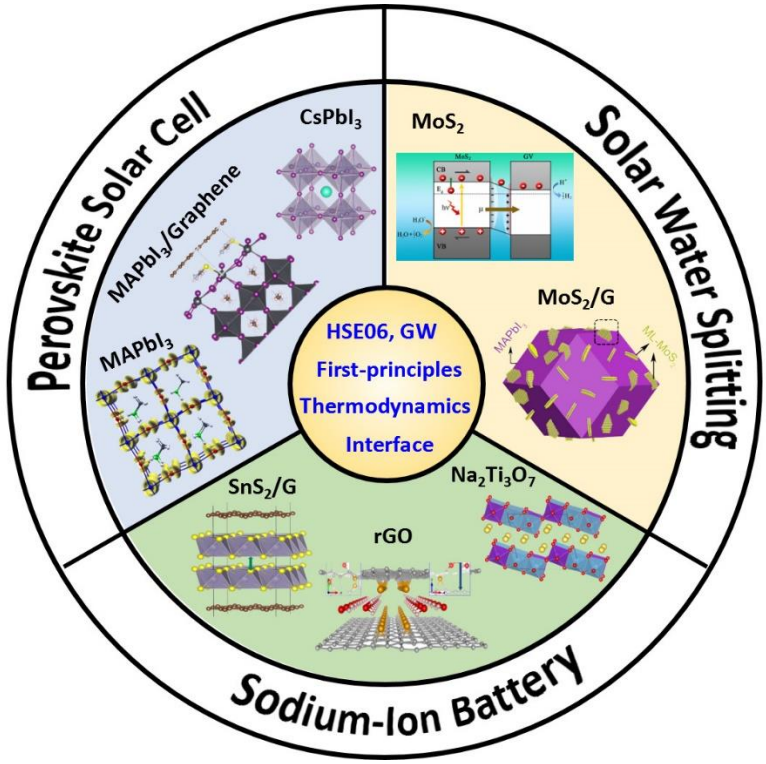

Illustration of various components used in the design of new functional energy materials with first-principles methods for energy applications including perovskite solar cell, sodium-ion battery and solar water splitting.

Abstract

Nowadays, the issue of climate change and global warming is more often highlighted in the mass media as one of the most serious global challenges that human beings face [**1**]. During the past centuries, vast amounts of greenhouse gases including carbon dioxide and methane have been released into air by human activity of extensive burning fossil fuels such as coal, wood, oil and natural gas to run industry, operate buildings and drive transports. Such excessive mining and consumption of fossil

fuels also cause the challenge for sufficient energy supplies. To mitigate the catastrophic effects of global warming and ensure sustainable energy supplies, more and more people and authorities are expressing a growing interest in renewable and clean energy sources, such that the majority of national and global energy policies include the exploitation of clean energy sources, such as solar energy, wind, hydraulic and tidal power. It is our ardent desire to develop innovative new functional energy materials, which make it possible for natural energy sources to become competitive with fossil fuels in the electricity market. In realizing our desire, we are applying the state-of-the-art first-principles methods to afford an insight into material properties and predict the shortest route for finding new functional materials, as atomistic modelling and simulation of materials have become an inevitable and powerful tool in materials development. We are focusing on halide perovskites as an energy harvesting material for a new type of perovskite solar cells (PSCs) [**2,3**], electrode materials for sodium-ion batteries (SIBs) [**4,5**], and photocatalysts for water-splitting hydrogen production. Although PSCs show rapid evolution of power conversion efficiency from 3.8% to over 25.5% during the past decade, the stability remains the critical problem due to the facile decomposition of methylammonium lead iodide perovskite ($MAPbI_3$), which is the key material as a light absorber of PSCs. By applying the first-principles methods combined with thermodynamics for defects, we provide the atomistic mechanism behind the degradation of $MAPbI_3$ under humid condition, presenting a strategy to overcome the negative effect of water on the performance and stability of halide perovskites [**2,3**]. The renewable and clean energy sources are often intermittent and thus require the advanced electrochemical energy storage systems with high efficiency, stability and reliability. With a merit of resource abundance of sodium on the Earth's crust, SIBs are believed to meet the requirements of stationary energy storage and electric vehicles as the most promising candidate of lithium-ion batteries. We design the cathode and anode active materials using the layered metal oxides and sulphides complexed with graphene or graphene oxides to develop commercially viable SIBs. With these efforts, we believe that we contribute to the construction of efficient clean energy economy for sustainable and green world.

Keywords: Energy materials; perovskite solar cell; sodium-ion battery; water-splitting; hydrogen evolution.

Acknowledgements

The work was supported as part of the basic research project "Design of Innovative Functional Materials for Energy and Environmental Application" (no. 2016-20) by the State Commission of Science and Technology, DPR Korea. Computations have been done on the HP Blade System C7000 (HP BL460c) that is owned by Faculty of Materials Science, Kim Il Sung University.

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Functional Characterization of Piezoelectric Materials: Application to Ultrasonic Transducers and Energy Harvesters

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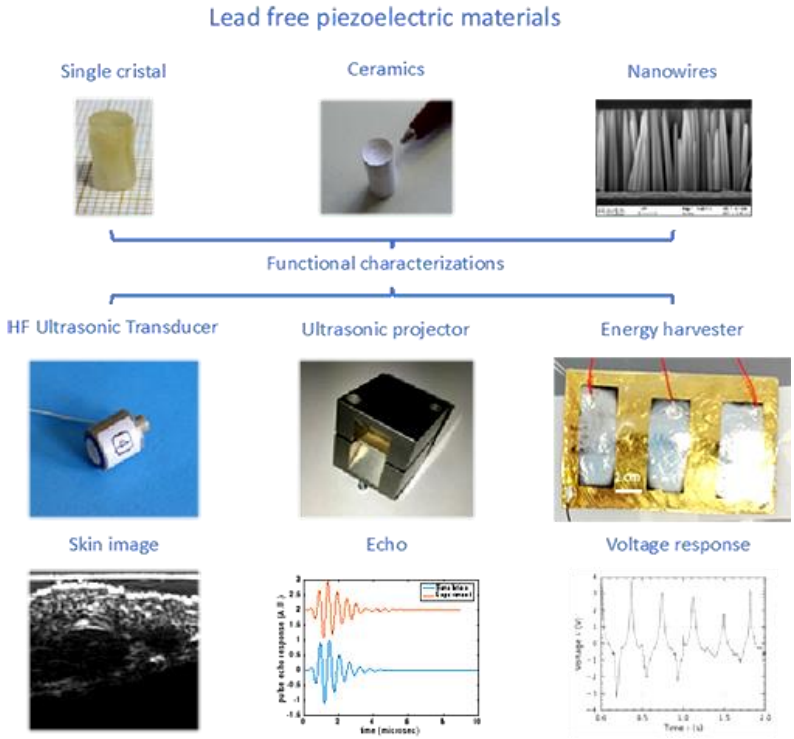
Graphical Abstract



Abstract

Piezoelectric materials, whether in the form of ceramics, composites or single crystals, are nowadays at the heart of a large number of energy conversion devices. They can be used as sensors, actuators or transducers where both direct and inverse effects of piezoelectricity are used. Starting from the materials, their elaboration and functional characterizations, we present several applications of these materials for ultrasonic transduction and energy harvesting. **Lead-free materials for ultrasonic transduction.** For ultrasonic transducer applications, the thickness mode is very often preferred in order to generate longitudinal waves in the propagation medium. The active materials used are generally lead-based ceramic, however due to environmental issues lead-free materials are developed both in the laboratories and by ceramic manufacturers. We report and discuss the manufacture of KNaNbO lead-free single crystals and thick films lead-free ceramics developed in

the laboratory and in an European company. On one side, centimeter size single crystal of (K,Na)(Nb,Ta)O_3 lead free system were successfully grown by floating zone melting in an optical furnace, while dense ceramics of the same compositions, obtained by Spark Plasma Sintering (SPS) were reproducibly synthesized. On the other side, doped ($K_{0.5}Na_{0.5}$)NbO_3 (KNN) based compositions obtained by conventional solid state synthesis was used to fabricate a curved high frequency thick film based transducer. In both cases, their functional properties are determined and compared to lead free commercial compositions. Coupling coefficients of 0.45 and a dielectric constants comprised between 600 and 700 for bulk doped ceramics and a coupling coefficient of 0.34 for thick films are reported for some compositions, which makes these materials suitable for transducer applications. Two examples of lead free ultrasonic based transducer for imaging, operating in the MHz range, are reported: The first is a high frequency transducer[1] for medical imaging and the second is based on a new design called acoustic projector[2]. For both types of transducers, electroacoustic responses are measured and, in the case of the high frequency transducer, an ultrasound image of the skin is made. **Materials for energy harvesting**. Mechanical energy harvesting utilizing piezoelectric materials has been widely studied over the past two decades. Thanks to the direct piezoelectric effect, piezoelectric materials are able to convert unused mechanical energy of our surroundings into electrical energy. Ambient mechanical sources are encountered on vehicles, industrial machines, passage ways, wind turbines, pipelines... or on human beings mainly through walk or hand movements. Among the various technologies of piezoelectric harvesters, we will present piezoelectric semiconducting zinc oxyde nanowires, which are usually integrated into multilayer composite devices called nanogenerators. We will present here a facile, cost-effective and industrially scalable process flow for the fabrication of flexible and stretchable nanogenerators on polydimethylsiloxane (PDMS) substrate. The 8 cm^2 nanogenerator[3] is able to produce a 35 µW peak power under a pressure of 100 kPa. This micro power supply can offer a viable solution to provide the energy required by wireless and mobile electronics in some specific applications, like health monitoring, medical implants, smart clothes or autonomous sensors

Keywords: Piezoelectric materials; characterisation; transducer; energy harvester.

Acknowledgements

The works on ZnO based nanogenerators were supported by the ECSEL JU from the European Union's H2020 research and innovation programme [grant agreement No 692482]; the French National Research Agency [grant agreement ANR-14-CE08-0010-01]; and the Region Centre [grant agreements 2011-00064272 and 2014-00091629].

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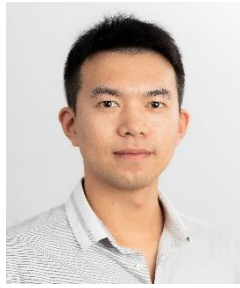
Computational Design for 3D Printing of Continuous Carbon Fibre Composites with Negative Poisson's Ratios



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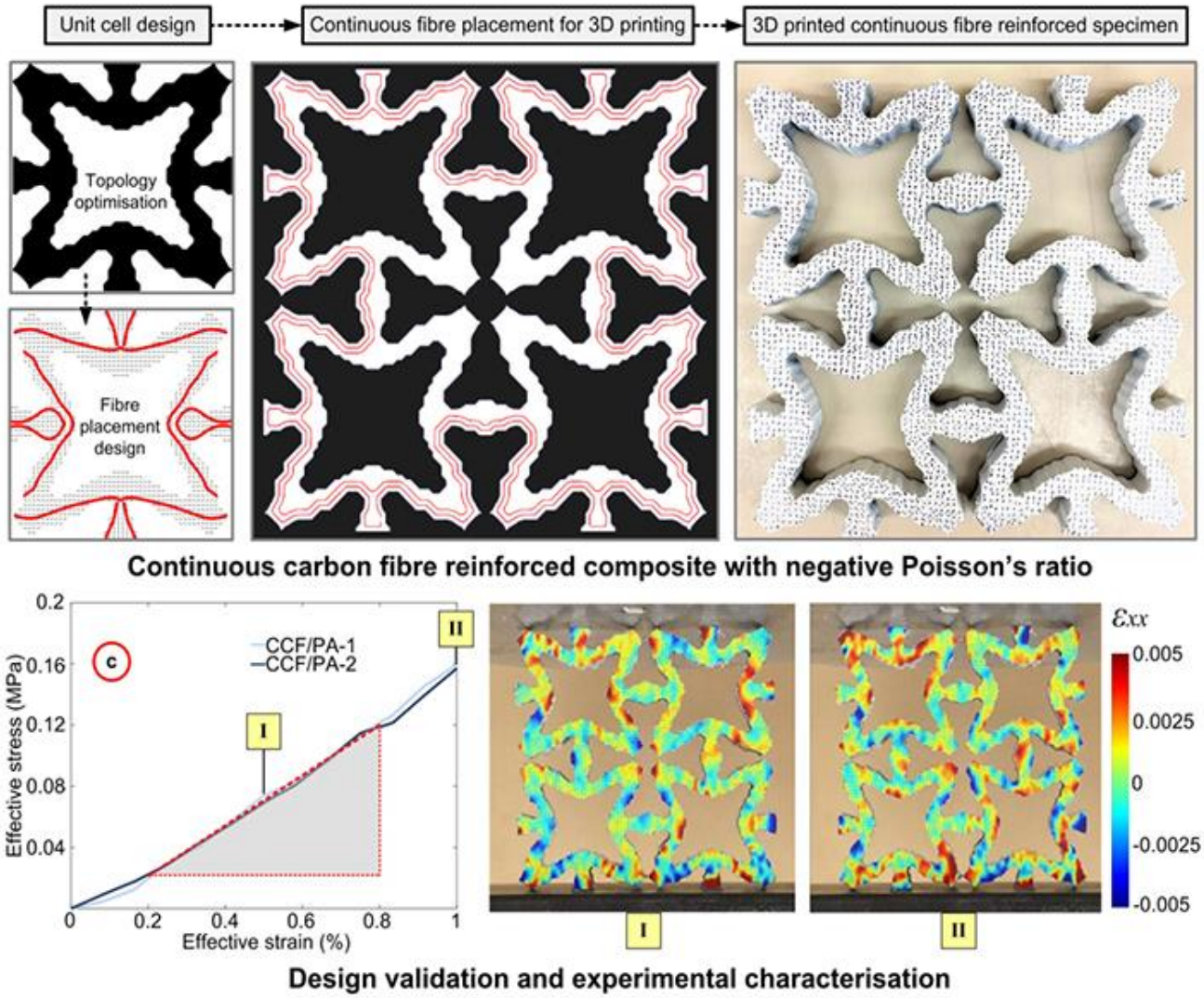
Graphical Abstract



Abstract

Auxetic or negative Poisson's ratio structures are attracting increasing attention and have a wide range of applications, i.e., smart materials, graded materials, shape memory alloys, and biomaterials [1]. Currently, most auxetic structures were designed or manufactured using isotropic materials such as polymers and metals. However, continuous carbon fibre (CCF) reinforced composites have demonstrated significant advantages when compared to isotropic materials [2, 3], but to date few relevant studies are reported.

This research developed an integrated computational design method with 3D printing to endow continuous carbon fibre composites with negative Poisson's ratios. First, CCF composites were designed using a multidisciplinary technique integrating homogenisation-based topology optimisation and fibre placement methodology for guiding the 3D printing set-up with fused filament fabrication. Then, specimens made of pure polyamide (PA), short carbon fibre reinforced polyamide (SCF/PA) and CCF reinforced nylon (CCF/PA) were fabricated and tested for a comparative analysis. Lastly, the effects of carbon fibre reinforcement were investigated, showing that a small addition of CCFs (VCCF = 0.23%) can enhance the negative Poisson's ratio from −0.24 of the PA auxetic specimens to −0.34. However, other greater CCF volume fraction would impair the auxetic behaviour.

Keywords: Additive manufacturing; topology optimisation; continuous carbon fibre; negative Poisson's ratio; polyamide.

Acknowledgements

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Tunable Acoustic Impedance of Helmholtz Resonators for Perfect Sound Absorption via Roughened Embedded Necks

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Abstract

Acoustic impedance regulation of a neck embedded Helmholtz resonator (NEHR) is realized by introducing surface roughness to the neck, so as to convert the initially non-perfect sound absorber to a perfect sound absorber. The proposed roughened-neck embedded Helmholtz resonator (R-NEHR) achieves perfect sound absorption ($\alpha > 0.999$) at 158 Hz across a deep subwavelength thickness of λ/42. Theoretical predictions of the R-NEHR's performance are validated against experimental measurements. Physically, surface roughness triggers periodic concentration effect of fluid vibration in the neck, thereby improving its acoustic mass and acoustic resistance and altering the resonant damping state of the absorber. As a result, the absorption peak position of the R-NEHR shifts by 16.0% to lower frequency, together with a peak value increase of 19.6%. This work provides an approach for perfect sound absorbers design and impedance regulation of acoustic metamaterials.

Keywords: Acoustic impedance regulation, perfect sound absorption, roughness effect, acoustic metamaterial.

High-amplitude Sound Propagation in Acoustic Transmission-Line Metamaterial

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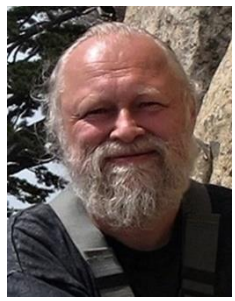
We report experiments on high-amplitude sound wave propagation in an acoustic metamaterial composed of an air-filled waveguide periodically side-loaded by holes. In addition to the linear viscothermal and radiation losses, high amplitude sound waves at the locations of the side holes introduce nonlinear losses. The latter result in an amplitude-dependent reflection, transmission, and absorption, which we experimentally characterize. First, we evidence that nonlinear losses change the nature of the device from a reflective to an absorbing one, showing the possibility to use the system as a nonlinear absorber. Second, we study the second-harmonic generation and its beating phenomenon both experimentally and analytically. We find that when considering the propagation of both the fundamental and the second harmonic, nonlinear losses cannot be neglected. Our results reveal the role of nonlinear losses in the proposed device and also provide a quite accurate analytical model to capture the effect of such losses.

Antimicrobial Polyhydroxybutyrate Submicron Fiber Mat Loaded with Extract of Hypericum Perforatum



Milos Beran[1,*], Aleš Horna[2], Viktor Vorisek[2], Eliska Berkova[1], Radka Korinkova[3], Vojtech Trousil[3], Marketa Hrubanova[4]

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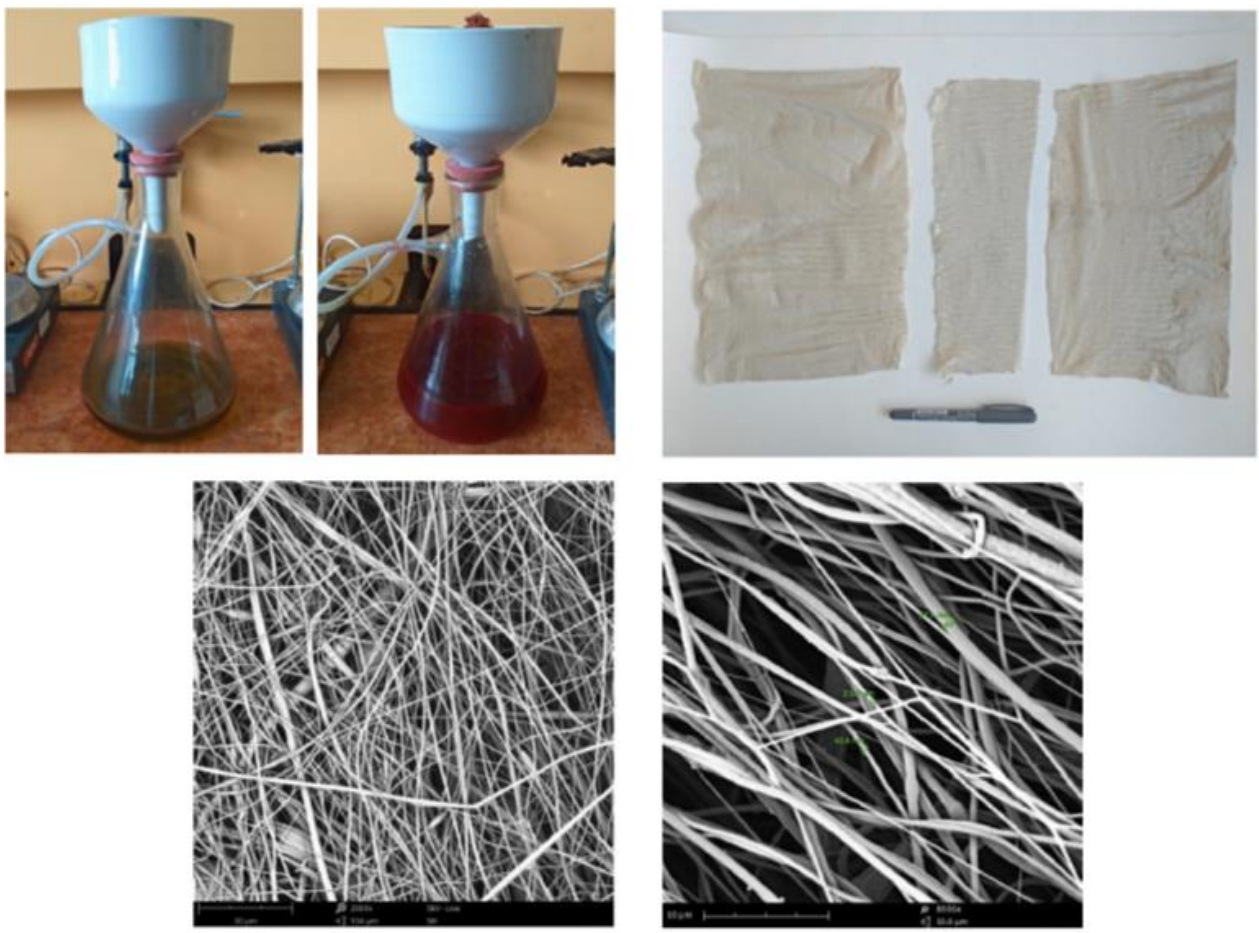
Graphical Abstract



Preparation of PHB submicron fiber mat loaded with extract of Hypericum perforatum.

Abstract

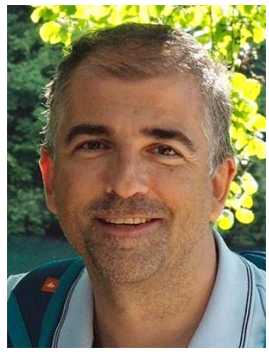
The aim of this work was to prepare a new biodegradable polyhydroxybutyrate submicron fiber mat loaded with *Hypericum perforatum* hypericin rich raw extract by centrifugal spinning technology, an alternative approach to fabricate nanofibers or microfibers from solutions at high speed and low cost. Hypericins in methanol/aceton extract of *H. perforatum* were determined by UHPLC-MS/MS and HPLC/PDA methods. Pure PHB and the *H. perforatum* extract enriched PHB submicron fiber mats were prepared using a pilot plant demonstrator for the centrifugal spinning technology and characterized by SEM. Singlet oxygen production was quantified by the 1,3-diphenylisobenzofuran method in hexan. The results proved a significant production of singlet oxygen by the prepared submicron fiber mat. We have also found a very significant antibacterial activity against *Escherichia coli CCM 5417* bacterial strain by a method in accordance with JIS Z 2801 / ISO 22196 tests. Determination of antiviral activities of the submicron fiber mats with *H. perforatum* extract against enveloped virus is in progress. The *H. perforatum* extract enriched PHB submicron fiber mats showed potential in development of self-cleaning and antimicrobial air filters.

Keywords: Hypericum perforatum; hypericins; nanofiber mats, photocatalytic, antibacterial.

Acknowledgements

This work was supported by the TACR project number TH03020466 and by the Institutional Development Fund of FRIP provided by the Ministry of Agriculture of the Czech Republic.

A New Approach to the Production of A High-Performance Silk Based Bioplastic



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Graphical Abstract

Abstract

Due to the unique combination of properties such as mechanical strength and toughness, biocompatibility, biodegradability, thermal stability, and easy processability [**1,2**], regenerated silk fibroin has been used as a functional biomaterial, adopted when a positive interaction with living tissue is required. While a plethora of micro and nanoscale architectures of silk fibroin have been explored in literature - films, fibers, microparticles, and gels[18], building larger, macroscale objects of fibroin has been challenging, since large dimension solid-fibroin material is required. Solid-fibroin is a bulk non-porous material usually prepared starting from a fibroin solution through a liquid to gel to solid transition by slow evaporation [**3**].

In this work we demonstrate the possibility to produce, in fast fashion, monoliths of solid-fibroin starting from a dry fibroin powder, in presence of water and under fast compression.

A full factorial design of experiment was used to understand the sintering process. We studied the material in the crucial phases of the procedure by DSC, FTIR and SEM, proving that the thermal-reflow can occur at low temperature if driven by a high-pressure process and in presence of water on a low crystallinity dry fibroin. Mechanical characterization and preliminary in vitro tests were conducted: human adipose-derived mesenchymal stem cells were cultured on both LTS fibroin samples and PCL samples (used as control material), to evaluate cell response. After each time point, cell adhesion, morphology and distribution were analyzed by confocal microscopy.

The analysis conducted with FTIR on the main stages of the process revealed that an excessive transition to β–parallel structure, due to a prolongated water treatment, doesn't allow the transition to the solid state. The transition occurs if the secondary structures are not enough stable to be able to re-organize themselves in more stable phases during the compression phase. Glass transition temperature was detected by DSC: interestingly, the rapid addition of water in the material through moisture absorption didn't change the Tg respect the lyophilized silk fibroin. SEM analysis at different time points in the compression phase proved the presence of a viscous flow, so we could deduce a decrease in the Tg under 40°C when moisturized lyophilized fibroin undergoes to compression. Preliminary biological results indicate a promising response of LTS fibroin samples in promoting cell adhesion and proliferation.

In this work we report a method to obtain a compact material form fibroin powder in a single compression mold step. We were able to optimize a fast, low temperature method to obtain large monoliths of solid – fibroin, reporting, for the first time a thermal – reflow at 40°C for lyophilized silk fibroin [**4**]. With this technique large objects can be produced in few minutes with a high reproducibility. The mild forming conditions allow the possibility to incorporate temperature degradable bioactive additives.

Keywords: Silk Fibroin; polymer sintering; biodegradable biopolymer, thermoplastic.

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Low-requirement Nanomaterials for Electrochemical Sensors

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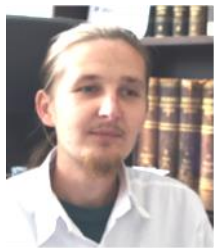

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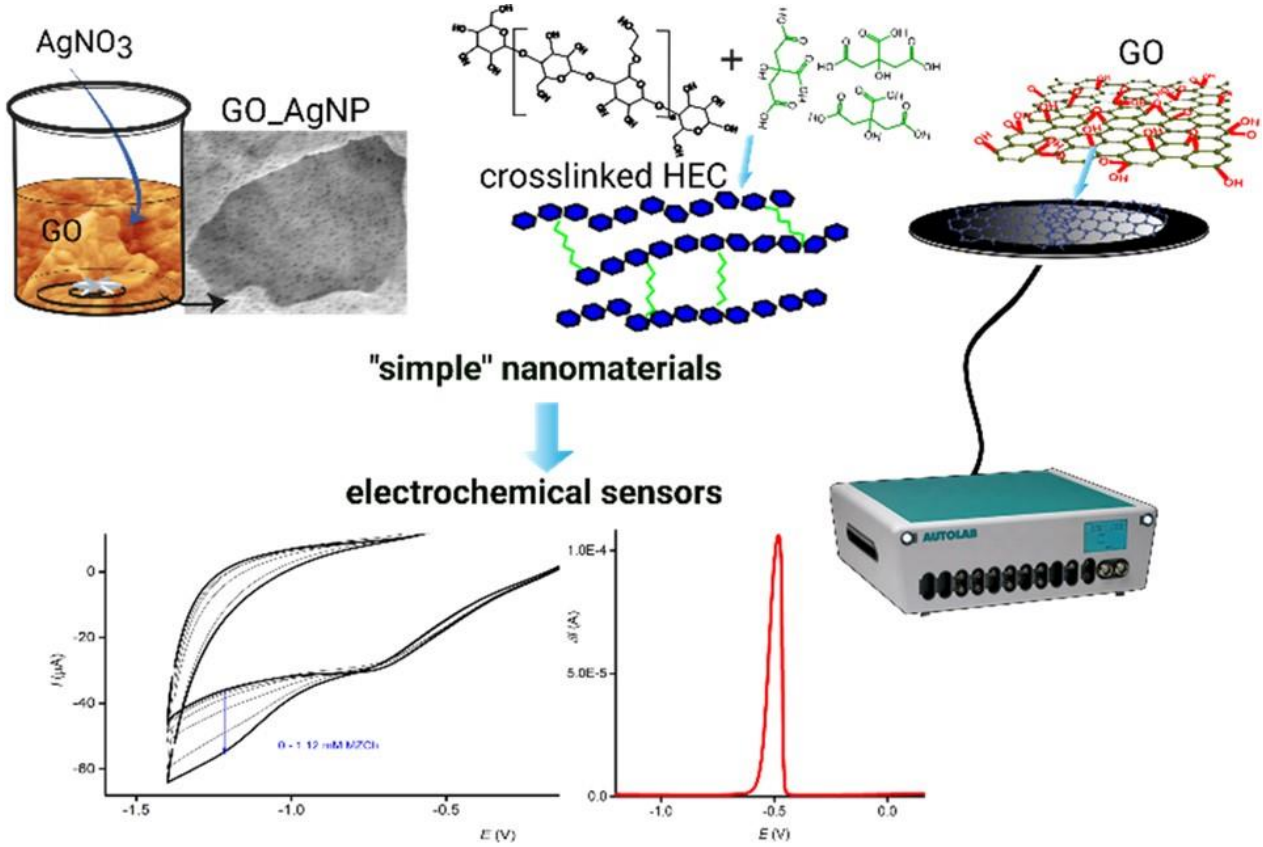
Graphical Abstract



Abstract

Graphene oxide (GO) has shown amazing applicability in electrochemical (bio)sensor. GO´s oxygen functionalities allow for attachment of biorecognition elements [**1**] and electrostatic interaction with biomolecules [**2**] or metal ions while the hydrophobic moieties allow for binding via hydrophobic π-π interactions [**3**]. Amount of these functionalities can be adjusted for example by electrochemical reduction, furthermore, GO can be considered as a mild reducing agent. All these features have been employed for development of sophisticated and multicomponent nanohybrid materials used for

modification of electrodes. On the other side, the preparation methods often used harmful chemical agents and/or multistep laborious fabrication protocol.

This work aims to reduction, simplification of GO application in electrochemical environmental sensors. First, silver nanoparticles (AgNPs) were synthesized in situ on GO surface without the need of any additional reducing agent. The preparation relied on simple incubation of aqueous GO dispersion with $AgNO_3$ solution. The prepared GO-AgNP nanoparticles were deposited on electrodes and employed for electrochemical determination of chlorides [**4**]. More importantly, GO-AgNP on the electrode surface (after the electrochemical reduction) could facilitate electrochemical reductive dechlorination of chloroacetanilide herbicide metazachlor and made its voltammetric determination possible [**5**].

In second experiment series, GO was simply deposited on screen printed electrodes (SPE) and, after short thermal treatment, the prepared GO/SPE were placed in flow cell and used for determination of heavy metals. The thermal treatment caused mild reduction of GO which allowed the sensor to operate in the negative potential windows needed for heavy metal determination.

The third way to simplify the sensors preparation was coating electrodes with hydroxyethyl cellulose (HEC). Since it is water-soluble, crosslinking had to be performed to obtain stable HEC film. Many studies investigated modification of cellulose derivatives by citric acid to achieve heavy metal sorbent, but we have prepared citric-acid crosslinked HEC film directly on electrode surface by very simple drop-casting of polymer + citric acid solution on electrode surface and consequent heating for 10-30 min in laboratory oven. The crosslinked HEC not only enhanced heavy metal sorption on electrode surface, it also turned out to be a sustainable binder for GO and GO-AgNP.

It can be concluded that there are ways to minimize the requirements (time, harmful chemicals…) for development of nanomaterials-based electrochemical sensors towards environmental pollutants. And it is worthy to follow them.

Keywords: Graphene oxide; hydroxyethyl cellulose; silver nanoparticles; electrochemical sensors

Acknowledgements

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Use of Conducting Polymer Composites in Biomedical Protocols

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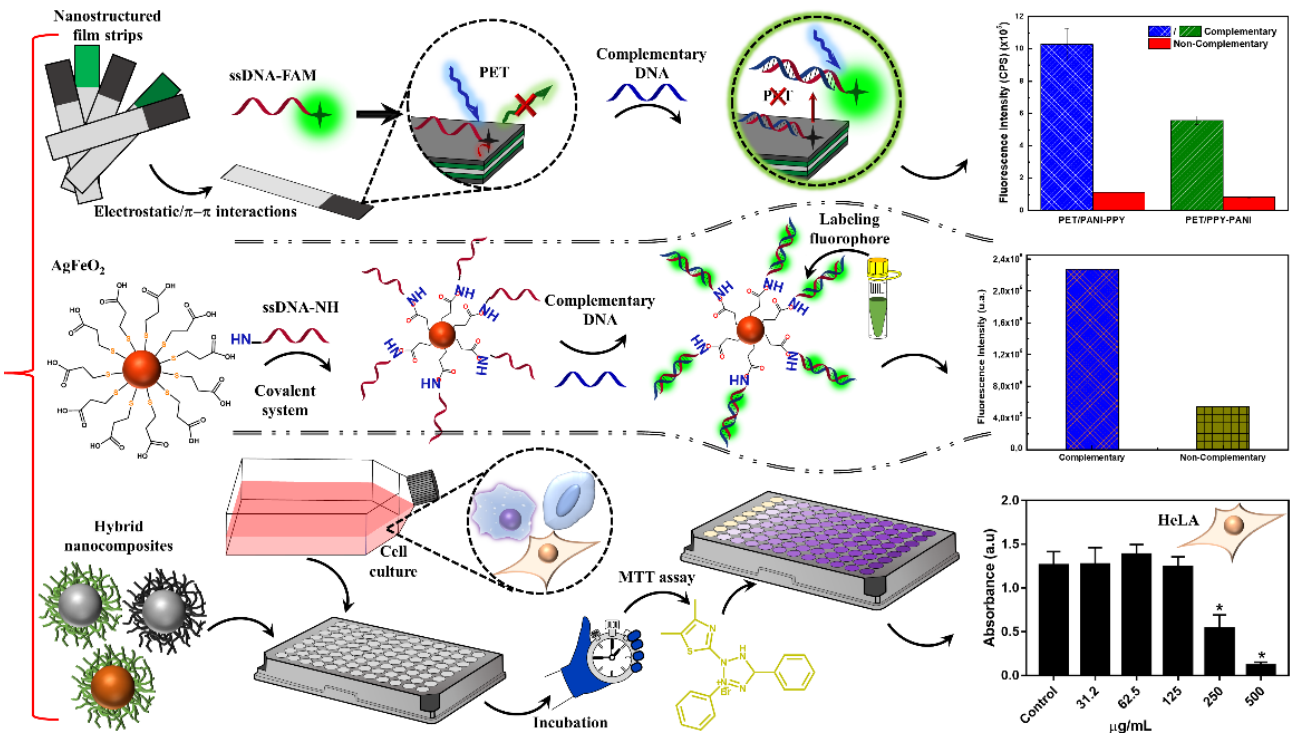
Graphical Abstract



Abstract

We present recent biomedical applications of nanostructured conducting polymer films and composites. First, we describe the use of magnetic $AgFeO_2$ particles in the covalent immobilization of single-stranded DNA chain (ssDNA) probes. The quenching of the fluorescence of a FAM-dye marked ssDNA, which follows hybridization with a complementary sequence, allows the identification of

pathogens and rapid diagnostic. Preliminary results using FAM-ssDNA of the *Salmonella s.p* pathogen immobilized on $AgFeO_2$ nanoparticles as model system show that this is an efficient procedure for covalent immobilization. The detection method proposed appears as a promising bifunctional fluorescent and magnetic platform for the development of fast, inexpensive, and efficient molecular diagnostic tests. We have also immobilized fluorophore-marked ssDNA probes on nanostructured polypyrrole (PPY) and polyaniline (PANI) films deposited on polyethylene terephthalate (PET) substrates. This allowed us to establish efficient molecular diagnostic protocols based on the selective detection of nucleic acids that exploit the quenching that may occur when fluorophores attach to films of conducting polymers. When a complementary sequence interacts with the immobilized probe, the newly formed ds-DNA chains detach from the polymeric film, causing the restoration of the fluorescence. This sensing system exhibits a low background signal and represents a simple, fast, and highly sensitive scheme for the recognition of target DNA fragments, which exhibits a limit of detection in the nM [pM] range for *Leishmania infantum* parasite [Zika virus]. Finally, we report the characterization of three different core-shell composites obtained by enveloping metal nanoparticles with chains of a conducting polymer. After preparing fluorescent Ag/PPY, Cu/PANI, and Ag/PANI nanocomposites through one-step *in situ* chemical syntheses at room temperature. We performed cytotoxicity assays of these hybrid composites, using three mammalian cell lines (macrophages, VERO cells, and fibroblasts). The Ag/PPY composite exhibited a viable cytotoxic concentration (CC_{50}) and selective antitumor activity against cancerous HeLa cells. For combining fluorescent properties and antitumor activity, these hybrid nanocomposites can find applications as theranostic agents. These results indicate that one can successfully develop efficient biomedical protocols based on the use of nanostructured conducting polymer films and (metal oxide)/(conducting polymer) composites as biological sensors and molecular diagnostic agents.

Keywords: Biomaterials; intrinsically conductive polymers; metal nanoparticles; molecular diagnosis; cytotoxicity.

Acknowledgements

CNPq, FACEPE, FUNASA

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PFPE Peroxide Decomposition as Universal Approach for PFPE Chain Grafting to Carbon Nanostructured Materials

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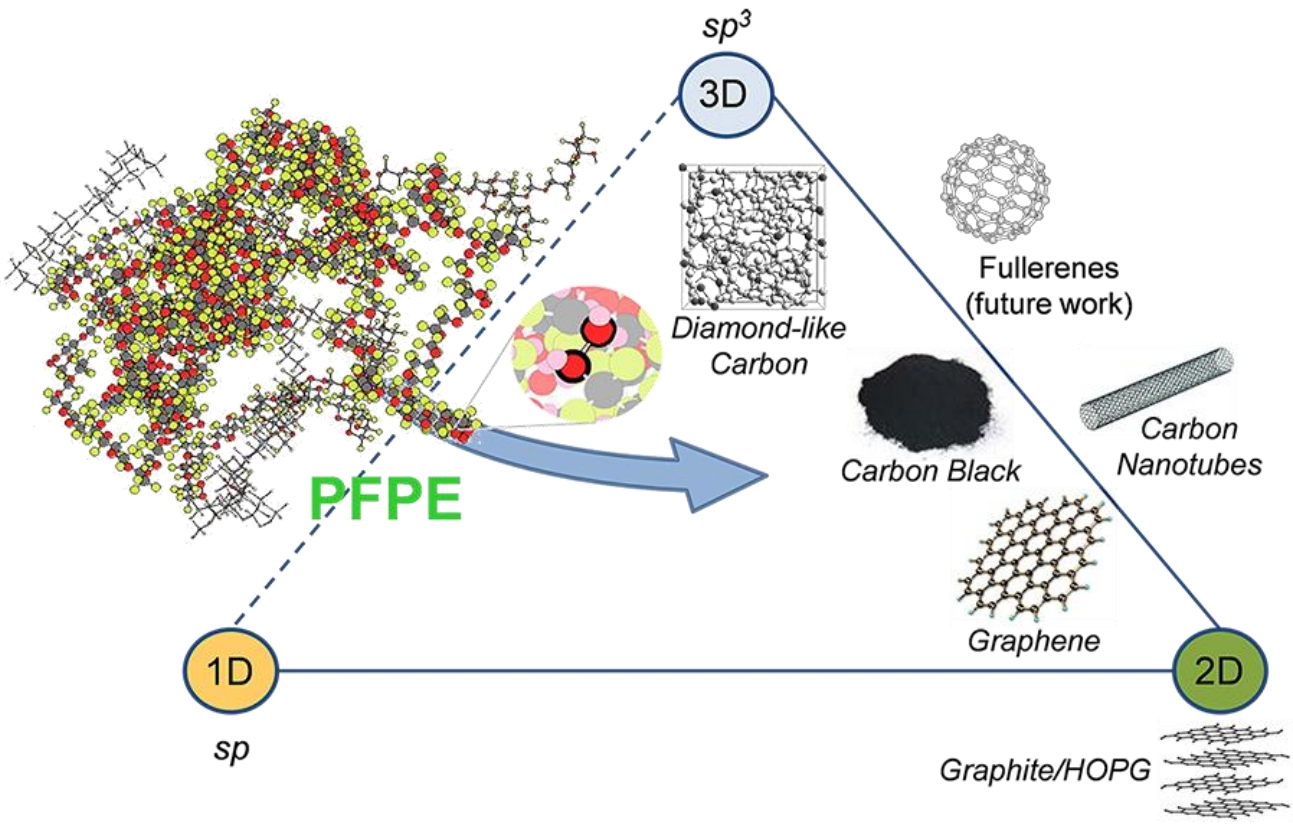
Graphical Abstract



Abstract

Carbon is fourth most abundant chemical element in universe and, thanks to its peculiar electronic structure, it is the main building block of organic chemistry giving rise to countless different molecules. Moreover, carbon atoms can arrange to build nanostructures of different dimensionality, shape and properties that are nowadays extensively exploited in many technologies and applications. Even more interestingly, carbon nanomaterials can be efficiently modified with functional molecules, altering their structural and electronic structure at various extension degrees, broadening the range of properties and widening fields of application. In this work, our experience on chemical grafting of perfluoropolyether (PFPE) chains to carbon nanostructures is reviewed and purposed as suitable and universal approach for PFPE covalent functionalization to the whole carbon nanostructure family. At first, carbon black (CB) functionalization was extensively investigated and a reaction mechanism, based on reactive PFPE radicals generated by thermal decomposition of peroxide moieties, was proposed [**1**-**3**]. A similar approach was also applied for PFPE grafting to carbon nanotube family, namely single-wall and multi-wall carbon nanotubes (SW-CNTs, MW-CNTs) [**4**]. The PFPE-modified SW/MW-CNTs were characterized by XPS, TGA, XRD, SEM and measurements of contact angle, surface area as well as resistivity at different applied pressures, resulting in tunable conductivity and hydrophobicity according to PFPE peroxide precursor concentration [**5**]. More recently, PFPE functionalization process was successfully employed for the treatment of the whole "graphene family". Single-layer graphene (SLG) and few-layer graphene (FLG), grown by CVD on copper and nickel substrate respectively, were used for this purpose as well as highly oriented pyrolytic graphite (HOPG), that can be considered as an infinite stacking of graphene planes. The perfluorinated layer was found to give hydrophobic properties to graphene without significantly altering its lattice structure, thus potentially keeping electrical properties intact, as confirmed by Raman spectroscopy, grazing angle FT-IR, XPS and contact angle measurement.

Keywords: Carbon allotropes; fluorinated materials; functionalization; surface chemistry.

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Vapor Deposition to Construct Particles and Scaffolding Materials for Regenerative Medicine

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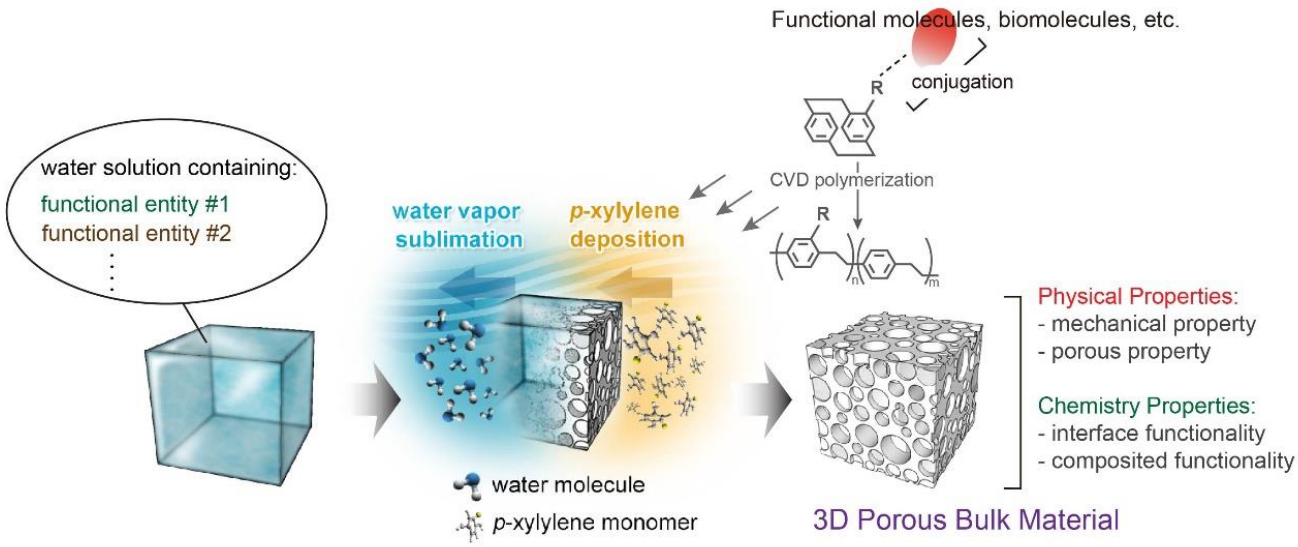
Graphical Abstract



Abstract

Functionalized poly(p-xylylenes) can be deposited via chemical vapor deposition (CVD) polymerization to generate ultra-thin films as conformal coatings and, due to the pre-defined chemical functionalities, provide a flexible solution to surface engineering challenges as they decouple surface design from bulk properties. Hence, the technology comprises essentially a one-step coating procedure to generate functionalized surfaces without requiring any kind of post-treatment once the films are deposited. Recently, three-dimensional porous structures are constructed via vapor deposition onto a sublimating solid template. Construction upon deposition of vapor-phase material occurs at a dynamic vapor–solid interface and is directed by the solid surface vanishing by sublimation. A proof-of-concept demonstration showed vapor depositions of poly-para-xylylenes on sublimating templates, including ice and mixtures with ethanol and hexane. The material construction macroscopically produces a replica architecture of the parent template. Characteristics of the pore structures are formed during the construction process as a result of the gas vapor and the space that is vacated by sublimation, thus enabling control of the porosity through regulation of the sublimation speed and/or the thermodynamic

properties of the templates. The technology introduced herein provides a novel approach for 3D porous material manufacturing and overturns the notion that vapor deposition necessarily forms dense thin films on substrates. Applications of using the vapor sublimation and deposition process were demonstrated for the productions of hierarchical micro- and nano-particles and shaped scaffolding materials with customizable interface and bulk properties, and potentials of applying these materials for regenerative medicine were also highlighted.

Keywords: Biomaterials; vapor deposition polymerization; biomolecular engineering; porous materials.

Acknowledgements

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Transparent Flower Petals and their Biomimetic Polymer Films for Optic Applications

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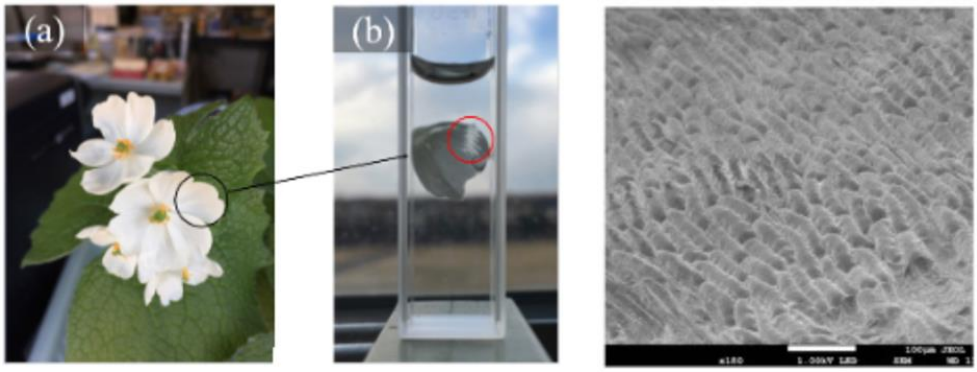
Graphical Abstract



Abstract

The skeleton flower *(Diphylleia grayi*), is a native flower to higher altitudes in Hokkaido. It has unimpressive six small white petals, that show a very unusual change in appearance: they turn translucent when wet. Here we report on the mechanism by observing the cross section and surface morphology of the petals in the scanning electron microscope (SEM) in both the dry and wet stages by the nanosuit method. The surface is covered with tube-like structures of a length of 100-200 μm and a width of 10-20 μm. By using a coating-on-water technique, we produced air-pocket containing thin films of poly(vinylidene fluoride) (PVDF) copolymers that also show a rapid change from turbid to transparent when immersed in water. Thus, this peculiar phenomenon of flower petals can be mimicked artificially and may give rise to applications in which a reliable, fast, and reversible change of transparency is required.

Keywords: Petals; porous membrane; transparency change; biomimetics.

Acknowledgements

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Silicon based Devices for in-vivo Applications

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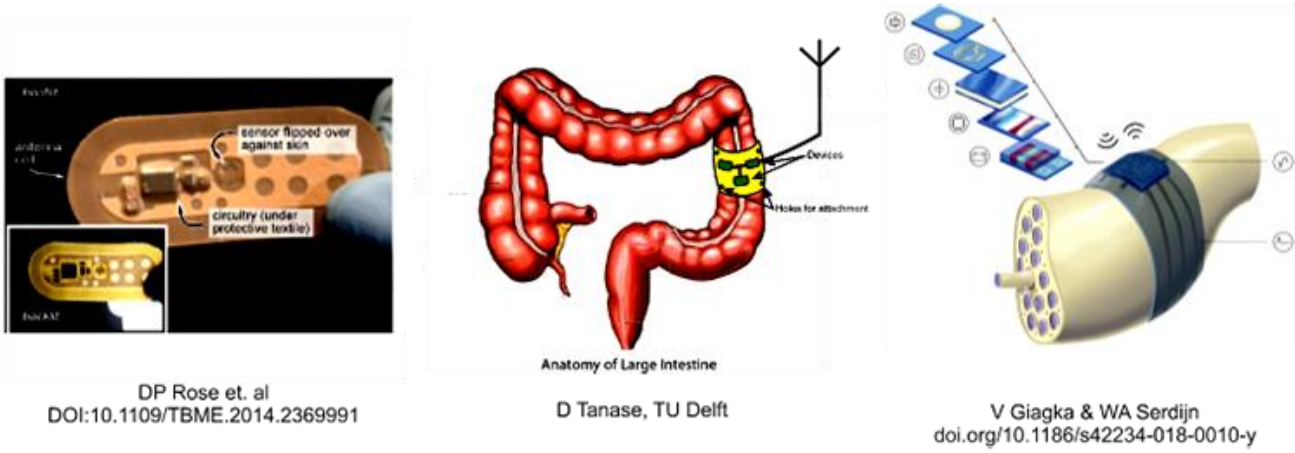
Graphical Abstract

Surface devices | Short term implant | Long term implant



DP Rose et. al
DOI:10.1109/TBME.2014.2369991

D Tanase, TU Delft

V Giagka & WA Serdijn
doi.org/10.1186/s42234-018-0010-y

Abstract

In-vivo sensors yield valuable information by measuring directly on the living tissue of a patient. These devices can be surface or implant devices. Electrical activity in the body, from organs or muscles can be measured using surface electrodes. Other surface devices can measure glucose, sweat, blood pressure, etc. [**1,2**]. These are often flexible devices in the form of a plaster, or some are fixed to the underside of a watch. For short term internal devices, catheters are used. These include cardiac catheter (in blood vessels) and bladder catheters. Due to the size and shape of the catheters, silicon devices provided an excellent solution for measurement. Since many cardiac catheters are disposables, the high volume led to lower prices of the silicon sensors. This was one of the first devices to take advantage of mass production in silicon. Many catheters use a single sensor, but silicon offers the opportunity to have multi sensors in a single catheter. Devices for longer term implantation presented additional challenges due to the harshness of the environment and the regulations for biocompatibility and safety. Some devices may be used for a short-to-medium period to monitor after an operation or injury. One example, is a sensor for measuring tissue viability after an operation [**3**]. Since this is required for less than 30 days, the FDA regulations are easier than long-term/permanent implants. Increasingly sensing devices are being applied to longer term implants for monitoring a range of parameters for chronic conditions, or for stimulation. Long-term stimulations include cochlear implants and nerve stimulators [**4,5**]. Silicon itself is not a biocompatible material and in silicon

processing a number of materials may be used, which are also unsuitable. However, coating layers may be used to protect the body from the silicon and also protect the silicon from the harsh in-vivo environment. This paper will examine the three main areas of application for in-vivo devices: surface devices, short-term and long-term implants. The issues of biocompatibility and safety will be discussed, as well as the different medical requirements.

Keywords: *In-vivo* sensor, implantable microsystems, sensor patches, medical devices.

Acknowledgements

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Innovative Usage and Application-Oriented Simulation of Veneer Based Hybrid Materials in Vehicle Structures

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Graphical Abstract

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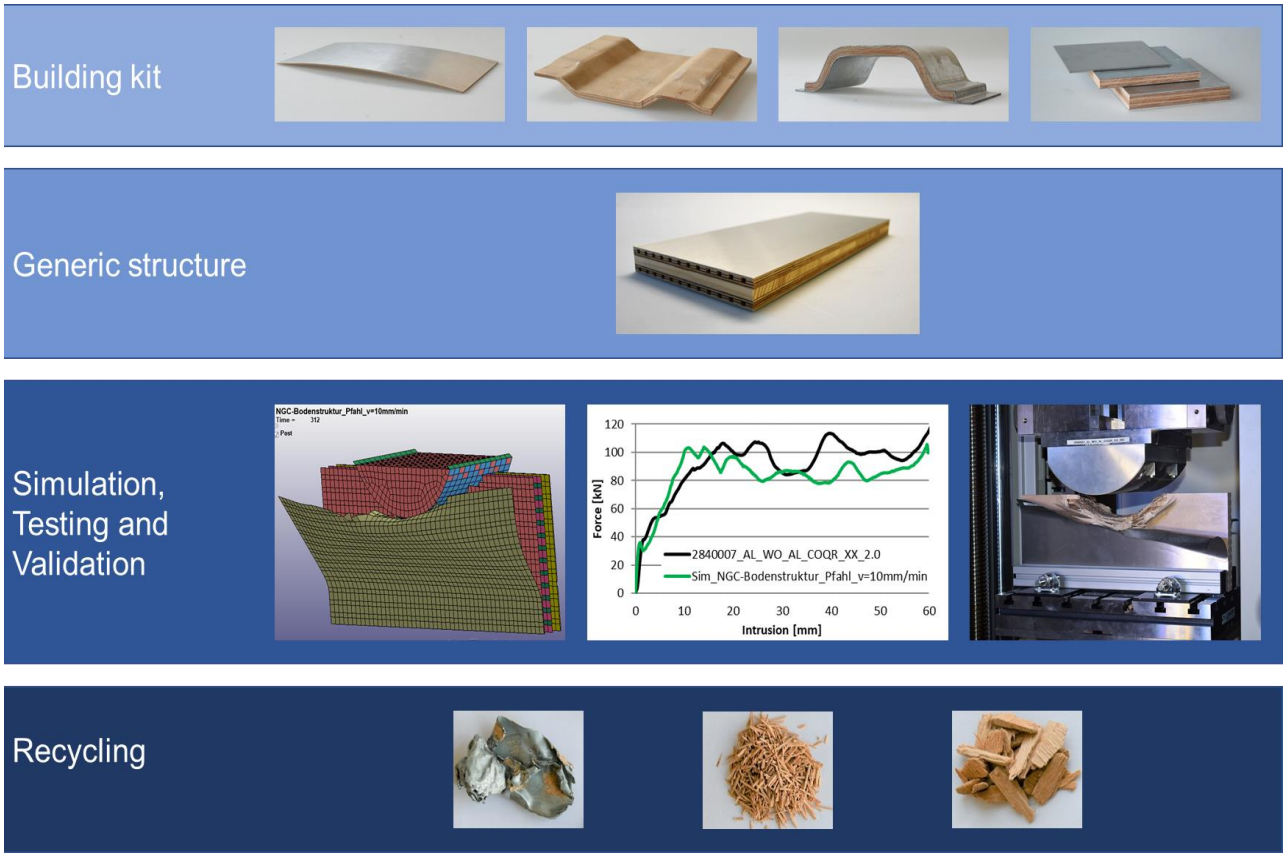

Abstract

Light-weighting in the rail and automotive industry is a key factor to meet the environmental policies combined with the increased public interest in green technologies. Multi-materials and hybrid-materials are effective approaches for the development of light-weight structures. The reduction of the

cradle-to-grave carbon footprint of those utilized materials is gaining importance given their global environmental impact. One promising approach for structural components is the utilization of biomaterials such as veneer-based hybrid materials. Wood is a natural carbon storage with high potential due to its specific properties that are comparable to conventional lightweight materials like aluminium and magnesium. Thus, wood-based components have the potential to be used in some structural and semi-structural components of a vehicle. Further advantages of wood are its low price, thermal and acoustic insulation. When required, the hybridization of veneer-based materials with traditional materials, such as metal sheets, can further increase its structural performance.

In cooperation with partners from research institutes and companies during the project "For(s)tschritt", the Institute of Vehicle Concepts of the German Aerospace Centre has developed a building kit to build veneer-based structures for rail and automotive vehicles. Through the hybridization of wood with aluminium and steel, it was possible to not only develop light but also sustainable solutions that can be recycled at the end of life. While it is technologically possible to implement such solutions, a key challenge for the implementation is the application-oriented simulation of those non-hybridized and hybridized wooden structures. Hence, a suitable simulation method and material model had to be developed and validated. The fully qualified simulation approach and material model contributes to the structural application of the proposed composites in modern vehicle structures.

After the project ended, further generic components were derived based on the building kit. In order to evaluate the proposed solutions some generic components were manufactured and tested to determine their mechanical performance and compared to the simulation results.

The talk gives an overview over different design and simulation approaches chosen and illustrates the high potential of veneer-based materials for vehicle body applications.

Keywords: Crash, simulation, veneer, structural.

Acknowledgements

The authors acknowledge the financial support by the German Federal Ministry for Economic Affairs and Energy (BMWi) through the TÜV Rheinland. We thank our colleagues from the project "For(s)tschritt" who provided insight and expertise that greatly assisted the research.

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Synthesis and Optical Properties of Two-Dimensional Materials And Heterostructures

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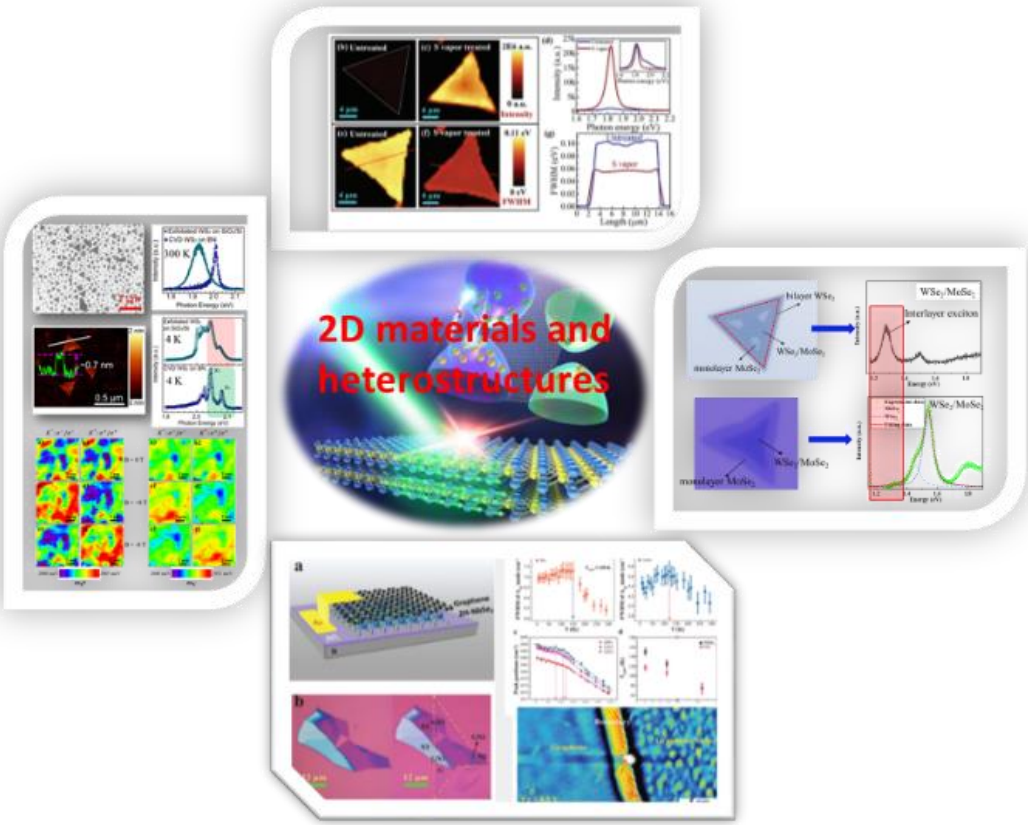
Graphical Abstract



Abstract

Two-dimensional (2D) materials and their van der Waals heterostructures have aroused great attentions due to their rich physics and novel properties as well as great potential applications in nanoelectronics and optoelectronics. In this talk, I will present our recent works on synthesis and optical properties of two-dimensional materials and their heterostructures. Remarkable quality

improvement of as-grown monolayer MS_2 (M=Mo, W) is realized by sulfur vapor pretreatment of SiO_2/Si substrate or epitaxial growth on hexagonal boron nitride (hBN) substrate. It is found that monolayer MoS_2 grown on sulfur vapor pretreated SiO_2/Si substrate has much lower density of sulfur vacancies. About 20 times enhancement in photoluminescence (PL) intensity is found in monolayer MoS_2 grown on sulfur vapor pretreated SiO_2/Si substrates than that on untreated substrates, as well as better electrical performance. The intrinsic light emission features and the valley Zeeman splitting of those high-quality monolayer MS_2 (M=Mo, W) directly grown on hBN substrate have been investigated by PL spectroscopy. The exciton and trion emissions of the as-grown monolayer WS_2 on hBN are well separated and their linewidths are only ~7 meV and ~10 meV, respectively. As well, in as-grown monolayer MoS_2 on hBN, a dramatically sharp peak appears at 1.96 eV with a linewidth of ~5.6 meV, which is much narrower than that of the exfoliated sample on SiO_2/Si. The intrinsic g-factors of these two promising 2D semiconductors are determined by the magnetic-field-dependent PL mapping. The van der Waals heterostructure of WSe_2/$MoSe_2$ with different interlayer coupling strength are tuned by the process of chemical vapor deposition. In addition, the anomalous charge density wave (CDW) states of 2H-$NbSe_2$ layers in graphene/$NbSe_2$ heterostructures prepared by dry transfer method are revealed by using in situ low temperature Raman spectroscopy and scanning tunneling (STM) microscopy. The evolution of Raman spectra demonstrates that the CDW phase transition temperatures are dramatically decreased when covering a single layer graphene onto $NbSe_2$ layers. The low temperature STM images show an exotic short-range ordered CDW patches from graphene/$NbSe_2$ heterostructure. The results presented here help in developing a better understanding of the physical and electronic properties of those 2D materials and their heterostructures.

Keywords: Two-dimensional semiconductors; transition metal dichalcogenides; heterostructures; optical properties; synthesis.

Acknowledgements

The work is supported by the National Key R&D Program of China (Grant No. 2018YFA0703700), the National Natural Science Foundation of China (Grant No. 61774040), the Shanghai Municipal Science and Technology Commission (Grant No. 18JC1410300), and the Shanghai Municipal Natural Science Foundation (Grant No. 16ZR1402500, 20ZR1403200).

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Microwave Chemistry: Rapid and Sustainable Routes for the Preparation of Energy Materials

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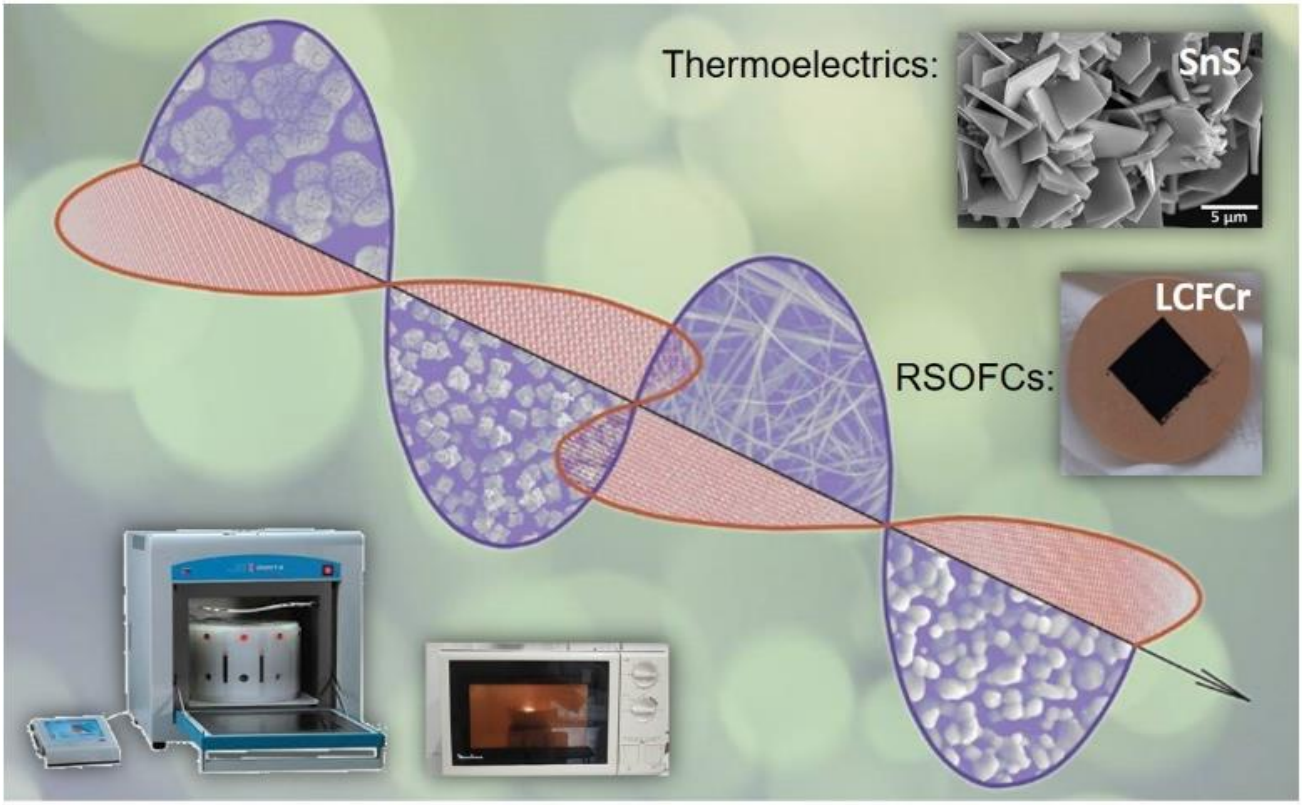
Graphical Abstract



Abstract

The use of microwaves to produce functional materials is an attractive option gaining interest because of their potential benefits such as energy saving, short processing times, increased product yields, economy and environment issues, etc. In a microwave process, an inverse heating profile is produced. The energy is directly transferred to the material through the interaction of the matter at the molecular level with the electromagnetic wave [**1,2**].

In this communication, we will show that a wide range of materials for energy applications can be synthesized by using microwave irradiation:

1) Materials for thermoelectric applications (SnS, SnSe) [**3**].
2) Materials for reversible solid oxide fuel cells (electrodes: $La_{0.3}Ca_{0.7}Fe_{0.7}Cr_{0.3}O_{3-d}$; electrolyte: $Ce_{1-x}RE_xO_{2-d}$).

Furthermore, synthetic aspects, structural characterization and physical properties of the different phases will be discussed as well.

Keywords: Microwave synthesis; energy; functional materials; RSOFCs; thermoelectrics.

Acknowledgements

This work has been supported by the Madrid Government (Comunidad de Madrid- Spain) under the Multiannual Agreement with Complutense University in the line Program to Stimulate Research for Young Doctors in the context of the V PRICIT (Regional Programme of Research and Technological Innovation): Project PR65/19-22459.

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Electrospun Nanofiber Fabric: An Efficient Moist-Electric Generator

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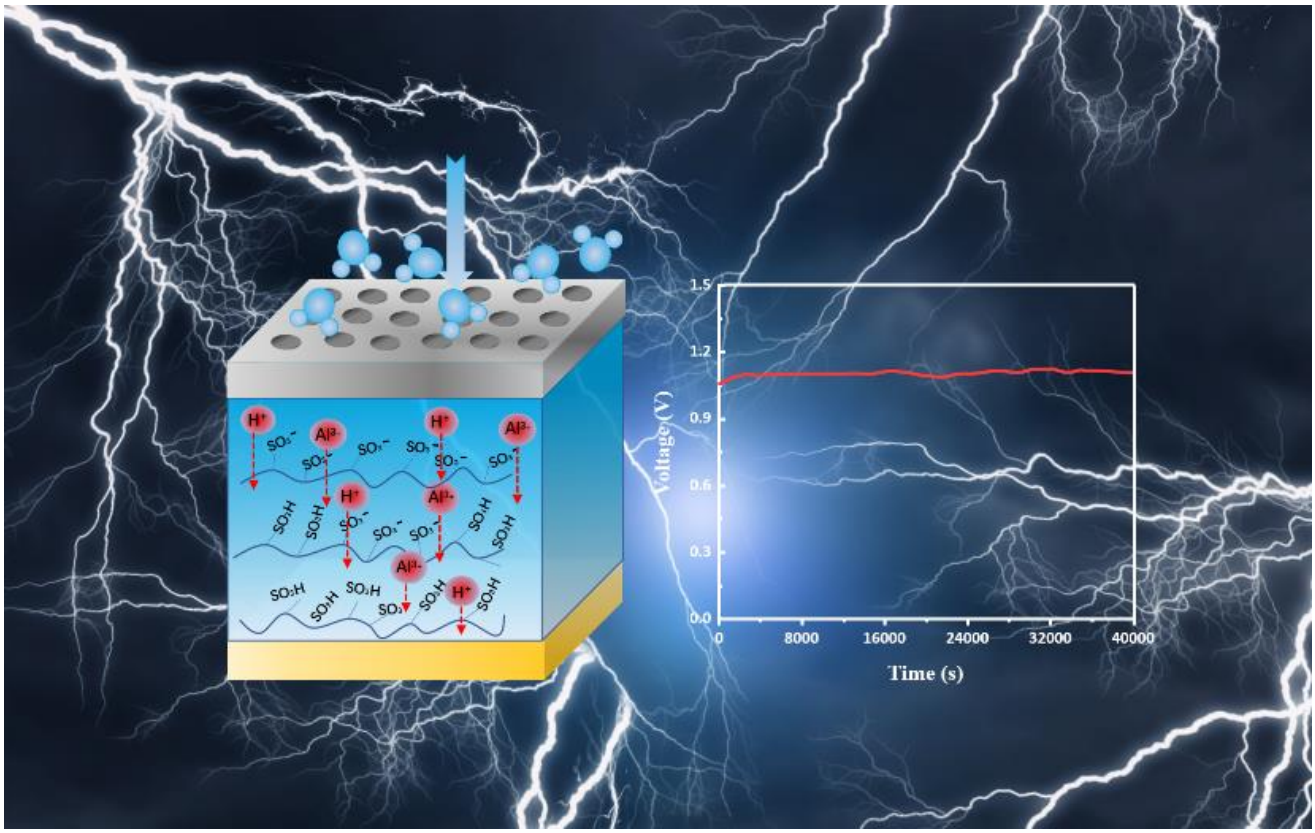
Graphical Abstract

An ion-gradient-enhanced moist-electric generator consisting of electrospun nanofiber fabric and porous active electrode was demonstrated to produce a sustained voltage output of 1.1 V for 40000 s without any weaken signs.



Abstract

Moisture-enabled electric generation as an emerging new energy-harvesting technology is one of the most fascinating and promising candidates for supplying renewable and clean power. However, existing moist-electric generators (MEGs) can only produce intermittent, brief bursts of power with

voltage output less than 1 V, severely restricting their practical applications. Therefore, an urgent requirement is proposed for next-generation MEG to develop devices with high efficiency and continuous energy harvesting property. In this work, an ion-gradient-enhanced MEG consisting of electrospun nanofiber fabric and porous active electrode was demonstrated to provide a perfect solution for solving instantaneous and low electric output at the same time. The assembled MEG can produce a sustained voltage output of 1.1 V for 40000 s without any weaken signs, reaching the highest level among all reported MEGs. This remarkable performance mainly arises from the higher concentration difference increased by the introduced active electrode which enhances the ions diffusion through the porous nanofiber fabric. Moreover, the co-existing streaming potential also contributes to the excellent performance. Beyond power generation, the electrospun nanofiber-based MEGs also demonstrate successful applications in self-powered sensors, including ammonia leak monitoring and moisture-temperature sensor for forest-fire detection. This study provides insight for the design of the innovative MEGs and opens a pioneering avenue for future energy conversion.

Keywords: Electrospinning; nanofibers; moist-electric generation.

Acknowledgements

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Reference

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Magnetoplasmonic Nanodomes as A Novel Structure for Biomedical Applications

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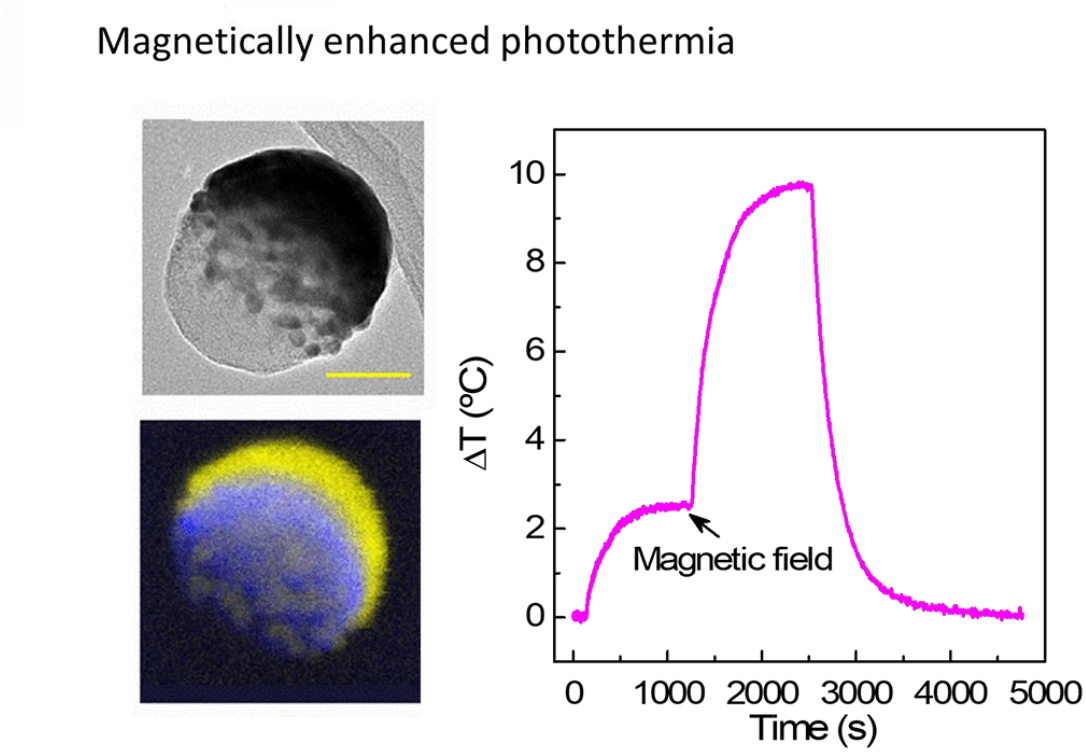
Graphical Abstract



Abstract

Advanced nanobiomedical applications have been traditionally based on chemically synthesized inorganic nanoparticles. Here we present a novel type of structure especially suited for diverse biomedical uses: magnetoplasmonic nanodomes [**1,2**]. The nanodomes are composed of a combined, magnetic and plasmonic, hemispherical shell deposited onto 100 nm diameter polystyrene beads. The variation of the materials and their thicknesses in the shell enables tuning both the optical and magnetic properties of the nanostructures. The very high plasmonic absorption of the nanodomes in

the near-infrared is used for very efficient local optical heating, i.e., photo-hyperthermia for cancer treatment [**1**]. The nanodomes magnetic character allows to remotely manipulate them to easily regulate the level of photo-hyperthermia. Moreover, given their asymmetric shape they exhibit strong optic and magnetic anisotropies. Thus, the rotation of the nanodomes using alternating magnetic fields can easily tracked optically using their different absorption depending on the orientation. Since the rotation of the nanoparticles depends strongly on the viscosity of the medium, which in turn depends on the temperature, the optical tracking of the rotation can be used to accurately determine the local temperature around the nanodomes, i.e., nanothermometry [**2**]. Combining the nanodomes efficient photo-hyperthermia with their nanothermometry capabilities, allows in-situ tracking the efficiency of photo-hyperthermia treatments.

Keywords: Magnetoplasmonic materials; hyperthermia; nanothermometry.

Acknowledgements

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Synthesis of Lithiated-SiOx Anode Materials for Lithium ion Battery using Mechanochemical Process

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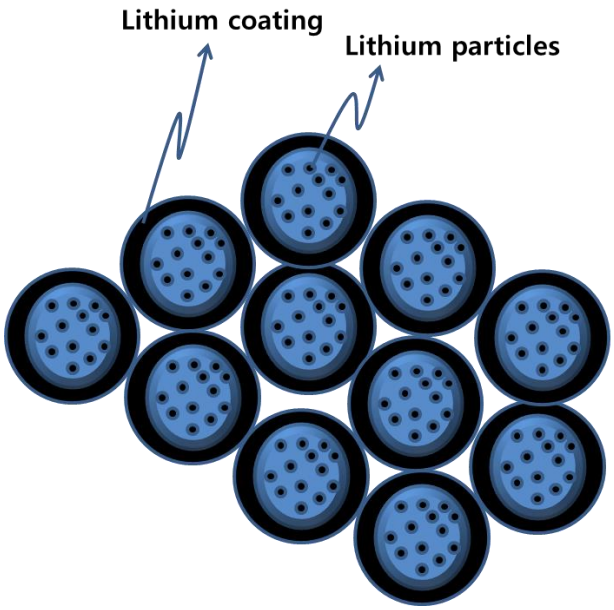
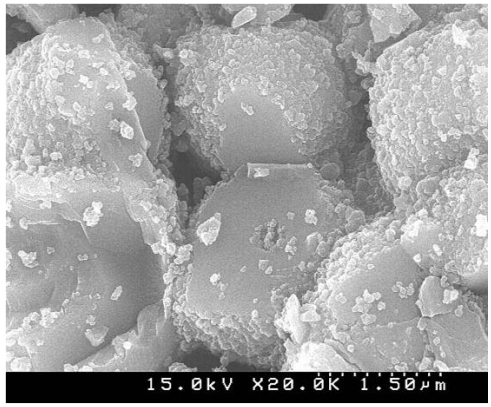
Graphical Abstract





SEM image of the lithiated SiOx

Abstract

A lithiated SiOx anode powder was synthesized by hydrothermal method and mechno-chemical processes using amorphous SiOx and $LiOH{\cdot}H_2O$ powder as a raw material. The lithiated SiOx particles consisted of 5μm SiOx and lithium composites with 50-100nm lithium particle, respectively and were identified amorphous SiOx structure having lithium elements obviously dissolved with meta-stable state into the SiOxr structure. The lithiated SiOx anode powder showed initial electrochemical lithium discharge capacity of 1,100mAh/g and revealed superior reversibility due to lithiation compared with the unlithiated SiOx. Also, the lithiated SiOx exhitbited the 89% ICE and good cycling performance because of the amorphous carbon into SiOx particels. The relationships between morphology and electrochemical properties have been discussed.

Keywords: SiOx anode; mechano-chemical process; lithiation.

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New Piezoresistive Composite Material Based on Nanographite in Glassy Matrix

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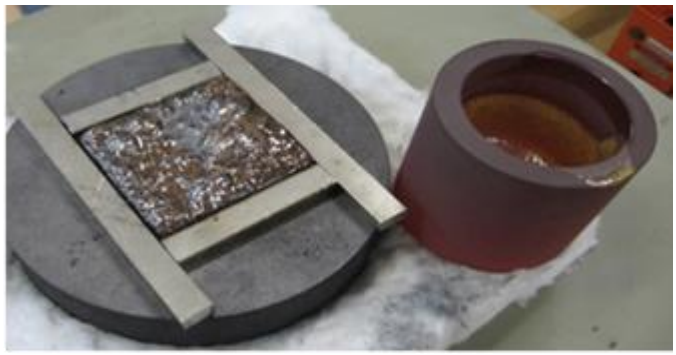
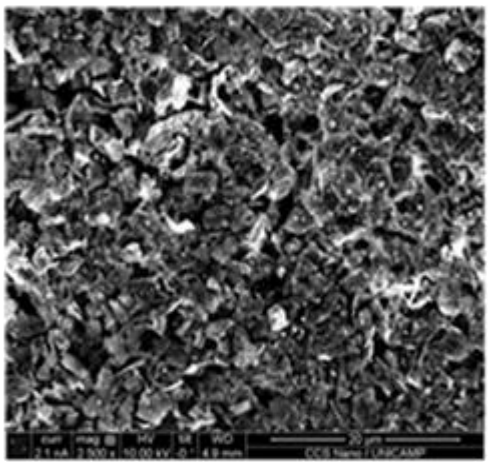
Graphical Abstract



Sintering of frit/nanographote mixture



SEM image of the composite material after sintering

Pressure sensor in Wheatstone bridge configuration

Abstract

There is a strong demand in automotive industry for development of low-cost and reliable piezoresistive pressure sensors. In the existing technology, composite materials based on porous glassy matrices (frits) and metal oxides like RuO_2 as conducive fillers are employed. The main limitations of the technology are due to extremely high cost of the ruthenium oxide and also its low natural abundance. A new methodology for producing films with a glassy matrix and multilayer graphene (MLG) / nanographite flakes as conductive fillers, was developed. The frit composition contains several Pb-free oxides: Bi_2O_3, B_2O_3, SiO_2, Al_2O_3 and ZnO. This composition allowed for obtaining reduced sintering temperature (near 600°C) for the composite material thus avoiding loss of graphite during thermal processing in air. The resistances of films (dimensions of 50 x 5 mm, thickness of 300 microns) deposited over alumina substrates, varied between ~ 1.2 and 142 kΩ. The developed material was successfully tested in pressure sensors with high sensitivity and durability. The results showed that films with MLG can replace films with RuO_2, usually employed for piezoresistive films preparation, with several critical advantages: i) thermal resistance, high conductivity, absence of electro migration and ii) very competitive price of nanographite as compared with that for RuO_2.

Keywords: Composite material; glassy matrix; nanographite; piezoresistive sensors.

Acknowledgements

The authors thank CNPq, FAPESP and SibratecNano-FINEP for financial support.

Reversible CO_2 Capture/Release of Sodium Manganate

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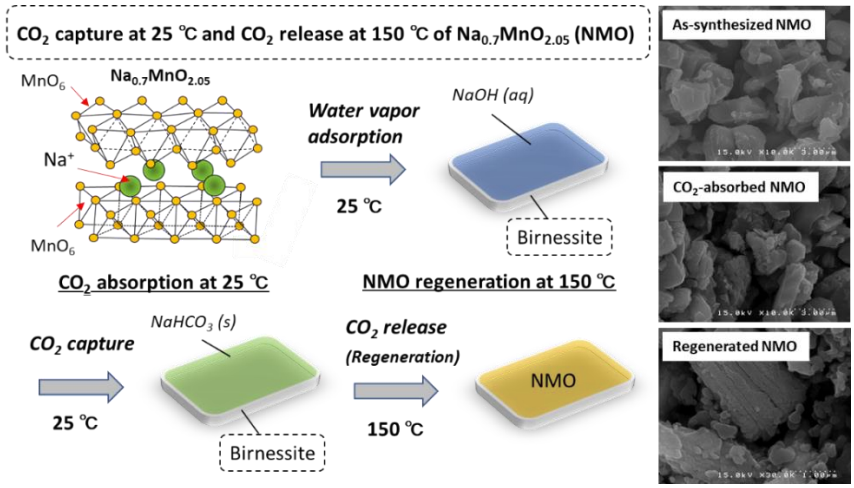
Graphical Abstract



Abstract

Sodium manganates with a layered structure, $Na_{0.7}MnO_{2.05}$, have been applied to a novel material for CCUS (CO_2 capture, utilization, and storage), capable of capturing CO_2 at 25 ℃ in the presence of water vapor and releasing CO_2 at 150 ℃. The temperatures of capturing and releasing CO_2 of $Na_{0.7}MnO_{2.05}$ were remarkably lower than those of other traditional metal oxides. The CO_2 absorption and desorption properties of $Na_{0.7}MnO_{2.05}$ were investigated by various methods, such as thermogravimetry, Fourier transform infrared spectroscopy, X-ray diffractometry, and gas chromatography. These investigations confirmed that $Na_{0.7}MnO_{2.05}$ absorbed CO_2 at 25 ℃ in the presence of water vapor to produce $NaHCO_3$ and a birnessite and the CO_2 absorption was promoted by increasing relative humidity and CO_2 concentration. The CO_2 absorption at 25 ℃ of $Na_{0.7}MnO_{2.05}$ was promoted by the formation of a strong basic solution on $Na_{0.7}MnO_{2.05}$, caused by the elution of Na ions from the interlayer of $Na_{0.7}MnO_{2.05}$ into water, adsorbed on the $Na_{0.7}MnO_{2.05}$ surface. Furthermore, $Na_{0.7}MnO_{2.05}$ was regenerated by heating the CO_2-absorbed $Na_{0.7}MnO_{2.05}$ at temperatures as low as 150 °C. The low-temperature regeneration indicates that $Na_{0.7}MnO_{2.05}$ can be a low-energy consumption material for capturing and releasing CO_2 at low temperatures.

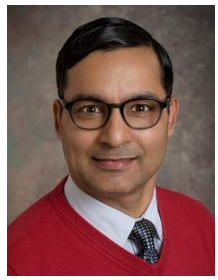
Keywords: Carbon dioxide; sodium manganate; water vapor; ambient temperature.

Acknowledgements

This work was supported by a Grant-in-Aid for Scientific Research (C) (21K05222) of Japan Society of the Promotion of Science (JSPS).

Altering Chemistry to Enhance the Solubility of A Slow-release Nanofertilizer

Yuriy Sakhno[1], Deb Jaisi[1,*]



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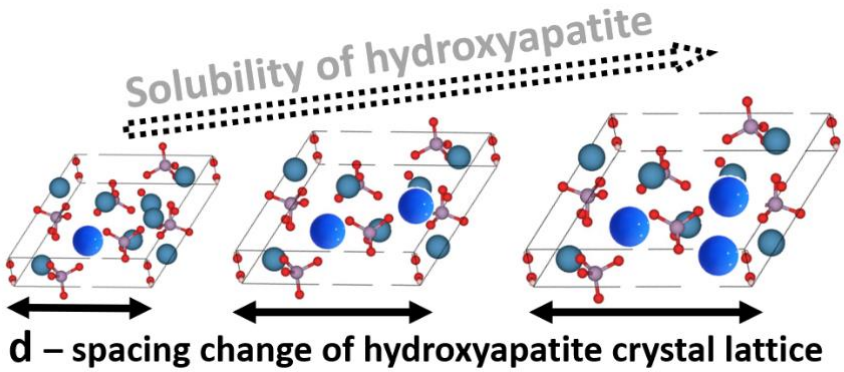
Graphical Abstract



Abstract

Modern agriculture has arrived at the crossroad of conflicting problems of keeping up the supplant food production and yet protecting water quality. Slow and controlled release fertilizers are developed towards minimizing the usage of natural resources and maximizing plant uptake. Research efforts on developing next generations of nanofertilizers are aimed to control the rate of release of nutrients and track transfer and transformation in soils and waters. Specifically, two approaches of tuning nanofertilizer are being investigated: altering crystal chemistry via substitution of cations and anions in structural sites in apatite and amorphous calcium phosphate and changing their surface properties including size, shape, and surface morphology. The structural incorporations of soluble ions and carbonate are found to enhance phosphorus release kinetics. Crystal defects created from altering the structural reorganization of a unit cell are likely dominating factors. The changes made in surface properties have counteracting effects. Inability to limit the number of variables among products complicates discrimination of the role of each parameter. Nonetheless, the current success made in optimizing the properties has aided in tuning the temporal need of phosphorus for plants.

Keywords: Hydroxyapatite nanoparticles, cation and anion substitution, lattice parameters, solubility.

Acknowledgments

This work was supported by a research grant from the U.S. Department of Agriculture (NIFA). We would like to acknowledge the Advanced Material Characterization Laboratory for providing access to FTIR, XRD, BET, and FE-SEM analyses of synthesized minerals.

Ordered Phase Transitions Triggered by Synchronous Conformational Changes in Riboswitch Crystals

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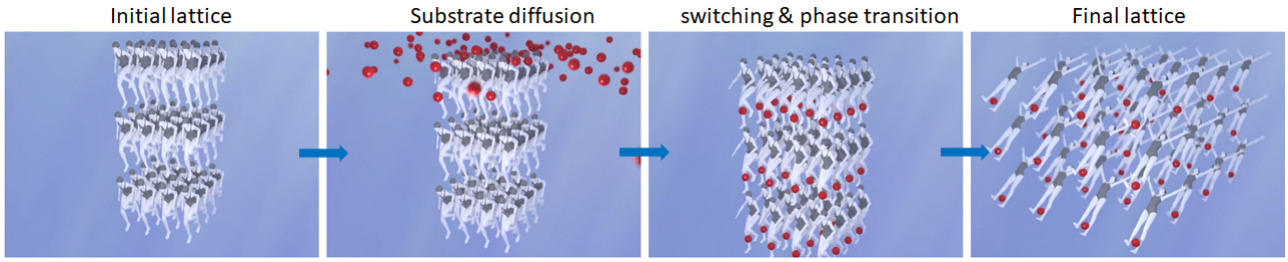
Graphical Abstract



The synchronized formation changes of simmers lead to the ordered rearrangement of the swimmers in unison. The red balls, swimmers and patterns symbolize substrate molecules, riboswitch molecules and lattices, respectively.

Abstract

Biomacromolecular crystals undergo solid-solid phase transitions as a result of conformational changes triggered by ligand binding. Here we report discovery of the synchronous behavior of the adenine riboswitch aptamer RNA (riboA) *in crystallo* during ligand-triggered isothermal phase transitions [**1,2**] (https://chemistrycommunity.nature.com/videos/several-millions-of-rna-molecules-move-in-unison). Direct visualization using polarized video microscopy (PVM) and atomic force microscopy (AFM) shows that the riboA molecules undergo cooperative rearrangements that maintain lattice order, whose cell parameters change distinctly as a function of time. The bulk lattice order throughout the transition is further supported by total diffraction from crystals using an X-ray free electron laser (XFEL). The synchronous molecular rearrangements in crystal provide the physical basis for studying large conformational changes using time-resolved crystallography and micro/nanocrystals. Our study also shows that synchronized behaviors are not unique to living systems[3], but are also present in isolated biomolecular systems, which may have profound implications that have not been explored.

Keywords: Solid-solid phase transition; synchronous; biomacromolecular crystals; riboswitch.

Acknowledgments

This research is supported by the NIH/NCI Intramural Research Fund (Y-X.W), the NSF-STC "BioXFEL" (NSF-1231306) (J.C.H.S.), the Maxwell computational resources operated at Deutsches Elektronen-Synchrotron (DESY) (H.N.C.).

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Mechanical and Thermal Properties of an AZ31 Alloy Subjected to Rotary Swaging

Zdeněk Drozd[1,*], Zuzanka Trojanová[1], Tomáš Škraban[1], Peter Minárik[1], Pavel Lukáč[1], Gergely Németh[1], Kristýna Halmešová[2], Ján Džugan[2]

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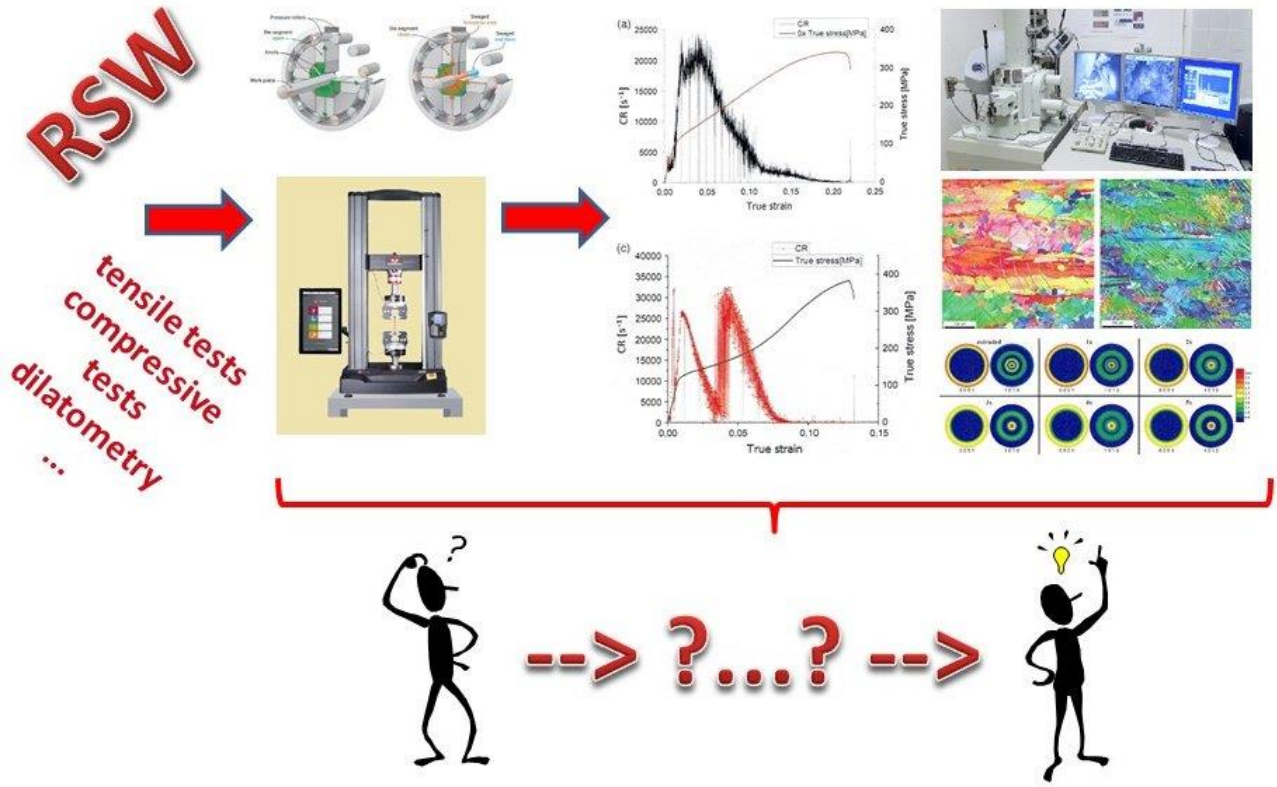
Graphical Abstract



Abstract

AZ31 magnesium alloy prepared by rotary swaging (RSW) technique was studied in this work. The technology which was used for material preparation in this study belongs to the methods of severe plastic deformation (SPD) and represents quite effective approach to refine the grain structure. Rotary swaging can be used for the precision forming of tubes, bars, and other cylindrical workpieces. The samples taken from rods prepared by rotary swaging in successive RSW passes (up to 5 passes) were subjected to tensile and compressive deformation tests conducted at room temperature with the initial strain rates from 10^{-5} s^{-1} to 10^{-1} s^{-1}. The yield stress and the ultimate

stress were determined from deformation tests. Acoustic emission was recorded in situ during these tests. True stress-true strain curves plotted together with the strain dependencies of count rates were obtained. Deformation mechanisms are connected with twinning and dislocation slip in non-basal planes. Vickers microhardness measurement was also used to probe the mechanical properties of the mentioned material. Microstructure of investigated material was studied using light microscopy and electron backscattered diffraction. Swaged samples exhibit refined microstructure. The linear thermal expansion of samples was measured using a Netzsch 410 dilatometer in the temperature range from room temperature to 400 °C. The thermal expansion curves were measured during 3-4 consequent heating and cooling cycles using the temperature rate of 0.9 K/min. Temperature dependencies of the thermal deformation and coefficient of thermal expansion were obtained from these measurements. Mechanical as well as thermomechanical properties are influenced by the texture of investigated material. The experimental results are analyzed and possible mechanisms of the observed mechanical and thermal properties are discussed. The aim of this discussion is to reveal the effect of RSW on the deformation processes occurring during tension and compression of the AZ31 magnesium alloy as well as on the other mechanical properties and microstructure features of this material.

Keywords: AZ31 alloy; rotary swaging; mechanical properties; thermal properties.

Cell-Silicon Hybrids for Bioelectrical Interrogation with Sub-cellular Resolution in 3D Tissues

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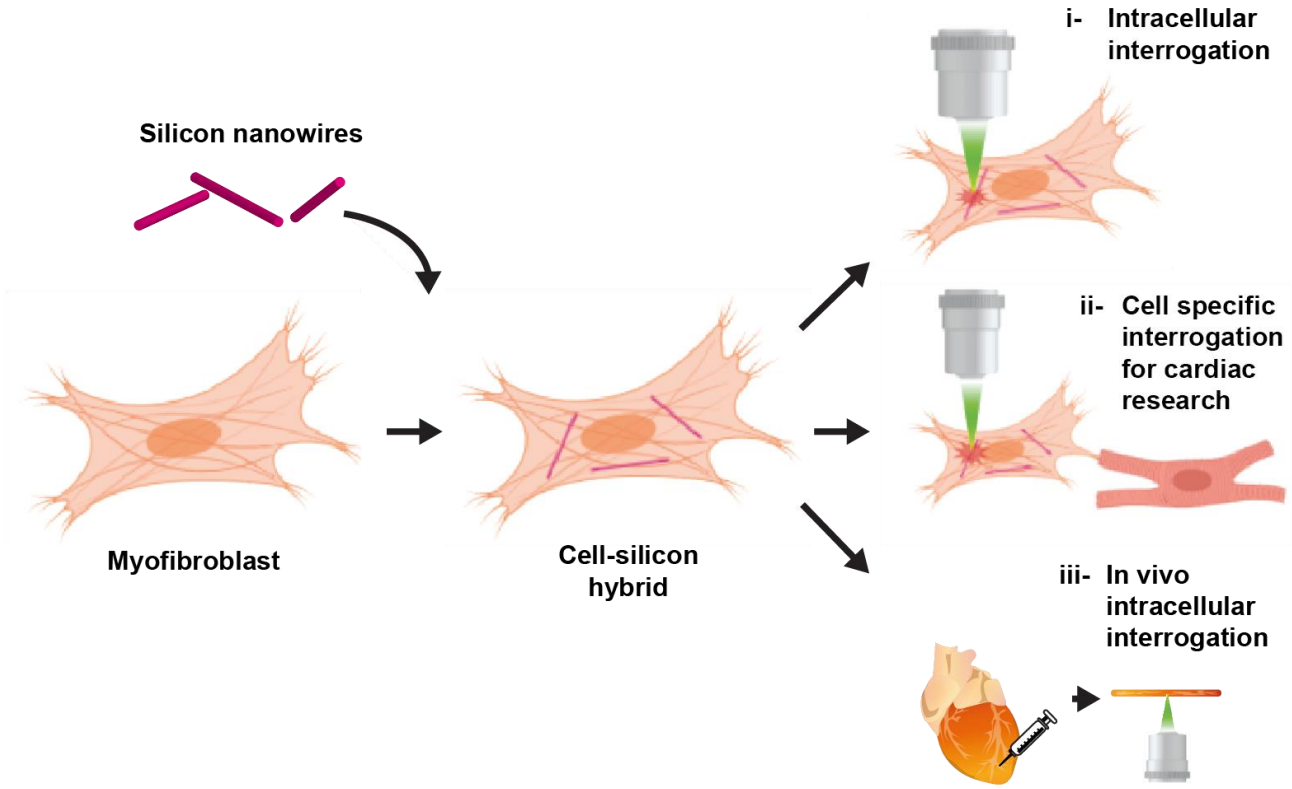
Graphical Abstract

Intracellular interrogation using silicon nanowires. Silicon nanowires can be spontaneously internalized by cells to form a cell-silicon hybrid. These hybrids can then be used for (i) intracellular electrical interrogation with subcellular resolution, (ii) cell specific interrogation in a co-culture to study intercellular coupling, or (iii) cell specific sub-cellular interrogation within the 3D volume of viable tissues.



Abstract

Traditional methodologies for bio-electrical interrogation are associated with interconnected leads and substrate-bound electrodes, which are mechanically invasive and lack intra-volumetric access [**1**]. Optogenetics, however, requires genetic modification, which limits its translational applications. Here we describe optically sensitive silicon nanowires (SiNWs) with p-i-n core shell configuration

that enable leadless, minimally invasive, and non-genetic photo-electrical modulation with unprecedented spatial resolution [**2,3**]. Moreover, this approach allows us to perform bioelectrical interrogation of specific cells that are located within the 3D volume of viable tissues, such as the cardiac tissue. To demonstrate the utility of this approach, we have used this methodology to investigate bioelectrical coupling in cardiac and brain cells. To this end, we hybridized cardiac myofibroblasts with label-free silicon nanowires by spontaneous internalization. Live imaging of the hybridisation process reviled that after internalization the cell-silicon hybrids were viable and active, and were able to undergo normal cell division in which the internalized SiNWs remained within one of the daughter cells. Then, we performed local stimulation with subcellular resolution by illuminating different nanowires that were internalized in a single cell. Consequently, transient calcium fluxes were induced, originating at the stimulation location demonstrating our ability to perform subcellular electrical interrogation. We then used these cell-silicon hybrids to study how myofibroblasts electrically couple to cardiomyocytes in vitro. Indeed, optical stimulation of the hybridized cells resulted in calcium propagation into neighbouring cells, which demonstrated that myofibroblasts electrically coupled to other myofibroblasts and to cardiomyocytes in vitro, via gap junctions. We then performed statistical analysis of the propagation speed and coupling efficiency using tailored image analysis apparatus. The culmination of this study was to address the long-standing debate of whether myofibroblasts electrically couple with cardiomyocytes in vivo. When hybrids were injected into the left ventricular wall, they establish a seamless integration with the native heart in vivo, as opposed to bare silicon nanowires that resulted in a severe immune-response, and fibrotic encapsulation. We then harvested the heart and applied local ex vivo cell-specific photo-stimulation of a specific pre-hybridized cell within the 3D tissue. Surpassingly, we found that hetero-cellular electrical coupling did not occur, as no calcium or electrical signal propagated from the stimulated myofibroblasts to the native tissue. Thus, we concluded that no electrical coupling between heterocellular myofibroblast-cardiomyocytes junction occurs in vivo as opposed to in vitro. To demonstrate the utility of these approach, we hybridised oligodendrocyte progenitor cells with SiNWs. The hybrids were then differentiated into oligodendrocyte and interacted with co-cultured neurons via myelin formation. Preliminary results demonstrate the ability of calcium transient to propagate from the hybrids to interfacing neurons, which suggest that they can be used for investigating the role of calcium transients in the myelination process. In summary, p-i-n SiNWs can be utilized for high spatial resolution optical modulation of cells for basic research investigations. It allows unprecedented spatial resolution in vitro, as well as within 3D viable tissues ex vivo.

Keywords: Silicon; nanowire, optical modulation, non-genetic, bioelectrical coupling.

Acknowledgements

This work was performed in the laboratory of prof. Bozhi Tian at the University of Chicago.

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Controlled Drug Release Kinetics from Rolled up Biocapsules based on Thermally Treated Gelatin Films

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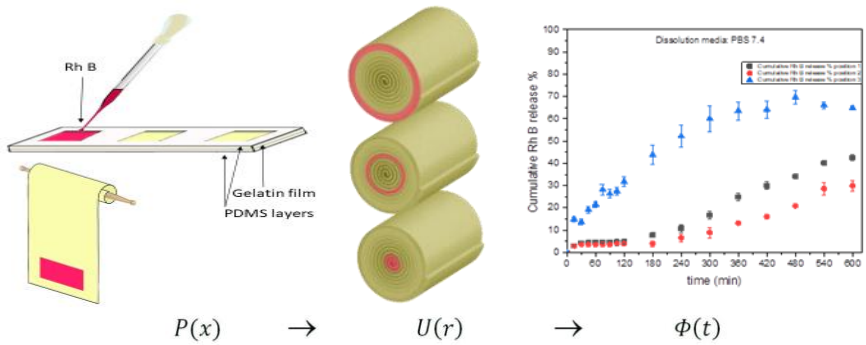
Graphical Abstract



Transformation of axial distribution of the drug model into radial distribution for release kinetic control

Abstract

Precision medicine is an emerging practice that has attracted the attention of many researchers over the recent years [**1**]. Herein, we design a new oral dosage form enabling chronomodulated drug release. We combine a theoretical idea [**2**] suggesting that a non-uniform distribution of a medicament in a micro/nanoporous matrix media can be explored for the programming of the drug release, with an experimental system [**3**] which consists in rolling a film, soluble in body fluids, and covered by a drug, in order to design a biopolymer-based capsules. Due to their unique and versatile characteristics, gelatin films are chosen to be the drug model matrix. First, focus is given to the influence of dehydrothermal treatment (DHT) [**4**] conditions on the physicochemical properties of gelatin films that present good prospects in the pharmaceutical field, e.g., as a drug delivery system. Atomic Force Microscopy (AFM), Brunauer-Emmett-Teller (BET) and Fourier Transform Infrared (FTIR) spectroscopy were used to investigate the physicochemiacal and mechanical properties of the gelatin films. Here, in contrast to typical DHT conditions, we show that 8 hours of heat treatment carried out at 150°C are efficient to obtain stable films insoluble in aqueous media at different pHs at 37°C. The treated films exhibit (with respect to untreated ones) a decrease in water absorption rate, an increase in contact angle and a reduced water uptake capacity with a limited mass loss. AFM

shows that the surface roughness remains almost invariant while mechanical properties are enhanced which is in accordance with tensile testing results. BET analysis show a slight decrease in pore size, in surface area and in N_2 adsorbed volume. No significant differences are detected among the FTIR spectra before and after DHT treatment except a peak, which appears at 1718 cm^{-1} potentially due to esterification. These capsules have been stabilized in the rolled-up geometry using Transglutaminase then dissolved using USP 4 apparatus in different media in physiological conditions. Results show that the arbitrary complex radial distribution of the drug model present complex release profiles via the diffusion-controlled and swelling-controlled mechanisms. Confocal Laser Scanning Microscopy (CLSM) and fluorescence spectroscopy determine drug diffusion profile during the delay of release period estimated to 3 hours for the inner and central positions. Computer simulation study is in progress.

Keywords: Gelatine; DHT; drug release.

Acknowledgements

The authors gratefully acknowledge financial support by the Frensh National Research Agency, award N° ANR-17-CE18-0021-01.

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Interface Characterisation for the Next Generation of Multi-materials Additive Manufacturing

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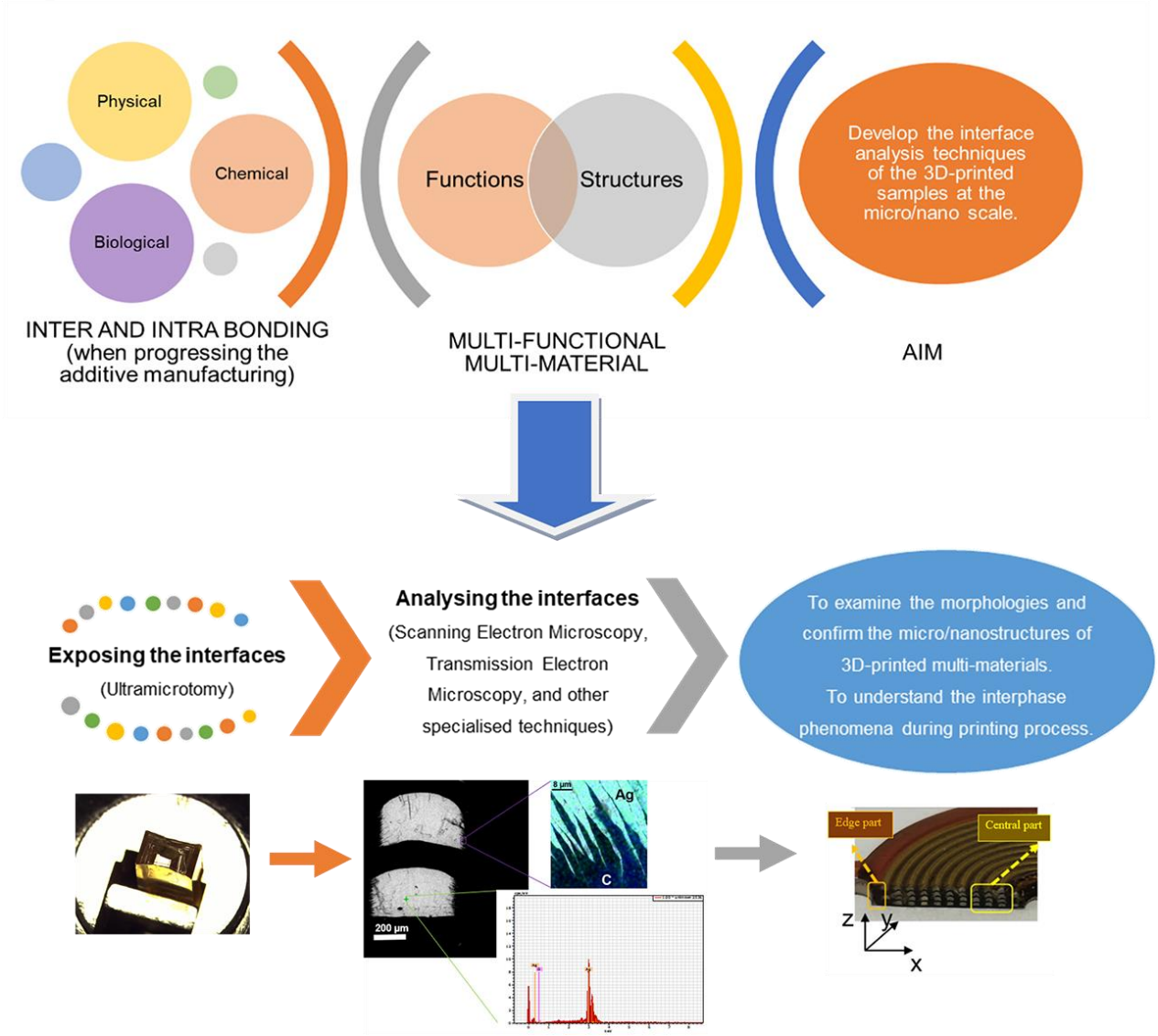
Graphical Abstract



Abstract

Multi-materials additive manufacturing allows the combination of different materials within a printed object to facilitate new functionality and/or enhance the performance of the final product [**1**]. Applications are foreseen in wide-ranging fields including automotive, engineering, healthcare, aerospace, and defense, and we are endeavoring to produce co-printed functional multi-materials particularly in pharmaceuticals and electronics [**2**]. To achieve this, potential physicochemical incompatibility of materials when concurrently or sequentially printed that may limit the efficiency and affordability of the 3D-printing technology needs to be understood and addressed [**3**]. Currently, the School of Pharmacy and the Centre for Additive Manufacturing from the University of Nottingham have been collaborating with various partners to design and develop the methodologies for co-printing and characterising the 3D-printed multi-functional multi-materials such as organic-inorganic materials in printed electronics or supportive/active materials in pharmaceuticals. Our project belongs to the Research Challenge 1 of the Programme Grant "Enabling Next Generation of Additive Manufacturing" (NextGen AM) [**4**]. We aim to develop robust characterisation approaches to study at the micro and nano scale the material interfaces and interphases of multi-material 3D prints. In this first phase of the project, we will present work on the development of suitable sample-preparation strategies to expose native material interfaces from within 3D-printed objects. As an example, we show data related to a commercialised 3D-printed inductor device ("DragonFly system" from Nano Dimension Company [**5**]). Ultramicrotomy was shown to be able to expose undamaged interfaces suitable for analysis by Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), and Transmission Electron Microscopy (TEM) to acquire morphological and structural data of the 3D-printed samples. Fourier-Transform Infrared Spectroscopy (FT-IR Spectroscopy) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) were also carried out to study interface composition and chemistry. We will show how the materials and chemical insights provided by these types of analysis can provide opportunities for improved multi-materials additive manufacturing and device functionalities.

Keywords: Interface characterisation; Multi-materials; Additive Manufacturing (3D-printing).

Acknowledgements

Programme Grant "Enabling Next Generation Additive Manufacturing" (EP/P031684/1) for funding the project. The School of Pharmacy, Centre for Additive Manufacturing, Nano and Micro Scale Research Centre (nmRC) at the University of Nottingham for the necessary facilities. The Nano Dimension Company for providing the commercialised electromagnet product.

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Effect of Processing Parameters on the Porosity Generation of Out-of-Autoclave Manufactured Laminated Thermoplastic Composites

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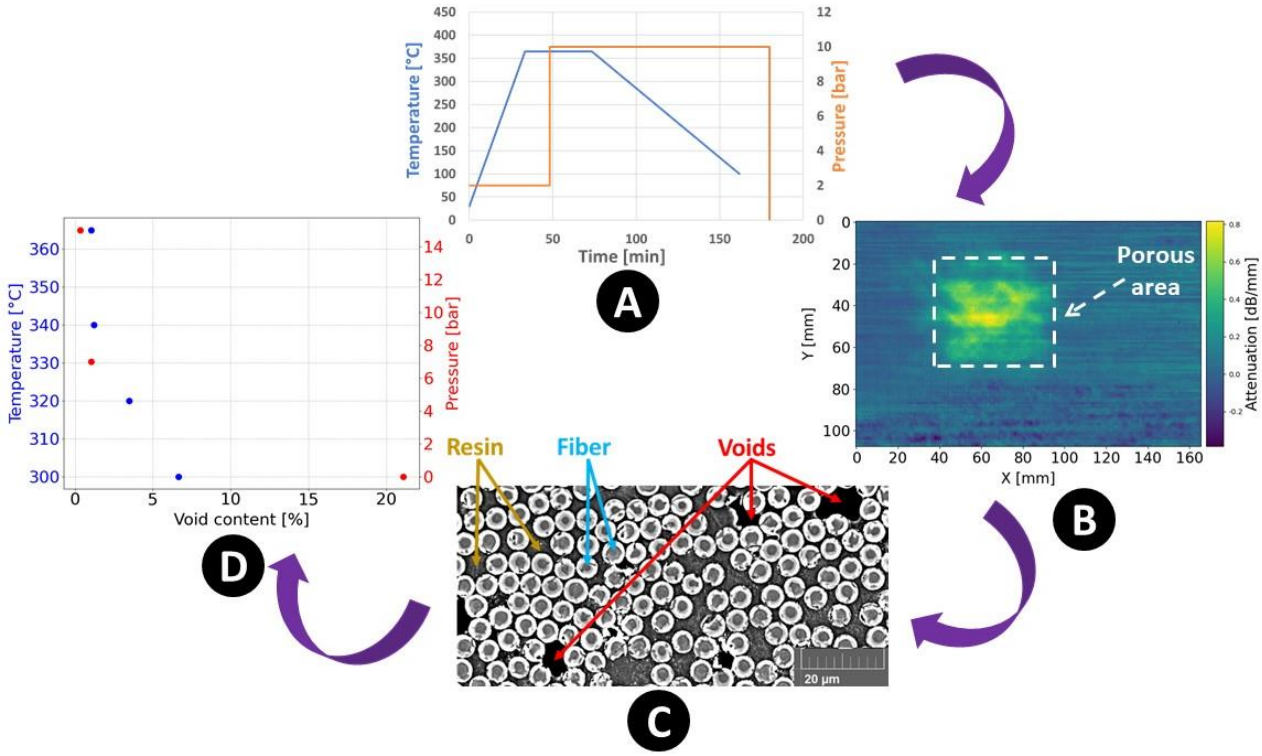
Graphical Abstract



A. Temperature and pressure cure cycle used to process Out-of-Autoclave composite prepreg.
B. Ultrasonic NDT image attenuation signal of a composite plate with porous area.
C. Micrographic cross section of the laminated thermoplastic composite.
D. Measured void contents as a function of cure pressures and temperatures.

Abstract

The increase of the aircraft production rate is strongly linked to the reduction of manufacturing costs especially with the use of organic matrix. The structures have increasingly complex shapes, which can be problematic in the development of these high temperature thermoplastic materials. The shaping of prepreg can induce, for example, high void content in intra-or inter-ply and in plane or out-of-plane

waviness. In addition, due to the high cost of autoclave processing, there is a heavy demand to develop cost effective Out of Autoclave (OoA) alternatives that provide equivalent properties. Vacuum Bag Only (VBO) prepreg processing is inherently low cost and scalable to large plates manufacturing [**1**]. Therefore, void reduction is one of the biggest criteria to achieve autoclave equivalent part properties. The goal of this study is to develop a fundamental approach of the void reduction mechanisms and develop process models that can be used to design and optimize the VBO processing cycle for thermoplastic laminates.

Firstly, the characterization of the material during consolidation step as well the numerical simulations of the manufacturing process were realized. For this purpose, plates were produced with and without porosity, subsequently, the samples were controlled by Nondestructive Testing (NDT). Finally, mechanical tests were carried out to validate the effect of void content on the mechanical behavior.

In this study, plates of laminated thermoplastic composite were manufactured by VBO and hot-press. Processing parameters (heating rate, dwell time and pressure) of the manufacturing cycles were altered to obtain different porosity levels within the laminates. Subsequently, the plates/coupons thus produced have been controlled by flash infrared thermography, ultrasonic NDT measurements, void content analysis, 2D microscopy and mechanical characterisation in order to measure and to confirm the presence and locate the porosity.

A range of porosity of 0–21% was reached, and the void content was measured by different methodologies and a good correlation between methods with only slight discrepancies was observed. A correlation was performed between the ultrasonic absorption coefficient [**2**], thermal diffusivity [**3**] and the void content in the laminate. These results show the possibility of evaluating the mechanical performance of thermoplastic structures from NDT and void content analysis, thereby reducing quality control costs and extra mechanical tests.

Moreover, in-plane airflow during the manufacturing process in the intra-ply is modelled using Darcy's flow that is representative of the porosity between adjacent layers and the ability to vent the gas at the part edge. The proposed mechanism model permits to evaluate manufacturing cycles for plane geometries in order to reduce void content. The optimum void content are equivalent to autoclave manufacturing for laminated thermoplastic composite [**4**].

Finally, for a better understanding of consolidation phenomena a study of the influence of manufacturing process parameters on the consolidation quality has been made. This criterion has been evaluated by mechanical tests (ILSS). In particular, the results show that temperature and pressure strongly influence the void content and thus the quality of consolidation of carbon fiber thermoplastic composite materials [**5**].

Keywords: Laminated thermoplastic composite, out-of-autoclave, in situ consolidation, porosity/ voids, NDT.

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Thermal Characterization of Fire-retardant Coated Green Biocomposite

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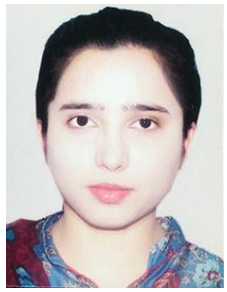

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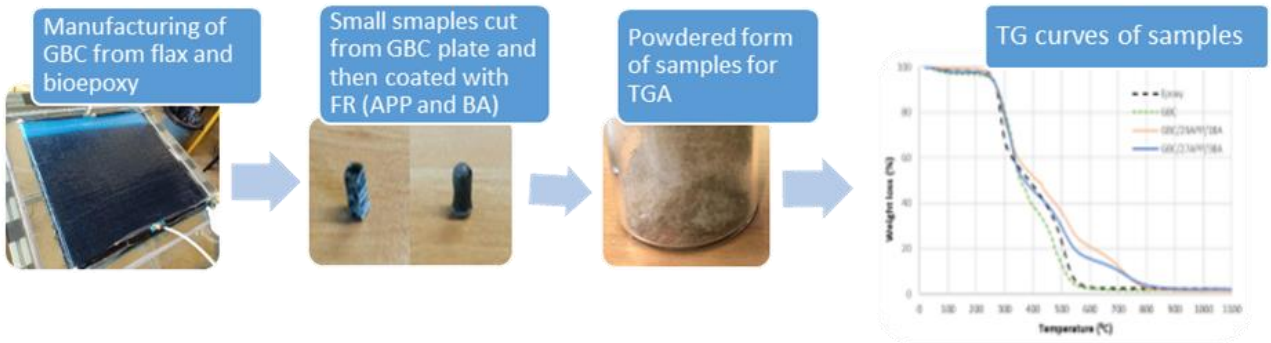
Graphical Abstract



Abstract

The use of biocomposites is rising exponentially due to their low weight to strength ratio, competitive mechanical strength and corrosion resisting behaviour [**1**]. Unfortunately, their application at the industrial level could not be materialised due to safety concerns in case of fire [**2**]. Therefore, fire-retardant (FR) treatment of green biocomposites (GBC) has become essential for their safe application in industrial environment. Intumescent fire retardant (IFR) system based on ammonium polyphosphate (APP) and boric acid (BA) was coated on the GBC that composed of flax laminates and 38% bio-epoxy resin. This ongoing study aims at carrying out thermal characterization of the GBC at matter (small: mg-mm), material (medium: g-cm) and product (large: kg-m) scales. Hence, thermogravimetric analysis (TGA) was performed between 20-1100°C under synthetic air with an airflow rate of 100 ml/min, and a non-isothermal heating rate of 10°C/min to investigate thermal degradation behaviour at matter scale. TG curves of epoxy, GBC, GBC/29APP/1BA and GBC/27APP/3BA reveals that addition of BA and APP improves fire retardant properties of GBC. Similar decomposition patterns for FR coating based on APP and BA have been reported [**3**]. The weight loss curves shown in graphical abstract exhibit that increasing the amount of boric acid from 1% to 3% has negative impact on fire retardancy of the GBC [**4**]. As compared to GBC and epoxy

that are fully decomposed at 590ºC with almost no residual mass left, the GBC coated with 29APP/1BA and 27APP/3BA FR had 22% and 16% residual mass at 590ºC.

Keywords: Biocomposites; TGA; fire retardant.

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Design and Fabrication of Highly Porous Graphene Oxide Composited Biopolymer Blends with Osteoinductive Properties

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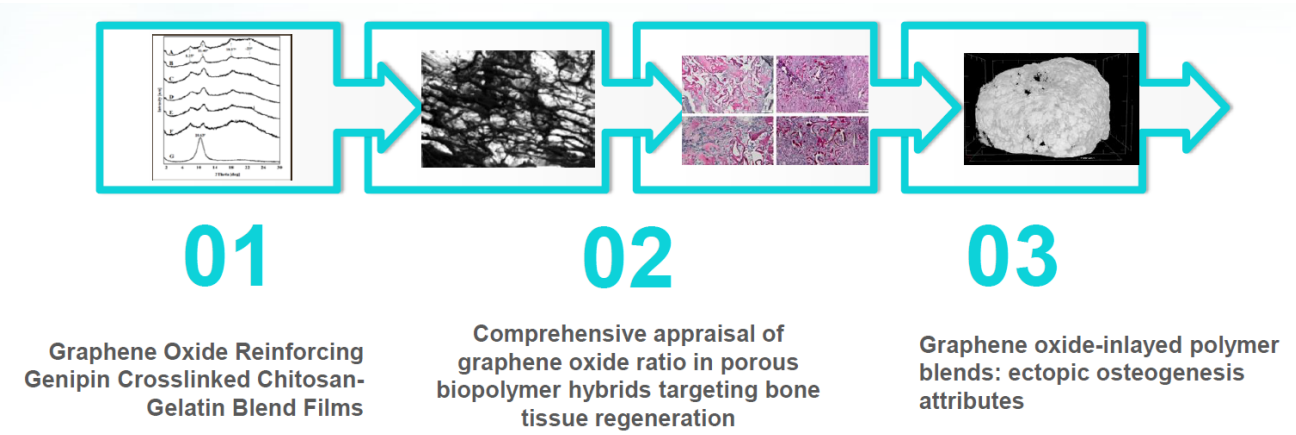
Graphical Abstract



Abstract

Herein, the synthesis and characterization of novel chitosan-gelatin highly porous scaffold reinforced with graphene oxide, crosslinked with genipin was targeted. This study addresses the potential boost of mineral-independent osteoinduction and osteodifferentiation featured by fish gelatin/chitosan (GCs) hybrids per graphene oxide (GO) reinforcement. Standard GCs formulation was referenced against genipin (Gp) crosslinked blend and 0.5 wt.% loaded GO composite (GCsGp/GO 0.5 wt%).

Suitable GO dispersion was ascertained within the biopolymer mix as nanolayers specific signals lack in both FTIR and XRD spectra and the specific spectral features of the polymers persisted with GO load enhancement. Overall, correlations between the GO induced material structuration, crystallinity variations and chemical interaction of the compounds can be correlated with the physical features and bioactivity of each composite formulation.

Exploratory mechanical investigations were performed before assessing in vitro osteodifferentiation (against MC 3T3-E1 pre-osteoblasts) and materials' osteoinductivity in vivo (CD1 mice). Specific biological staining revealed collagen formation and Ca^{2+} deposits, validated by µCT. runx2 and opn markers determination stressed on the osteogenic phenotype of the cells populating the

implanted materials. The aftereffects of implantation in *ex vivo* materials were studied from the angle of *in situ* biomineralization and morphology alterations. X-ray diffraction and Fourier-transform infrared spectroscopy underlined the novel material structuration in the mineralized extracellular matrix.

This data supports the GO bioactivity in osteogenesis mechanisms as being self-sufficient to boost osteoblast differentiation and bone formation in ectopic sites. Hence, the synthesis route of a natural polymer blend/graphene oxide composite material is anticipated to emerge as influential formulation in bone tissue engineering.

Keywords: graphene oxide, biopolymer blends, ectopic bone formation, osteoinduction, ex vivo analysis.

Acknowledgements

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Electron Spin as A Key Factor for Improving the Treatment of Genetically-Based Diseases Like Cancer

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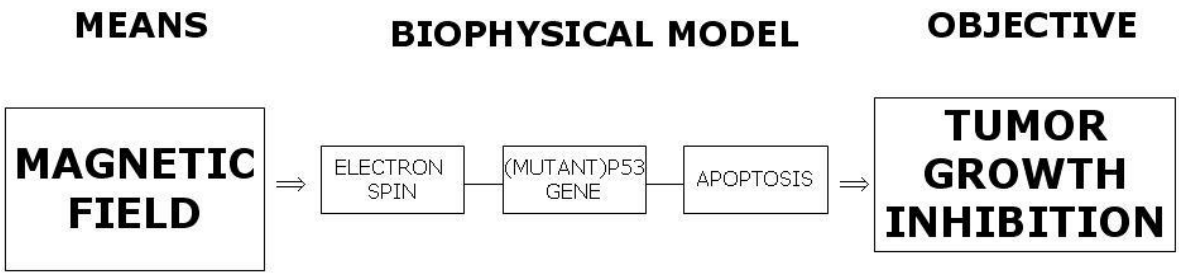
Graphical Abstract



Abstract

From a thorough analysis, based on quantum physics, the electron spin, as a key factor governing cell genetic stability, appears to play an important role. The electron spin and its properties may be important to impact positively on the knowledge gap facing biomedical science today, the one between the atomic level and the cellular level [**1**]. Diminishing this gap may help to improve the development of medical therapies in the so important area of genetically based diseases like cancer.

The spin state has a pivotal role in all the reduction-oxidation (or *redox*) reactions that are at the core of our metabolic machinery. Redox reactions involve the transfer of electrons from one reactant to another. This kind of reactions is so important that our life depends on them.

During normal cellular respiration, electrons are passed through a series of mithocondrial complex to the terminal electron acceptor, molecular oxygen. Reactive oxygen species (ROS), oxygen free radicals, are then formed as a natural byproduct and have important roles in cell signaling and homeostasis.

It has been shown that oxidative stress conditions, i.e., elevated intracellular levels of ROS, may control the very important genes such as tumor suppressor genes p53 and (DNA) repair genes [**2**].

Being the spin a purely physical entity, its energy states can be theoretically better influenced by physical means (i.e., magnetic-electromagnetic fields) than by chemical reactions. So appropriate magnetic fields were hypnotized to influence cancer cell functions through en effect on the rate of recombination of spin correlated radical pair [**3**]. The hypothesis that specific magnetic fields can change rate of ROS recombination has been recently experimentally validated [**4**].

Different authors have studied the use of static and extremely low-frequency magnetic fields as a potential antitumor agent as well as an adjuvant agent to chemotherapy and radiotherapy with promising laboratory results. Overall, the published data support the presence of antitumor efficacy in many cancer models using different human cancer cells including those of adenocarcinoma, breast cancer, melanoma and neuroblastoma, lung cancer, gastric cancer and pancreatic cancer [**5,6**].

Overall, the available data suggest that this new approach based on physics, specifically quantum physics, could open new frontiers in biological and medical research for possible improvement of available therapies, mainly in the area of genetically based diseases like cancer.

Keywords: Magnetic fields, antitumor effects, ROS, apoptosis, p53 expression.

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Elaboration of Silica Ceramics by Indirect Additive Manufacturing and Aqueous Gelcasting

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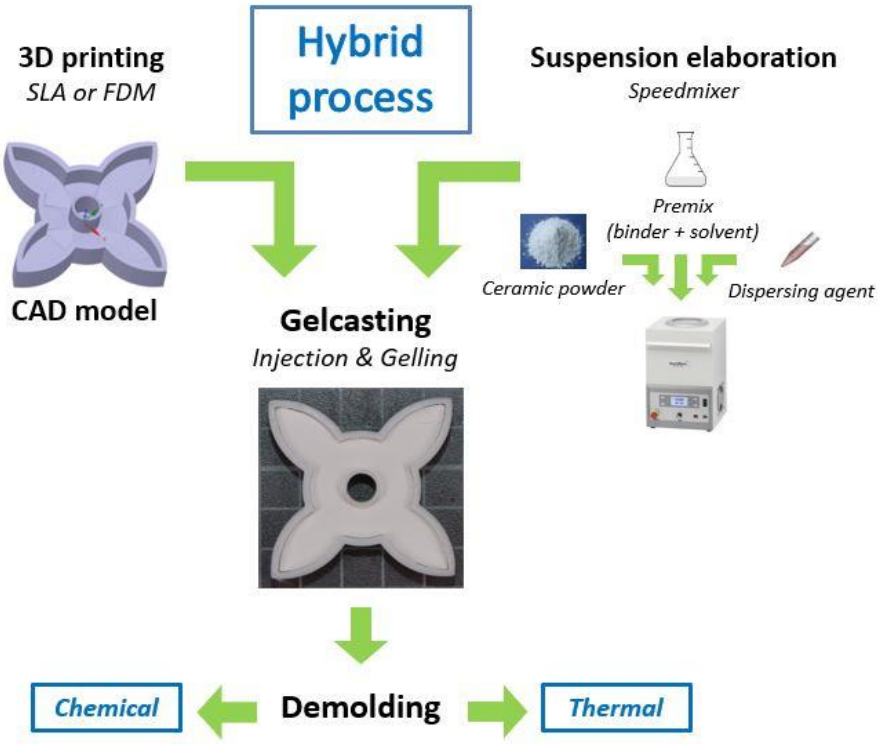
Graphical Abstract

Fabrication of complex shaped silica ceramic parts by a hybrid process using the additive manufacturing of molds and the gelcasting.



Abstract

The "gelcasting" process developed in the 1990s by Omatete and Janney, [**1**] overcomes the disadvantages of the classical production of ceramic parts by the ceramic injection molding (CIM) method: a relatively long debinding time and a high cost for the realization of the tools used, making it impossible to manufacture small series of parts at a competitive price. [**2**] However, most of the studies relating to the manufacture of ceramic parts by gelcasting show that the green bodies are demolded before drying and sintering using silicone or metal molds that can be separated into several parts. In the case of complex shapes, demolding is a critical step. It cannot be carried out mechanically

and it is necessary to destroy the mold thermally or chemically. The combination of additive manufacturing of molds with the gelcasting process allows the production of complex parts. [**3-4**] Despite the fact that many articles deal with the production of ceramics from gelcasting, very few are devoted to the thermal or chemical demolding of the parts. Moreover, among all the literature research carried out on the manufacture of ceramic parts using the gelcasting process, the vast majority of studies concern the use of alumina powders and very few are those dealing with silica powders. To our knowledge, no study has yet been carried out on obtaining silica ceramic parts by combining gelcasting with the additive manufacturing of molds and by chemical demolding. This hybrid process was used in this study to fabricate ceramic parts of complex geometry from an aqueous ceramic suspension with a high silica filler content (> 50%vol) and a low viscosity (< 1.5 Pa.s) allowing its injection into molds printed by StereoLithography Apparatus (SLA) and Fused Deposition Modeling (FDM). The gelling and curing of the green parts are ensured by the use of the MAM/MBAM low toxicity gelling system. The evolution of gelling kinetics as a function of temperature as well as initiator and catalyst content is presented in this study. The rheological properties of the suspensions as a function of the loading rate are studied and the advantages and disadvantages of thermal or chemical demolding are exposed. The use of FDM PLA molds allowed them to be dissolved in a dichloromethane bath without damaging the raw parts, unlike SLA printed PLA molds which cause mechanical stress during removal. Nevertheless, the printing resolution of these FDM molds is not as high as for the SLA process, inducing surface defects on the parts. Thermal demolding obtained by the SLA process with a commercial burn-out resin has made it possible to obtain dense ceramic parts with a good surface finish. However, the need to dry before demolding is a bottleneck for obtaining parts with even more complex geometries. The use of chemical demolding makes it possible to avoid this critical step, but it is necessary to improve the printing resolution of the molds.

Keywords: Indirect additive manufacturing; gelcasting; MAM/MBAM; silica; hybrid process.

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Microwave-Induced Titanate Nanotubes for Visible-Light-Driven Hydrogen Production

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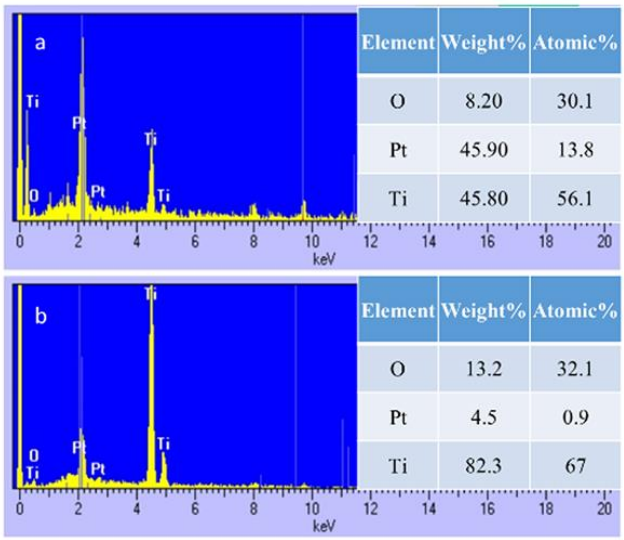
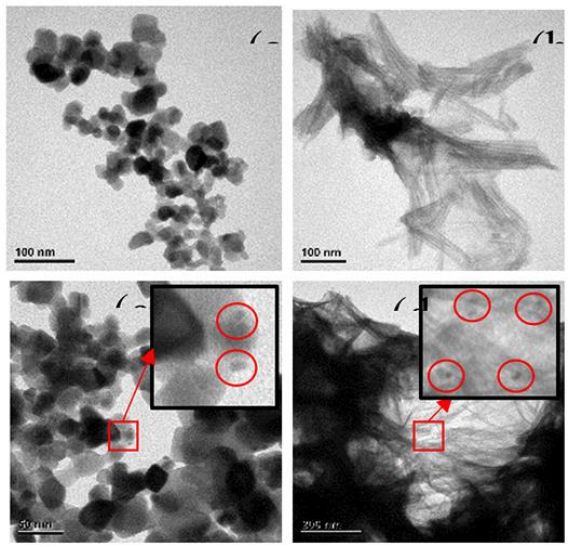
Graphical Abstract



SEM images of (a) Pt/TNTs, (b) Pt/TiO_2



TEM images of (a) TiO_2, (b) TNTs, (c) Pt/TiO_2, (d) Pt/TNTs

Abstract

Titanate nanotubes (TNTs) fabricated through microwave-assisted synthesis were examined for their ability to catalyze hydrogen production under UV and visible light irradiation. The UV-Vis spectral analyses of the TNT composites showed greater shifts toward the visible region after co-catalysts loading than the spectra of TiO_2. The photocatalytic performances were evaluated by measuring the hydrogen production, and Pt loaded on TiO_2 and TNTs were examined for their ability to catalyze hydrogen production. The experimental results showed that Pt/TNTs exhibited higher activity than Pt/TiO_2 from an aqueous solution containing 20 vol% methanol solution under UV and visible light irradiation. Furthermore, the presumed mechanism of the photocatalytic conversion of a methanol solution to H2 is the oxidation of methanol and transformation to formaldehyde and then formic acid. Then, formic acid is transformed to CO and H_2O or CO_2 and H_2. Because bare TNTs and Pt/TNTs showed lower CO generation than bare TiO2 and Pt/TiO2, TNT composites enhanced the photocatalytic selectivity for H_2 generation from formic acid to a greater extent than Pt/TiO_2. Because

the kinetic diameter of CO (0.38 nm) is larger than that of CO_2 (0.33 nm), this result may be attributed to the inability of CO to diffuse into the pores of TNTs because of the diameter difference.

To enhance the photocatalytic performances from an aqueous solution containing 10 vol% formic acid solution under visible light irradiation, the composites formed from Pt, CdS, and titanate nanotubes (TNTs) were examined. Experimental results showed that CdS/TNTs exhibited much higher activity than CdS/TiO_2. And TNT composites with Pt loading by the photo-deposition method had a significantly enhanced photoactivity and exhibited a hydrogen production rate of 661.1 μmol g^{-1} h^{-1}, which is approximately 3.6 times higher than that observed for Pt deposited by the thermal impregnation method. This result indicates that smaller and more uniform Pt nanoparticles efficiently promoted the separation of photogenerated charges. XPS results showed negative shifts of the Pt binding energies and positive shifts of Ti binding energies due to the strong metal-support interaction between Pt and TNTs. And the TNT composites showed no significant amount of oxidized S^0 or S(VI) on the catalyst surface even after 3 h of reaction. Thus, the photocorrosion of CdS was inhibited when combined with TNTs during the photocatalytic reactions.

Keywords: Titanate nanotubes, hydrogen production, strong metal-support interaction, photocorrosion of cadium sulfide.

Acknowledgements

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Metal Oxide Nanowires and Nanofibers for Solar Water Splitting

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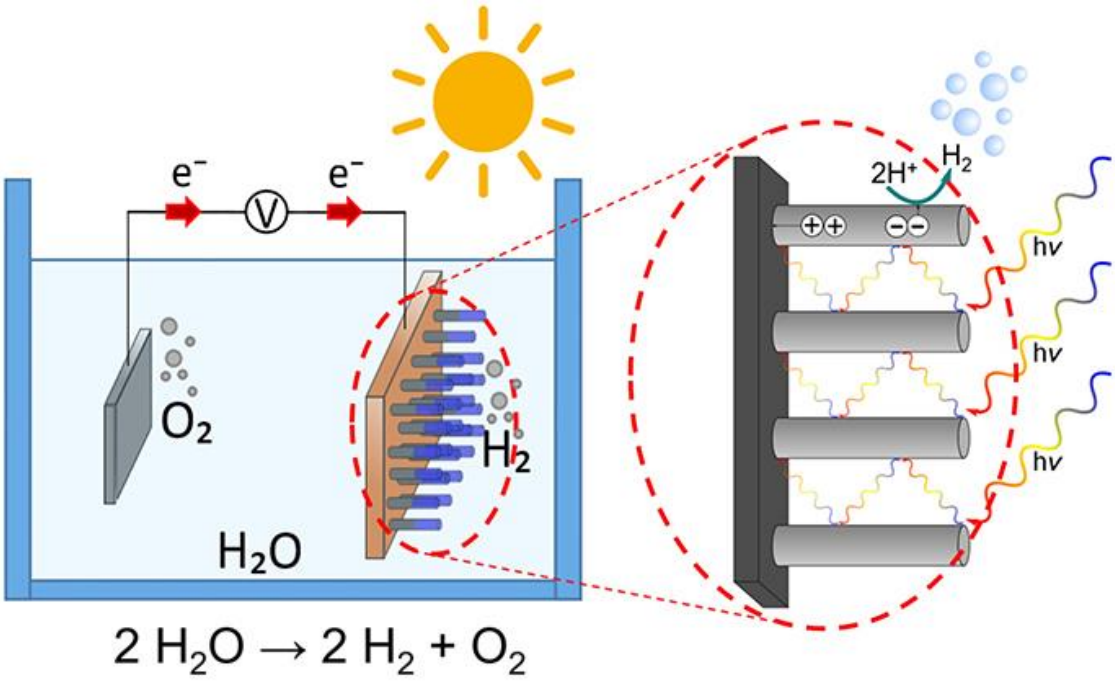
Graphical Abstract



Abstract

The unique physical and chemical properties of quasi one-dimensional nanostructures that arise by their high surface-to-volume ratio make these nanostructures very promising for many applications, including solar water splitting. Furthermore, the physical properties of most semiconductors also demand the use of such elongated nanostructures for photo(electro)chemical applications. For instance, the diffusion length of minority charge carriers (i.e., electrons for a p-type semiconductor or holes for an n-type semiconductor) in Cu_2O is only 20-100 nm, while the absorption depth near the bandgap is approximately 10 µm. This means, that with the use of one-dimensional nanostructures, a maximum of solar light can be absorbed over the nanowire length, while the nanowire diameter is small enough for efficient electron and hole diffusion, and therefore high

efficiency. This concept forms the basis of the research that is performed within my group. In the past, we for instance successfully developed ZnO and Cu_2O nanowires and nanowire networks that presented a significantly improved PEC performance when compared to their thin film counterparts [**1,2**]. And currently, we are for instance focused on the development of core-shell Cu_2O@MOF nanowires [**3**], $CuBi_2O_4$ nanowires and nanofibers via templated electrodeposition and electrospinning, respectively, and we are also investigating the use of the more traditional PV-materials Si and $CuGaSe_2$/$CuGa_3Se_5$ for photoelectrochemical water splitting [**4,5**].

Within this presentation, I will focus on two of our recent achievements, namely (i) the synthesis and characterization of interconnected $CuBi_2O_4$ nanowires via templated electrodeposition and (ii) the synthesis and characterization of nanofibers consisting of several different materials (e.g., $CuBi_2O_4$, $BiVO_4$ and $CuFeO_2$) via electrospinning. Both types of nanostructures are developed and investigated for their improved solar-to-hydrogen efficiencies when compared to their thin film counterparts.

Keywords: (photo)electrochemistry, water splitting, $CuBi_2O_4$, templated electrodeposition, electrospinning.

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Electrospun Core-shell Nanofibers for Protection against Corrosion

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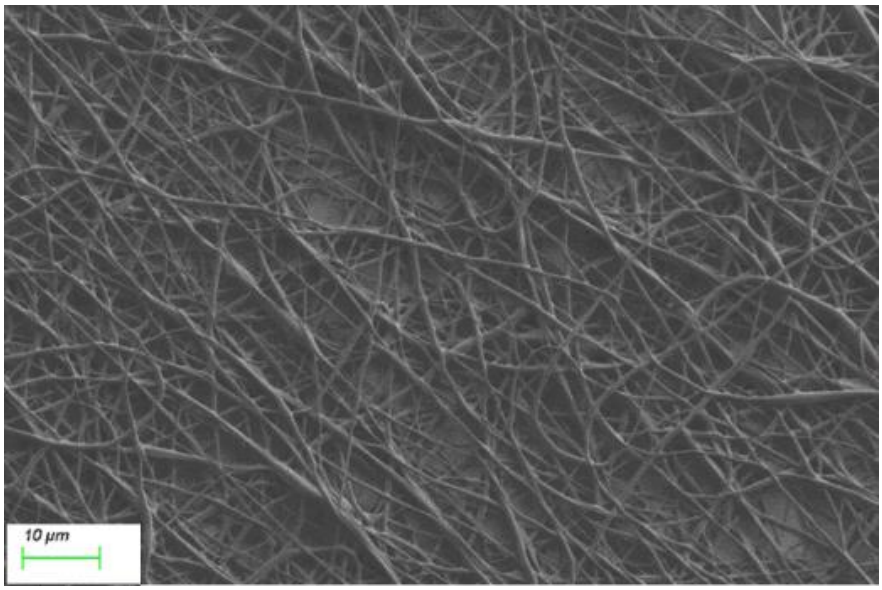
Graphical Abstract



Core-shell nanofibers

Abstract

Aluminium is an active metal and its resistance to corrosion depends on its capability to form protective oxide films. Currently, the most widely used strategy is based on the application of anodization processes. Anodized layers with additional sealing are already on the industrial market and provide enhanced corrosion protection, but there is place for improvements. An innovative way of counteracting corrosion is proposed: electrospun core-shell nanofibers.

Core-shell polyurethane/oil nanofibers were produced using the coaxial electrospinning set-up. Optimization of the electrospinning parameters was done in order to achieve the formation of beads free nanofibers. The distance between the co-axial needle and the collector was tailored between 80 mm and 180 mm. Flow rate for the oil was also tailored from 0.01ml/h to 0.07ml/h. Co-axial electrospinning experiments were performed at ambient temperature.

Electrospun nanofiber mats were placed either directly on the Al substrates after removing the native oxide (degreasing and pickling) either in between two commercially available coating layers. The morphology of the electrospun nanofibers was observed by means of scanning electron

microscopy (SEM). The core-shell nanofibers layer thickness as measured by focused ion beam (FIB) was tailored between 1 and 20 µm as a function of deposition time. Surface wettability of various surfaces (nanofibers, nanofibers incorporated in the coating) was investigated by means of contact angel measurements. Adhesion of the commercially available coating with and without core-shell nanofibers was measured by performing cross cuts test according to ISO 2409. IR and Raman measurements were performed on PU and PU/oil core-shell nanofibers for comparison. Additionally, electrochemical impedance spectroscopy (EIS) measurements in NaCl solution and open circuit potential measurements were performed to characterize the performance of the core-shell nanofibers against corrosion.

Keywords: Core-shell nanofibers; corrosion; coatings.

Acknowledgements

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Multi-scale Computational Modeling of Flow of Hybrid Composites

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Abstract

Overmolding, or in other words the injection of long fiber thermoplastics (LFT) over a continuous fiber reinforced thermoplastic composite insert, is gaining in popularity. This technology can be applied to both simple and complex parts and is of interest to many of industries and fields of applications such as: automotive, aeronautics and electronics. During the injection step, the fluid pressure may displace or deform the insert. The development of this process is hindered by a lack of numerical simulation solutions to insert position and fiber orientation. This process involves multi-physics coupling (fluid flow, fluid/fluid interaction and heat transfer).

A numerical study is carried out at macroscale to investigate the mechanical interactions between the flowing LFT and the melt composite insert. The focus will be on the predictions of the fiber orientation patterns in 2D/3D geometrical features. The numerical modeling of short fiber suspensions flows requires a description of the micro-structural evolution that can be related to fiber orientation which affects the flow kinematics and that is itself governed by this kinematics. Several approaches have been proposed in the literature to describe the micro-structural state including the use of orientation tensors which requires closure approximation techniques; the novelty of the proposed approach is to describe the fiber orientation state from its probability density whose evolution is described by the Fokker–Planck equation. It is worth to note that the orientation probability density $\phi(\mathbf{x}, \mathbf{p})$ depends on the fiber position $\mathbf{x}$ in a Cartesian coordinate system and the angle of orientation $\mathbf{p}$. As result two kinds of discretization can be looked at separately: angular discretization and spatial discretization. Many angular discretization techniques have been applied to solve similar problems, such as the discrete ordinates method (DOM). This technique is adopted here to discretize over a unit sphere S and capture all possible fiber orientations, while using the finite element method to discretize the fokker-planck equation spatially.

Keywords: Overmolding process, numerical simulation, multiphase flows, fiber suspension, fiber orientation, finite element methods, discrete ordinates methods.

Ammonium Citrate Carbon Dots Naturally Have a High Selectivity to *Helicobacter pylori*

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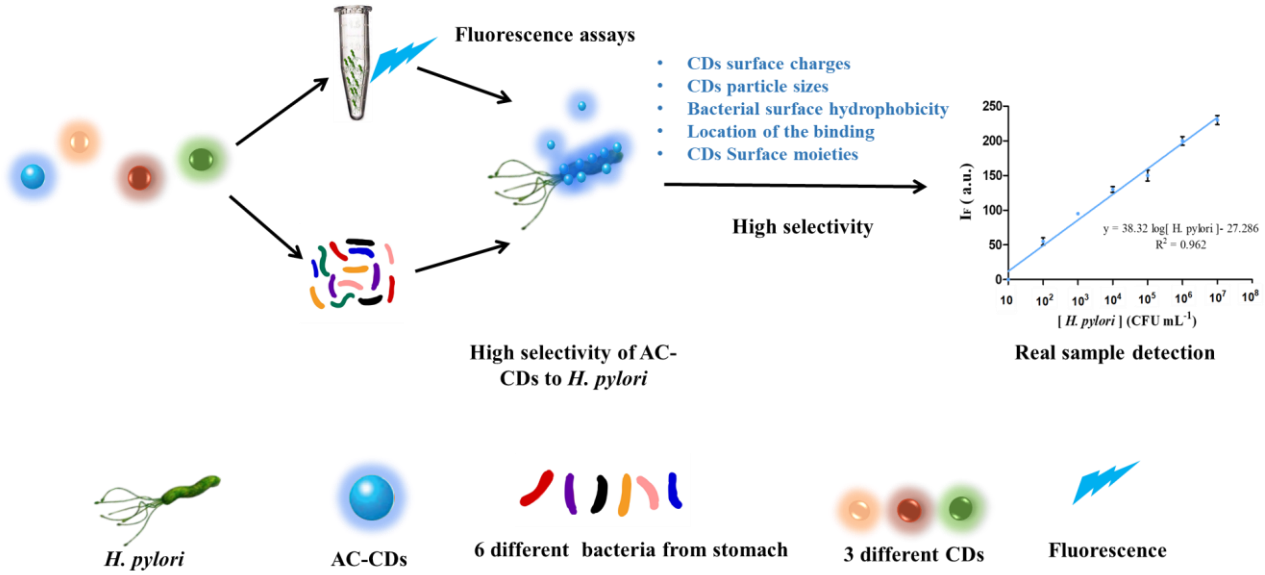
Graphical Abstract



Abstract

Helicobacter pylori is a highly pathogenic bacterium and closely related to various gastric diseases including gastric cancer. Accurate detection of *H. pylori* is very important to reflect the effects of drug administration for medical purposes. In the clinic, the evaluation of *H. pylori* infection is mainly relied on the ^{13}C-urea breath test. However, this test can't be casted on younger children and pregnant women for its radioactivity. Therefore, endeavors are still being made to develop the rapid and precise ex vivo detecting systems for *H. pylori*. Carbon Dots are emerging photoluminescent nanomaterials. However, it has been argued that CDs lack the specificity that will severely limit their medical applications. It is of great significance to discover CDs that naturally have high selectivity to *H. pylori*. Herein, four kinds of CDs, including Ammonium Citrate -CDs (AC-CDs), Citric Acid -CDs (CA-CDs), Glucose -CDs (Glu-CDs) and *H. pylori* -CDs (Hp-CDs) were prepared. It was found that the AC-CDs with a better binding capacity to *H. pylori* is 3 folds of those for the rest CDs. Meanwhile, the binding ability of AC-CDs to each of the seven bacteria isolated from the stomach,

including *H. pylori*, *Escherichia coli, Streptococcus gordonii, StapHylococcus hominis, Shigella dysenteriae, Lactobacillus johnsonii, and Ralstonia pickettii* were compared. The results revealed that the number of AC-CDs bound on *H. pylori* was seven-folds higher than those for the rest bacteria, indicating that the AC-CDs had the highest selectivity to *H. pylori*. Furtherly, we investigated the reasons for the high selectivity. We implemented successive treatments to *H. pylori* cells, which were firstly protease K digestion to *H. pylori* outer membrane protein, subsequently EDTA to remove the outer membrane, and at last, lysozyme to remove peptidoglycan layers. After each step, AC-CDs were incubated with the treated cells and their binding were tested. It was found that the outer membrane proteins of *H. pylori* were likely to be the binding sites of AC-CDs. Furthermore, through the competitive binding experiment for the binding of AC-CDs to *H. pylori* and the Nessler assay, ammonium ions on the surface of AC-CDs were postulated to contribute to the selectivity to H. pylori by AC-CDs. Finally, we explored the detection sensitivity of AC-CDs to *H. pylori*, and found that the detection signal value was still good when the concentration of *H. pylori* was as low as 5 CFU mL^{-1}. This study exclusively reported that AC-CDs spontaneously exhibited a high selectivity to *H. pylori* without pre-tailoring or post-modifications. Unravelling the mechanism of this high selectivity may lead to easy design of CDs that have targeting abilities.

Keywords: *H. pylori*; Carbon Dots, high selectivity.

Acknowledgements

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Thermal Endurance of Swelling Anti-Fire Composites Equipped with Rfid Technology

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Graphical Abstract

Abstract

Passive fire protection is one of the key safety systems which is installed in modern buildings. Its aims are to eliminate or minimize negative influence of expanding fire, spreading smoke and high temperature on people and building itself. To enhance effectiveness of the mentioned fire protection measures it is crucial to use appropriate swelling composites. These composite materials should allow to prevent against fire and smoke spreading for a period of time dependent on a selected fire resistance class. In this paper, such prepared swelling materials used e.g., in intumescent pipe wrap, fire rate intumescent coat, intumescent grille, are presented. The second issue addressed is an identification method of these fire protection after their installation in buildings. In order to verify its presence it is often required to demolish some parts of buildings and after inspection rebuilding. Therefore, it is beneficial to identify them wirelessly with using Radio Frequency Identification (RFID) technique bearing that in mind that selected RFID tags have to exhibit sufficient thermal endurance. The results achieved in this study showed that the designed swelling materials behaved as expected and fulfilled the whole protected space when exposed to high temperature. There were observed small differences in temperature distribution across the tested passive protections. The applied RFID tags showed to be capable to identify the fire protections as well as to withstand high temperature, in particular when a gasket sealant or a high-temperature silicone were utilized for their encapsulation. It was possible to establish communication even after several minutes after their

placement in high temperature. The critical temperature revealed to be about 120°C, but applying higher temperature did not cause total damage of the tags, even in a long term. After a subsequent cooling process of the RFID tags installed into passive fire protections data exchange between reader and tags was restored.

Keywords: Passive fire protection, swelling composites, RFID, pipe collar, intumescent grille.

Acknowledgements

This work was supported by the National Centre for Research and Development, Poland [project's number: POIR.01.01.01-00-0627/15].

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A Versatile Modeling Method in Electromechanics – The Canonical Equivalent Circuit Representation of a Clamped-free Piezoceramic Multilayered Bending Transducer

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Graphical Abstract

$$\frac{d^4\underline{v}(x)}{dx^4} - \omega^2 \frac{\mu}{C}\underline{v}(x) + j\frac{\omega}{C} r_a \underline{v}(x) = j\frac{\omega}{C}\underline{f}(x) \quad (1)$$

$$\underline{v}(x) = \sum_{m=1}^{\infty} X_m(x)\underline{v}_m \quad (2)$$

$$\underline{v}_m\left[\frac{(k_m l)^4}{j\omega n_0} + j\omega m + r\right] = \frac{\int_0^l \underline{f}(x) X_m dx}{\int_0^l X_m^2 dx} \quad (3)$$

$$\begin{pmatrix} \underline{v}_1 \\ \underline{\Omega}_1 \\ \underline{v}_2 \\ \underline{\Omega}_2 \end{pmatrix} = \underbrace{\begin{pmatrix} \underline{h}_{11} & \underline{h}_{12} & \underline{h}_{13} & \underline{h}_{14} \\ \underline{h}_{21} & \underline{h}_{22} & \underline{h}_{23} & \underline{h}_{24} \\ \underline{h}_{31} & \underline{h}_{32} & \underline{h}_{33} & \underline{h}_{34} \\ \underline{h}_{41} & \underline{h}_{42} & \underline{h}_{43} & \underline{h}_{44} \end{pmatrix}}_{\underline{\mathbf{H}}} \cdot \begin{pmatrix} \underline{F}_1 \\ \underline{M}_1 \\ \underline{F}_2 \\ \underline{M}_2 \end{pmatrix} \quad (4)$$

$$\underline{T}_{1,i} = c^E_{11,i}\underline{S}_1 - e_{31,i}\underline{E}_{3,i} \quad (5)$$

$$\underline{D}_{3,i} = \varepsilon^T_{33,i}\underline{E}_{3,i} + d_{31,i}\underline{T}_{1,i}$$

$$\begin{pmatrix} 0 \\ 0 \\ \underline{v}_s \\ \underline{\Omega}_w \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \underline{h}_{33} & \underline{h}_{34} \\ 0 & 0 & \underline{h}_{43} & \underline{h}_{44} \end{pmatrix} \cdot \begin{pmatrix} \underline{F}_1 \\ \underline{M}_1 - \underline{M}_w \\ \underline{F}_s \\ -\underline{M}_w \end{pmatrix} \quad (6)$$

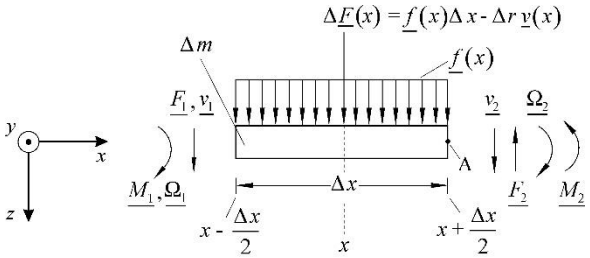

Fig. 1. Differential beam element.

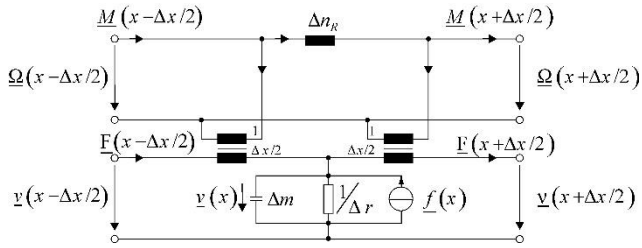

Fig. 2. Equivalent circuit representation of a differential beam element.

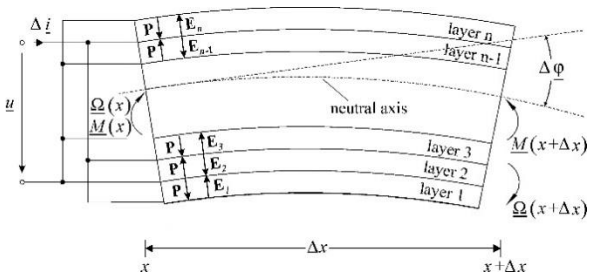

Fig. 3. Piezoceramic multilayered beam segment.

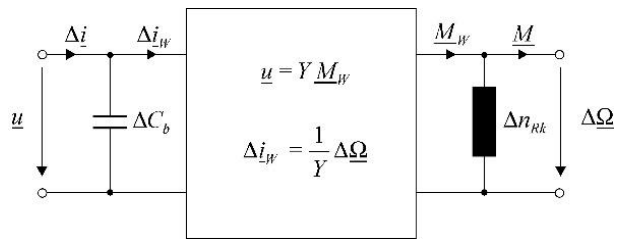

Fig. 4. Equivalent circuit representation of a multilayered piezoceramic beam segment.

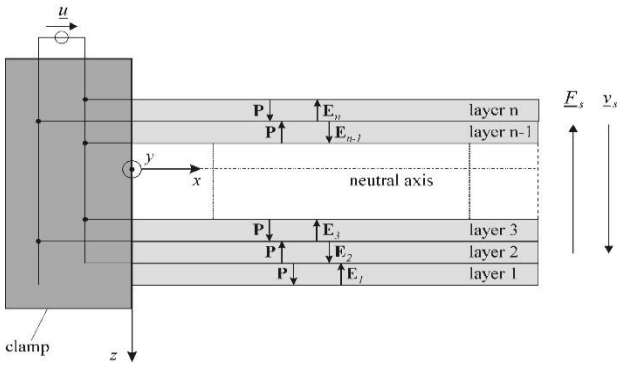

Fig. 5: Clamped-free piezoceramic multilayered transducer**.**

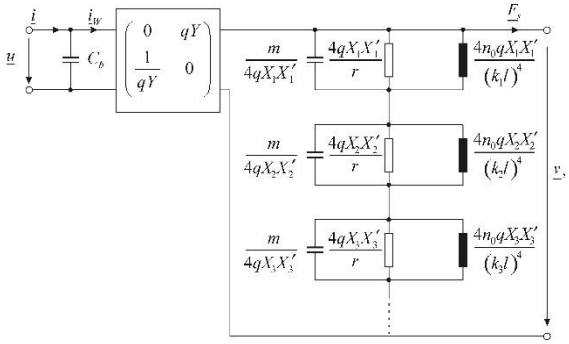

Fig. 6. Canonical equivalent circuit representation of a clamped-free piezoceramic multilayered transducer.

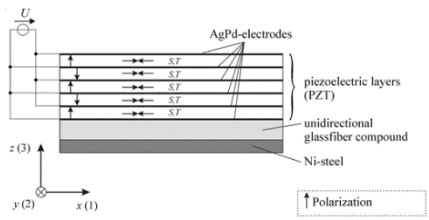

Fig. 7. Used piezoelectric actuator for experimental investigations.

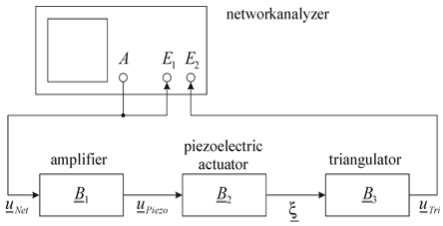

Fig. 8. Measurement setup for the experimental verification of the canonical equivalent circuit.

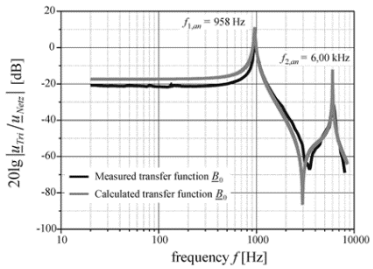

Fig. 9. Measured and calculated transfer function.

Abstract

In this paper the systematic derivation of the equivalent electromechanical circuit for any kind of clamped-free piezoceramic multilayered bending transducer with respect to Rayleigh's dissipation function is presented. In recent publications only bimorphs and triple layer piezoelectric benders have been represented by electrical equivalent circuits assuming a corresponding admittance matrix [**1-4**]. The aspects of the equivalent viscous damping in the sense of Rayleigh's dissipation function and the different vibration modes have not been taken into account yet.

Starting point of the consideration is a differential homogeneous beam element affected at both ends by as well complex-valued translatory quantities (velocity $\underline{v}$, force $\underline{F}$) as rotary quantities (angle velocity $\underline{\Omega}$, Moment $\underline{M}$) represents the starting point of considerations [**Fig. 1**]. In order to determine the dynamic behaviour of the beam element, the mass Δm, the equivalent viscous damping Δr and a continuous load $f(x)$ are taken into account. Assuming that the mass, the friction force and the load can be considered to be concentrated in the middle of the beam element, the inner structure of the differential beam element can be determined [**Fig. 2**]. This structure can also be described by the complex-valued partial differential equation for beam bending movements (eq. 1) where C, ω, μ and r_a represent the flexural rigidity, the angular frequency and the mass and friction per unit length. The solution of the differential equation can be described by an infinite series (eq. 2) where $X_m(x)$ and $\underline{v}_m$ represent the displacement and velocity functions according to the m-th vibration mode [**5**]. The orthogonality properties of the displacement functions result in a general solution (eq. 3) which is the base for the determination of the dynamic admittance matrix $\underline{\mathbf{H}}$ (eq. 4).

In order to proceed to the piezoceramic transducer a multilayered beam segment with piezoelectric layers in bending deformation is considered [**Fig. 3**]. In combination with the piezoelectric constitutive equations (eq. 5) the connection between electrical and mechanical quantities can be described by an electromechanical circuit with two ports [**Fig. 4**] that can be implemented directly into to the equivalent circuit of a differential beam element [**Fig. 2**]. Assuming a piezoceramic multilayered cantilever [**Fig. 5**], the dynamic admittance matrix can be calculated (eq. 6) and the canonical electromechanical circuit representation of a clamped-free piezoceramic multilayered bending transducer can be derived [**Fig. 6**].

For the experimental investigations a specially developed piezoceramic multilayered bending transducer is used [**Fig. 7**]. In order to verify the canonical electromechanical circuit the emphasis is laid on the experimental determination of the dynamic deflection characteristics $\underline{\xi}$ of the bender's tip as a function of the driving voltage $\underline{u}$. The used measurement setup is shown in **Fig. 8**. The measurement results compared to the analytical calculations are shown in **Fig. 9**.

Keywords: Piezoceramic bending actuator; dynamic admittance matrix; canonical equivalent circuit representation; electromechanics; Rayleigh's dissipation function.

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Chloride-Sulfate Exchange Mechanisms in $(LiCl)Al_2(OH)_6$ Type Layered Double Hydroxides

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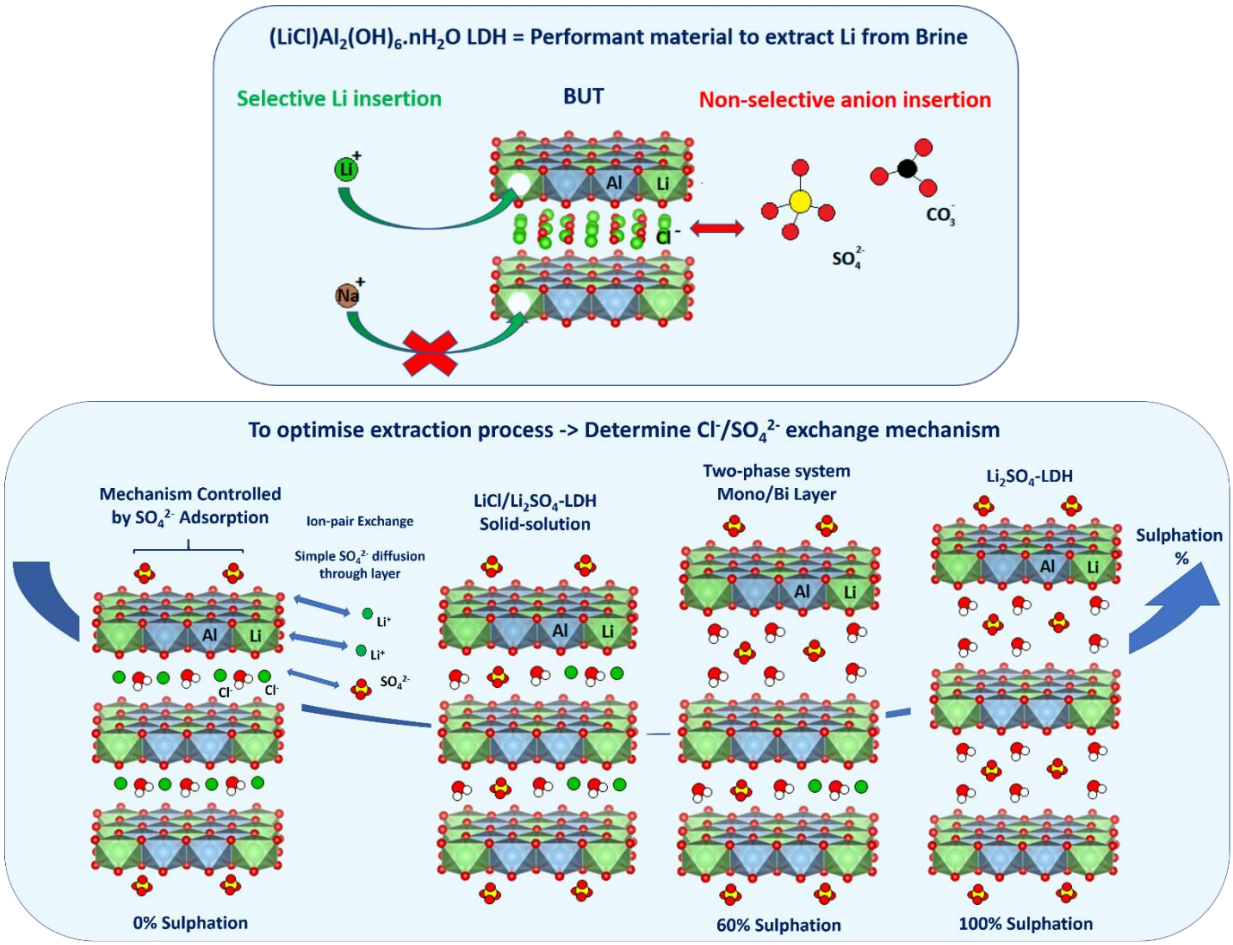
Graphical Abstract



Abstract

The brines of the South American salars are the most important lithium resources in the world. Lithium is most often extracted at industrial scale according to conventional process based on natural evaporation with a high environmental footprint, high quantity of salts precipitation and low overall

performance. Processes based on the selective extraction of lithium by ion exchange are extensively developed as an alternative to the conventional process [**1**]. In particular lithiated aluminium hydroxides, appear as performant functional materials for extracting lithium salts.

While the insertion of lithium is very selective from most of brine cations because it occupies a precise crystallographic site, the insertion of chloride, placed in the hydrated interlayer space, competes with other anions (sulfates, nitrates, carbonates…). The diffusion of lithium is strongly correlated with that of the anion. Understanding the exchange and diffusion mechanisms is therefore essential to optimize the process and adapt it to a wide variety of brines. We present here a study on the exchange of chloride for sulfate in these Li/Al-Cl Layered Double Hydroxides (LDH) one of the impurities present in South American brines. Up to now, only the (de)insertion mechanisms between sulfates and aluminum hydroxides have already been studied [**2**]. However, no studies have been conducted on sulfate exchange in already lithiated aluminum hydroxides.

A mapping of the brine was carried out first to determine the influence of the brine composition on the equilibria starting from Li/Al-Cl LDH, and in particular the influence of $[Li^+]$, $[Cl^-]$ and $[SO_4^{2-}]$. These contents in solution and solid were determined by elemental analysis, and structural analysis of the solid was also performed. Then, in order to get insights on the exchange mechanism, kinetics studies by conductimetry and in-situ infrared spectroscopy were carried out.

There are two trends depending on the $[Cl^-]/[SO_4^{2-}]$ ratio of the brine, defined by the parameter $xSO_4^{2-}{}_{solution} = 2nSO_4^{2-} / (2nSO_4^{2-} + nCl^-)$: for high $[Cl^-]/[SO_4^{2-}]$ ratio ($xSO_4^{2-}{}_{solution}$ <0,08), a sulphate adsorption regime is observed and for low $[Cl^-]/[SO_4^{2-}]$ ratio ($xSO_4^{2-}{}_{solution}$ >0.08), a sulphate insertion regime is then observed.

An accurate analysis of the diffractograms of sulfated materials suggests that sulphate insertion is a continuous process initially carried out without deformation of the material structure (solid solution) until 60% solid sulphation. Then, a two-phase system appears in which the quantity of water inserted increases causing a swelling of the material.

Analyses of sulphation kinetics regards to Avrami-Erofeev [**3**] and Sharp-Hancock models [**4**] show that sulphation mechanism is entirely controlled by the diffusion of the sulfate into the layer which is expected for a hydrated layered material. However, no classical model can explain the diffusion of sulphates in the intersheet. Despite this, empirical sorption models [**5**], often used for the adsorption of pollutants by various materials, can describe sulphation kinetics fairly well. In particular, the Ho & McKay model[5] best describes sulphation kinetics and suggests that the sorption mechanism is controlled by adsorption, which is consistent with the two regimes discussed above.

Keywords: Lithium recovery; layered materials; ion exchange.

Acknowledgements

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Carbon Nanotube Hybrid Fabric – Manufacturing and Applications

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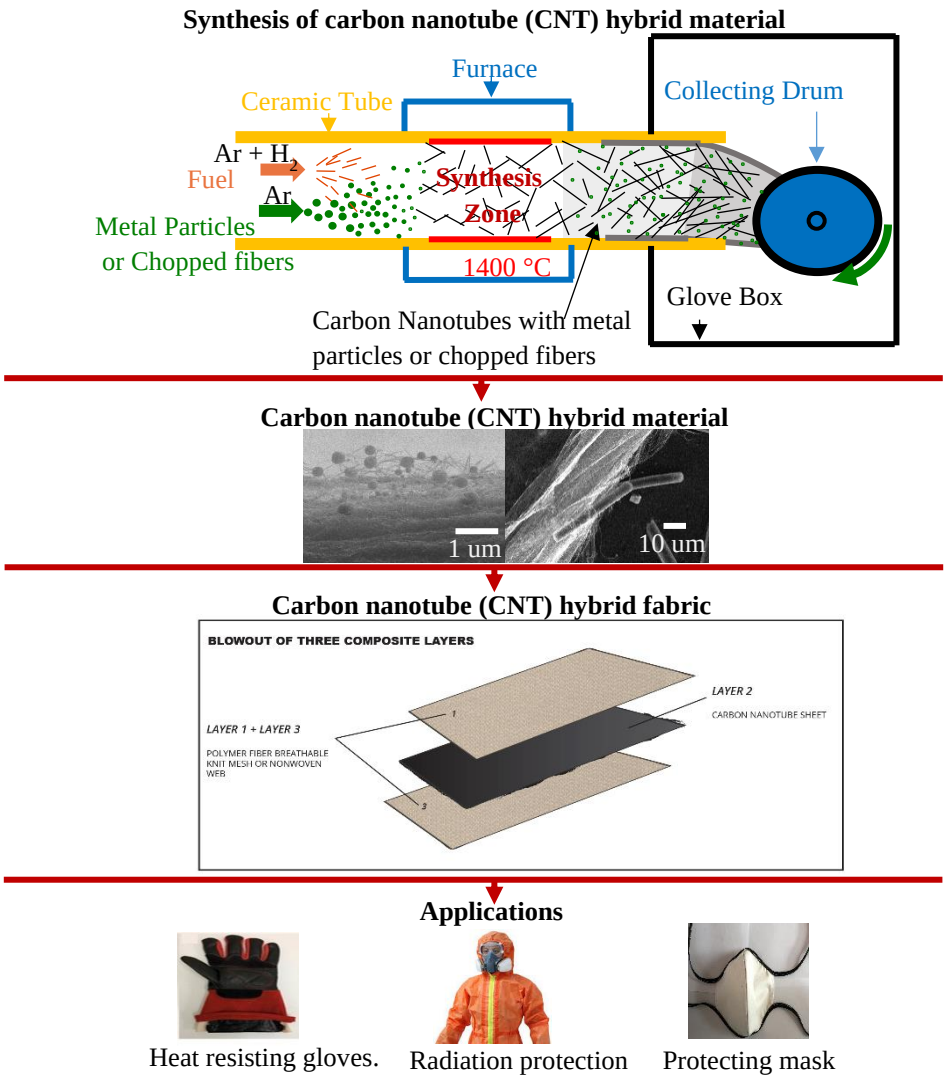
Graphical Abstract



Abstract

Since the discovery of carbon nanotubes (CNTs), they are a vast research field. The extraordinary properties of CNTs have enable to integrate CNTs in supercapacitors, patch antennas, and fibre-reinforced composite applications [**1,2**] , to mention a few among the different industrial, commercial and defence applications. Synthesis of carbon nanotubes (CNTs) by the floating catalyst chemical vapor deposition (FC-CVD) method is apt to meet demands of the growing field of CNT applications [**3,4**], among other CNT synthesis methods. Carbon nanotubes are produced using different synthesis methods and usually have reasonable properties. However, it is very difficult to achieve the extraordinary properties of single wall carbon nanotubes when integrated into macroscopic CNT sheets. To improve their properties in macro-structure form, CNTs can be integrated with other nanoparticles and microfibers which enable them to enhance their properties at the macroscopic level [**5**]. There are different methods to integrate metals into CNT sheet and yarn, such as sputtering, electrolysis, physical vapor deposition, plasma functionalization. All the mentioned methods are two step processes. In this work, we use a single step in situ method to integrate metal and non-metals in CNT sheet. We propose a in situ process of integrating CNTs with nanoparticles (NPs) and microfibers to form CNT hybrid material with new/improved properties and lower cost using the floating catalyst CVD method. Various metal, ceramic, and chemical compounds can be used to synthesis the CNT hybrid material. The nanoparticles or the nanofibers are introduced inside the CNT synthesis reactor with a particle feeder and fuel injector systems. The injected nanoparticles or the nanofibers integrates in the macroscopic web of CNTs right in the reactor during the synthesis process. The synthesized flexible CNT hybrid fabric can be used for clothing, filters, and other textile applications. This paper gives an overview of methods of forming various CNT hybrid materials and discusses several applications.

Keywords: Carbon nanotube (CNT); FC-CVD; CNT-hybrid fabric; Radiation shielding.

Acknowledgements

This research study was supported by the National Institute for Occupational Safety and Health through the Pilot Research Project Training Program of the University of Cincinnati Education and Research Center Grant #T42OH008432.

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Extraction of Polyoxotantalate in basic Medium by Layered Double Hydroxide: Capacity and Mechanism Studies

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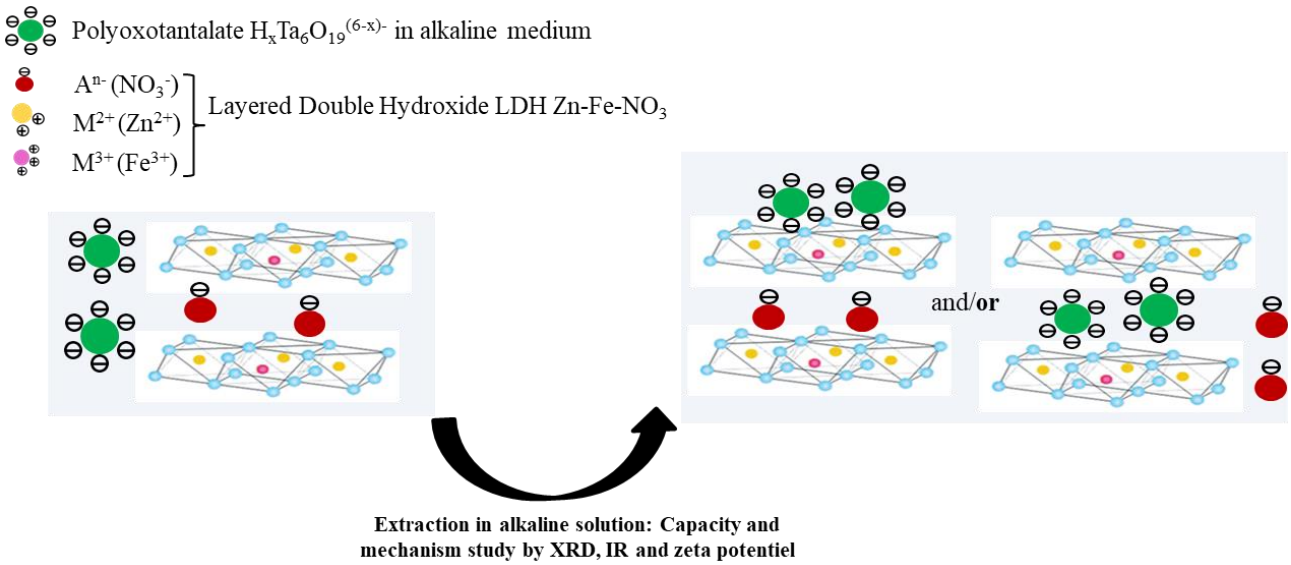
Graphical Abstract



Abstract

Polyoxometallates (POM) are formed mainly by refractory metals (V, Nb, Ta, Mo, W) and are known for their fascinating structures and wide range of applications. Layered Double Hydroxide (LDHs), a class of anions clays, exist as naturally occurring minerals, they are also easy and economical to synthesize. The structure of LDHs is based on positively charged brucite sheets whose charge is balanced by anions intercalated in the hydrated interlayer, leading to the general formula $[M_{1-x}^{2+}\ M_x^{3+}(OH)_2]^{x+}(A^{n-})_{x/n}.mH_2O$.

A strong interaction between POMs and LDHs is expected, due to the very high negative charge of POMs, favourable to their insertion between the positively charged layers. Nevertheless, other reactions have been observed, such as their adsorption on the surface of the particles [**1-3**]. The extraction of POMs from V, Mo and W by LDHs has been widely studied in the literature but to date no studies have been done for Tantalum. Ta(V) is a critical metal soluble as POM of hexatantale

species ($H_xTa_6O_{19}^{(6-x)-}$) in alkaline solutions [**4**] and a new extraction processes from electronic waste or ores could be developed using LDHs. Thus, the aim of this study is to investigate the feasibility of extraction/desextraction of polyoxotantalates by LDH Zn-Fe-NO_3, to highlight the different influential parameters, and to identify the extraction mechanism(s) based on structural characterizations.

Keywords: Layered double hydroxide; polyoxotantalates; sorption capacity, mechanism study.

Acknowledgements

PSL Valorisation is thanked for the funding of the project Lix_LDH.

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New Titanium-composite Bipolar Plate Material for Electrolyzer

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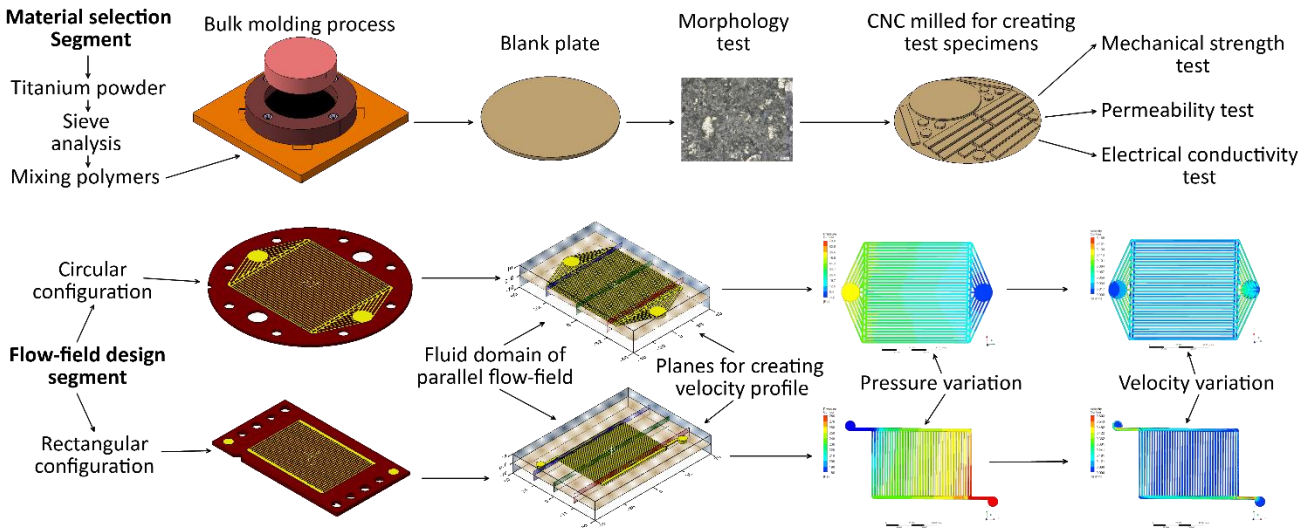

Abstract

Motivation: Alternative sustainable energy generation seem to be a promising approach to tackle the present carbon gas emission problem. However, investigations shows that the electricity generated from renewable energy sources is extremely fluctuating to satisfy the demand. Therefore, a storage system has to be developed by converting electrical energy to chemical energy in the form of hydrogen, as it possesses higher potential to store energy in large megawatt scale [**1**]. Hydrogen can be produced from renewable sources through the process of electrolysis and as a result labelled as green hydrogen. But its contribution is very negligible due to high cost of production. To make it competitive, the electricity cost from renewable sources and the material cost of the electrolyzer system itself have to be reduced. There are different electrolyzer technologies available, but this study emphasis on low temperature proton exchange membrane electrolyzer as it is regarded as a significant competitor. Thus, focusing particularly on the selection of bipolar plate material and flow-field design while they account for 30 % of the total cost of the stack [**2**].

Material selection: There are various bipolar plate materials available, among them, composite materials have obtained favourable attention as they can incorporate the advantages of its individual materials and consequently improve the performance. Investigations were carried out on conductive titanium powders, categorised from type 1 to type 6 based on their grain sizes and shapes, along with different polymers like thermoplastic - polyvinylidene fluoride (PVDF) and thermosetting plastic - epoxy resin to produce twelve different types of composite plates, each in the ratio: 78 wt.% metal and 22 wt.% polymers. Here, the categorisation of the titanium powders was done via sieve analysis. The composite plates were manufactured using bulk molding process and later milled to required dimension using computerised numerical control machining. Subsequently, these composite plates were subjected to morphology, mechanical strength, permeability and electrical conductivity analysis to determine compatibility with US Department of Energy norms. From the analysis, it was observed that the titanium powders having grain sizes ranging between 0-150 µm with uniform grain shape showed reliable results along with PVDF as they either satisfied the US DOE norms as in case of mechanical bending test or were very close to the targeted values with reference to permeability or electrical conductivity [**3,4**].

Flow-field design: Numerical simulation were carried out by employing four types of flow-field designs, namely parallel, pin-flow, serpentine and broken serpentine to study the influence of the different inlet and outlet manifolds in two types of bipolar plate configurations such as rectangular and circular. The output of the numerical simulation revealed that the velocity profile and the pressure drop in the rectangular configuration were non-uniform due to the diagonal flow profile observed across the inlet and outlet manifold. Whereas in circular configuration because of proper positioning of the manifolds, especially with parallel and serpentine flow-field design, more consistent flow profile was witnessed. Eventually, making it a promising design for bipolar plate [**5**].

Keywords: Electrolyzer; composite material; titanium; PVDF; epoxy resin.

Acknowledgements

This work was supported by Department of Fuel Cell Research and Development laboratory of Eisenhuth GmbH & Co.KG.

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Oxime-Functionalized Nanodiamonds as A Platform for Treatment of Organophosphate Poisoning

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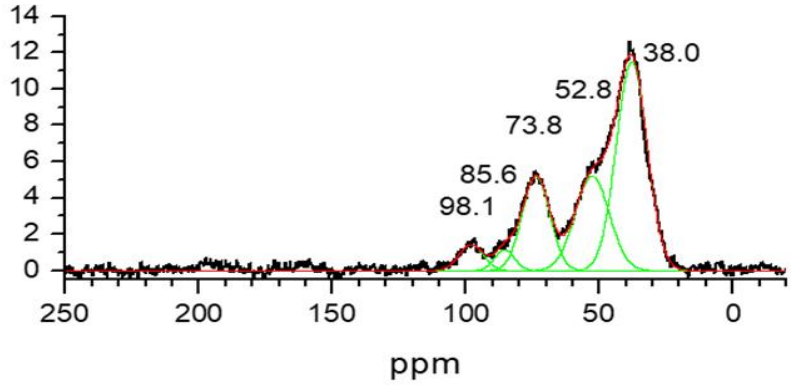

Fig. The ^{13}C MAS NMR spectrum of the starting Nanodiamonds.

Abstract

Nanoscience drastically changed our classical understanding of chemistry, biology, physics, and molecular interactions, allows us to try new pathways for drug delivery and use of bioactive compounds for nanomedicine.

In recent years, different carbon nanoparticles (CNP) were used for biomedical applications [**1**]. They were studied as a potential treatment, as well as a drug delivery platform. In this study, we used the nanodiamonds (NDs) which showed the least toxicity amongst other CNP [**2**]. The nanopowder made of ca. 5nm diamond particles with large accessible surface and tailorable surface chemistry shows extraordinary optical, mechanical, electronic, and thermal properties on the nanoscale. Inert and biocompatible NDs could be used in nanomedicine and biotechnology to improve the therapeutic value of various drugs [**3**]. The coating of drugs on NDs increases their bioavailability, solubility, retention time, efficacy, tolerability, and drug therapeutic index [**1**].

We tried to design the most beneficial method of the preparation of drug-coated harmless NDs for treatment of organophosphate poisoning. Developing potent antidotes towards acetylcholinesterase (ACHE) inhibited by OP in the central nervous system remains a challenging task. The pre-treated detonated NDs bear carboxylic groups on their surface. This allowed us to perform coating using traditional methods of organic synthesis. Continuing our previous work on design of oxime-functionalized

reactivators [**4**], we synthesized several bioactive compounds and purified them, followed by attaching/coating on NDs' surface. The modified NDs were studied by different techniques (ssNMR, FTIR, DLS, SEM) and tested in the collaborator's biomedical laboratories for reactivity towards inhibited ACHE and toxicity screening against the mammalian cells. Its permeability across the blood-brain barrier was carefully investigated.

Acknowledgements

This research is partially supported by NATO SPS MYP G5565.

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One Step Synthesis of High-Quality Carbon Nanofabric

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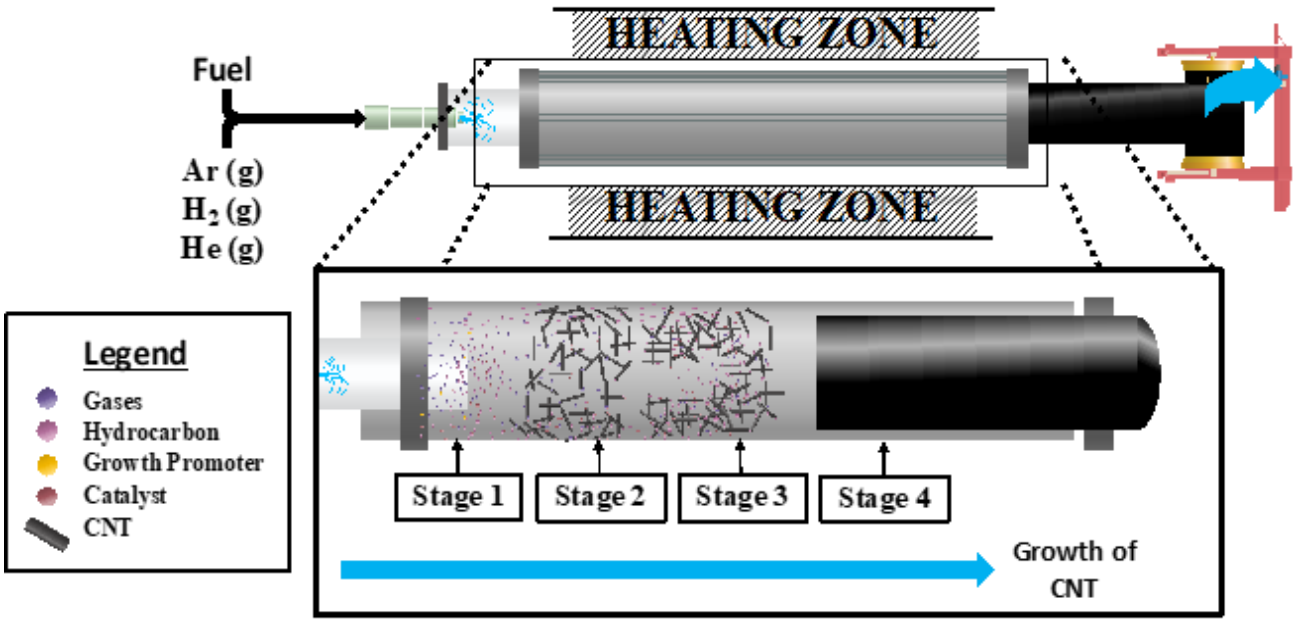
Graphical Abstract



Abstract

In recent years, with the emerging market and awareness of nanotechnology, the demand for high quality carbon nanotubes (CNTs) in industry has increased. Generally, the appearance of the radial breathing mode (RBM) and high G/D ratio is an indication of graphitic carbon. To reduce the amount of amorphous carbon, understanding and controlling the parameters in the pyrolysis method is fundamental to producing high quality macroproducts. In this study, an aerosol injection containing ferrocene, as a catalytic precursor, is used to continuously grow CNTs that can be wounded into nanofabric. The quality and morphology of the samples were analyzed by Raman spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). Characterization analysis revealed extremely high G/D ratio of about 100, majority single-walled, and uniform diameter were produced at 1400°C compared with traditional methods. The high quality may be attributed to the following factors: (i) Improved aerosol

nebulization of the iron/sulfur particles; (ii) Pre-conditioning the fuel/gas mixture entering the reactor; (iii) High temperature synthesis at 1400°C; and (iv) Short growth time.

Keywords: Chemical Vapor Deposition (CVD); carbon hybrid nanofabric; synthesis.

Acknowledgements

This research study was supported by the National Institute for Occupational Safety and Health (NIOSH) through the University of Cincinnati Education Research Center (ERC) Grant #T42OH008432 (Pilot Research Project Training Program and Occupational Safety Health Engineering Fellowship). It was, also, broadly supported by ONR Award #N00014-15-1-2473 and I-Corps@Ohio 2017 Cohort.

Study of the Aging of Lithium-ion Coin Cells with Impedance and Noise Measurements

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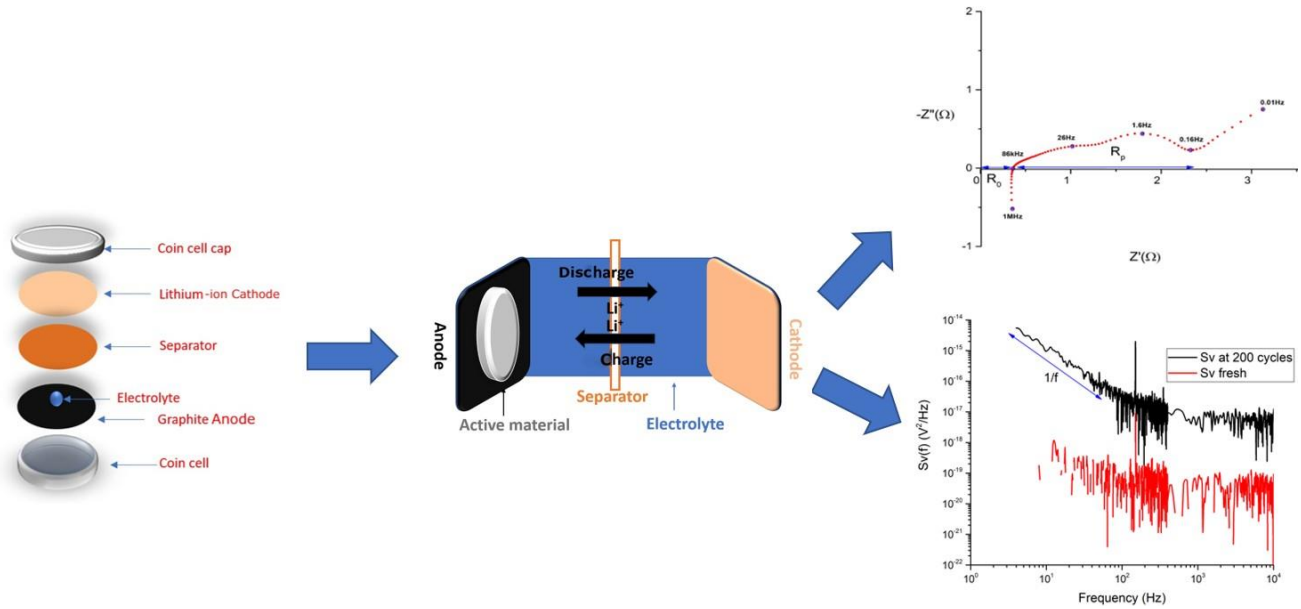

Abstract

The growth of the electrochemical power sources expects new techniques for estimating batteries state of health (SOH) and state of charge (SOC). Thus, a new approachable technology is developed like the electrochemical noise (ECN) measurement [**1**]. In this work, we study the aging of commercial lithium-ion coin cells by performing successive cycles of charging and discharging until the depletion of the battery. We perform different duration of discharging (and charging): short (30mins), average (2h) and long (20h). Electrochemical noise and impedance measurements have been carried out at each cycle number in wide range of frequency typically from 0.01 Hz to 1 MHz. In the context of this work, we notice that the aging leads to a strong increase of the resistance R_p and not in the resistance R_0 and to the capacity fade that tends towards 0 when the battery is out of order. In addition, the levels of the noise measurements in low frequencies in $1/f^{\gamma}$ ($1<\gamma<2$) increase with the evolution of cycle numbers. However, we observe the decrease of noise level with the decrease of SOC values.

Keywords: Lithium-ion, battery, cycles, impedance, noise, electrochemical reactions.

Acknowledgements

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Experimental and Numerical Identification of Frictional Effects in Mode II Delamination of Composites

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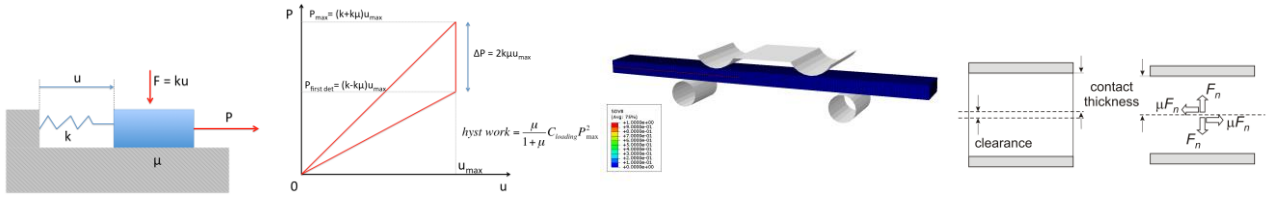
Graphical Abstract



(a) (b) (c) (d)

(a) Simplified Model, (b) Response with hysteresis, (c) Non linear Finite Element Model, (d) Modelling of the contact with friction

Abstract

Mode II delamination propagation is one of the most common mechanisms for the development of interlaminar damage in realistic load conditions. Despite the advantages of the 4-point ENF test for the characterization of this phenomenon, like the stable propagation of the crack, its use is still not widespread. This is mainly due to the effect of friction between the faces of the crack, which leads to a not reliable estimation of the interlaminar toughness [**1**]. In this work a method is proposed to take into account for the effect of the friction in 4 point ENF test. The approach is based on the measurement of the friction effect by means of some hysteresis cycles performed by loading and unloading the specimen without propagating the crack. Initially, a hysteresis function is defined by analyzing a simplified form of the problem. Thereafter, a general form of the function is provided, which depends on the specimen compliance, *C(a)*, and on a set of coefficients that must be evaluated by fitting the experimental results, as shown in the following equation:

$$f_{hysteresis} = C(a)\left(k_1 P_{\max}^2 + k_2 P_{\max}\right)$$

Once calibrated, the function quantifies the energy dissipated by frictional forces and is inserted as a dissipation energy term in the energetic balance, so to correct the apparent interlaminar toughness evaluated by means of conventional data reduction schemes.

The method is applied to experiments on composite unidirectional specimens and the results are interpreted by developing detailed Finite Element Model of the tests, where the contact between the two sliding surfaces is modelled and the interlaminar toughness is represented by means of finite thickness elements implementing a Cohesive Zone Model [**2**]. A comparison of the results is carried out also by means of analytical models present in the literature [**3**], which requires in advance the measure of the friction coefficient. The results indicate that the method represents an efficient tool to evaluate directly the effect of the friction during a 4-point ENF tests, without requiring the knowledge of the surface properties.

Keywords: Composite delamination; friction; ENF test; interlaminar toughness; characterization.

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Biography of Presenting Author

Pietro Ballarin awarded his Master Degree in Aeronautical Engineering in 2019 at Politecnico di Milano. His PhD in Aerospace Engineering started in November 2020 and it is in cooperation with the Department of Management Engineering of Politecnico di Milano. His main research topic is the impact assessment of Structural Health Monitoring systems on the lifecycle of aerospace composite structures. Other research fields of Pietro Ballarin are the Morphing Structures and Composite Materials.

Nanopapers based on Lignocellulose Nanofibers and their Potential use in Water Treatment Contaminated with Metal Cations

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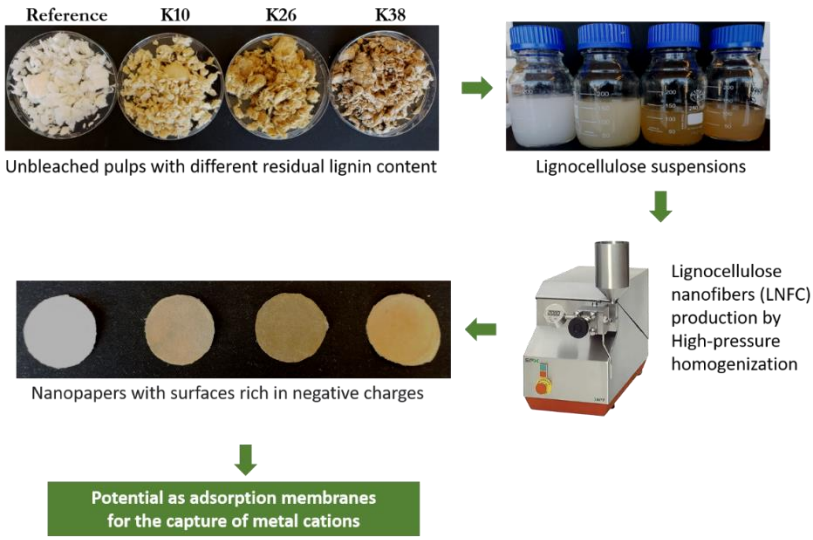
Graphical Abstract



Abstract

The lignocellulose nanofibers (LCNF) differ from cellulose nanofibers (CNF) by presenting lignin and hemicellulose residual contents on their surface [**1**]. Recent studies have reported the use of LCNF in the nanopapers production. These nanopapers are characterized by having a greater specific surface area and more homogeneous pore diameters [**2**], desirable characteristics in adsorption membranes. Lignin is a phenolic polymer with a three-dimensional structure present in wood, whose content is 20-40%. This polymer presents a complex structure composed of randomly linked non-linear phenylpropane units, rich in hydroxyl and hydrophilic carboxy groups exhibiting ion adsorption capacity metallic [**3**]. In this way, the richness of functional groups presents in lignin and thus also in hemicellulose, allows us to suggest that nanopapers based on LCNF will present better adsorption capacity for metal cations than nanopapers based on CNF.

In this work, the LCNF production was carried out from unbleached pulp with different contents of residual lignin and hemicellulose. The fibrillation process used corresponded to high-pressure homogenization, whose working conditions were 500 bar and 10 steps.

To the studying the physical properties of the membranes it was possible to observe the decrease in thickness, lower grammages, increased bulk density and reduced membrane porosity as the residual lignin and hemicellulose content is higher. The presence of residual lignin and hemicellulose was evident in the spectra FTIR obtained for the K26 and K38 membranes, where 3 characteristic signals of the residual lignin and hemicellulose.

Through SEM microscopy it was possible to observe clear differences in the morphology of the membranes manufactured. As the residual lignin and hemicellulose content increases, it becomes more difficult look at cellulose fibers, this is because lignin forms a type of matrix in which the cellulose fibers are embedded (this has been reported in other studies). In addition, the results obtained by SEM showed a decrease in both fiber and pore size as lignin and hemicellulose content increases residual, highlighting the membranes obtained from K26, where a distribution of quite narrow pore size. This is of great relevance, since it can be suggested that the presence of residual lignin and hemicellulose allow to obtain a homogeneous pore size (38nm), being able to infer that its presence allows to control this parameter, which is very difficult to control when manufacturing NFC-based nanopapers. This constitutes one of the main disadvantages of CNF-based membranes for water treatment.

Finally, by studying the magnitude of the surface electrical charges (**Fig. 1**) of the fabricated membranes it was possible to infer that the K26 membrane could act as a membrane adsorption for water treatment, as it is expected to present a surface rich in negative charges capable of capturing cations, such as Cu^{2+} by electrostatic attraction. I know concludes that non-delignified / bleached cellulose pulps are an excellent material raw material for the manufacture of absorption membranes.

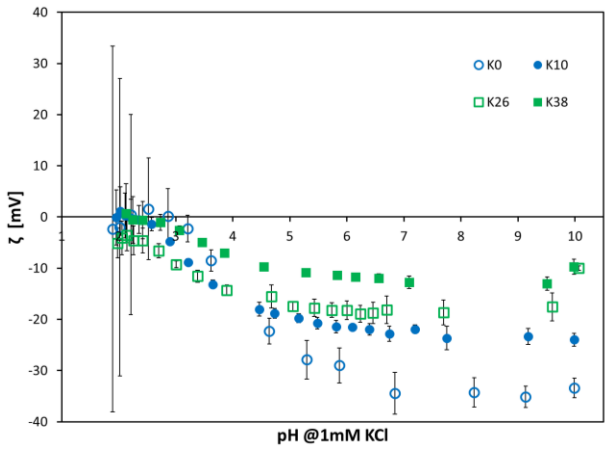


Fig. 1. Transmission of zeta potential (ζ) as a function of pH for manufactured nanopapers.

Keywords: LCNF; nanopaper; high-pressure homogenization.

Acknowledgements

Agencia Nacional de Investigación y Desarrollo (ANID)

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Measurement of Material Levels Inside a Silo using a Hotspot Detector and Artificial Neural Network and Optimization of Measurement Points using Genetic Algorithm

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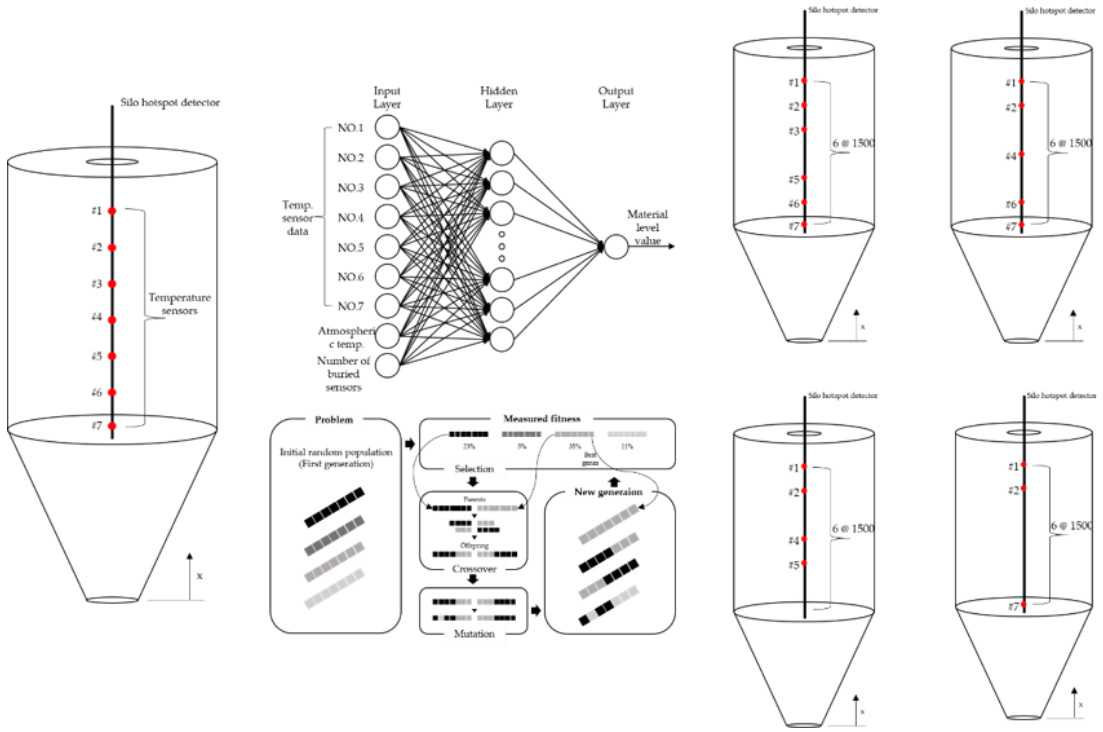
Graphical Abstract



Abstract

Resources such as coal, biomass, etc. are essential energy sources in modern society. These essential energy sources are stored in a silo structure and used as much as needed to efficiently consume resources. To this end, the amount of resources stored in silos must be accurately predicted and managed. In order to manage the amount of stored resources, height of internal resources is typically measured and managed, and methods used to do so include guided wave radar (GWR), laser meters, load cells, and thru-air radar (TAR). However, these methods are not applicable due to internal silo

dust problems and silo-largement, or are economically inefficient even if they are applied. To address this, this work utilizes silo hotspot detector, a detector that monitors silo internal temperature. Analyzing the temperature data measured by the detector confirmed that the temperature distribution was bounded, which was related to the height of the material. However, simply dividing them and determining the height of the material often leads to large errors. To overcome this, we apply an artificial neural network (ANN), which has the advantage of accurately predicting the relationship between data of nonlinear relationships with algorithms depicting the human brain. We compare the predicted results with the ground truth and confirm that we show an accuracy of 97%. Furthermore, we combine the ANN model with the generic algorithm (GA), an optimization algorithm that mimics the natural evolutionary principles of living organisms, to optimize the silo internal temperature measurement position and number of predictive accuracy improvements. As a result, the error was reduced by approximately 50%, and we found that it was sufficiently predictable even if the number of temperature measurement points decreased from 7 points to 4 or 5 points. These findings can be utilized to build systems that enable silo internal temperature monitoring and internal material level management economically and efficiently.

Keywords: Silo hotspot detector; temperature measurement; artificial neural network; genetic algorithm.

Acknowledgements

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Development and Production of Organic-Inorganic Nano Composite Coating Materials

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Fraunhofer IKTS Hermsdorf develops sol-gel materials for several decades. At the beginning inorganic sols were used to develop and produce inorganic separation membranes. For about 20 years the experience in sol-gel technology is used to develop and produce the so called nanocomposites. Application areas are scratch and corrosion resistant coatings, non-stick coatings even for elevated temperatures, the unique PLASMAGEL coatings. Up to 10 tons per year of liquid coating material for the protection of concrete and natural stone were produced. The lecture shows the general chemistry and some “tricks” that were necessary to obtain the required quality. Using different building blocks with more than one functional group tailor made materials are possible.

Electrospun Fibers as a Support for Oxidoreductase Immobilization: Improving Stability of the Produced Biocatalysts

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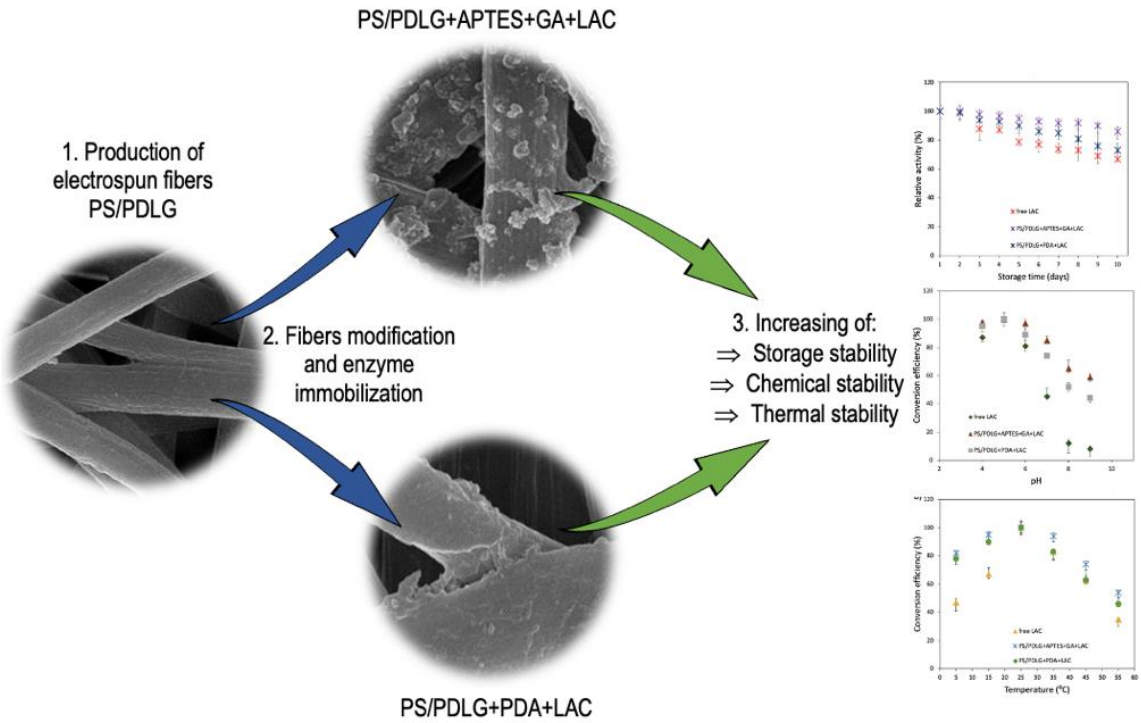
Graphical Abstract



Abstract

Immobilized enzymes are applied in various areas such as food production, pharmacy, medicine and even environmental protection. However new materials predestined to be supports for enzyme immobilization are still being sought. Supports, which are widely described in recently published studies, include mainly metal oxides, silicas or activated carbons [**1,2**]. These materials despite their

advantages, possess limitation, for example insufficient inner surface area or lack of specific functional moieties, which could affect enzyme immobilization and final catalytic activity [**3**]. Therefore, the properly selected support and type of surface's modifier seem to be the best way to obtain biocatalysts characterized by relatively good catalytic activity in various reaction conditions. In our work we proposed production of electrospun fibers from polystyrene/poly(D,L-lactide-*co*-glycolide) as a support for oxidoreductase immobilization by covalent binding using (3-aminopropyl) triethoxysilane/glutaraldehyde (APTES/GA) and polydopamine (PDA), separately, as surface modifiers. The fabricated PS/PDLG fibers, before and after enzyme attachment were characterized in terms of the presence of specific functional moieties on their surface and their porosity. Moreover, the catalytic activity of the biocatalyst was measured after 10 storage days and at various values of pH and temperature. It could be seen that laccase, regardless of its form, possessed the highest catalytic activity at pH 5 and 25 °C. Moreover, that system PS/PDLG+APTES+GA+LAC possessed the highest catalytic activities at various process conditions, compared to the native biomolecule and laccase immobilized onto electrospun fibers using PDA as a linker. PS/PDLG+APTES+GA+laccase showed 86% of its initial catalytic activity after 10 days of storage, whereas biomolecule immobilized onto the system PS/PDLG+PDA and its free form possessed 73% and 67% its catalytic activity, respectively. The obtained results showed that produced electrospun material PS/PDLG can find application as a support for enzyme immobilization. Comparison of two approaches of laccase immobilization allows to choose the best way of enzyme attachment to the electrospun support. However, it is still necessary to continue this research by evaluation of reusability of immobilized laccase and application of the produced biosystem in real reactions, such as degradation of phenolic pollutants from wastewaters.

Keywords: Electrospinning; enzyme immobilization; catalytic stability and stability.

Acknowledgements

This research was supported by the Polish National Agency for Academic Exchange, the Iwanowska Programme.

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A Novel Graphene Base Heterojunction Transistor with Saturated Output Current

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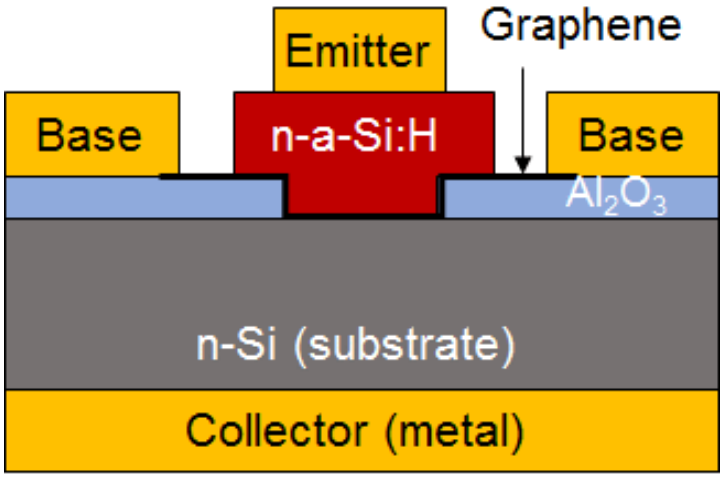
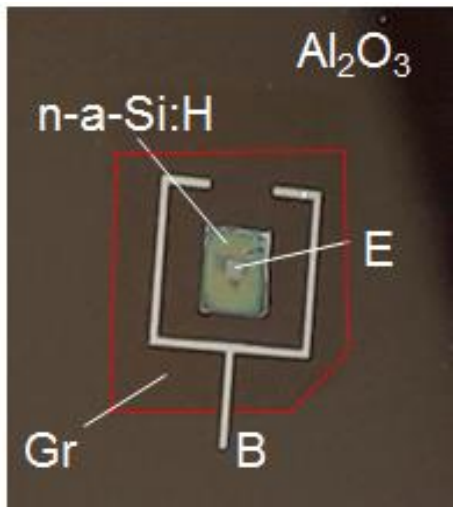
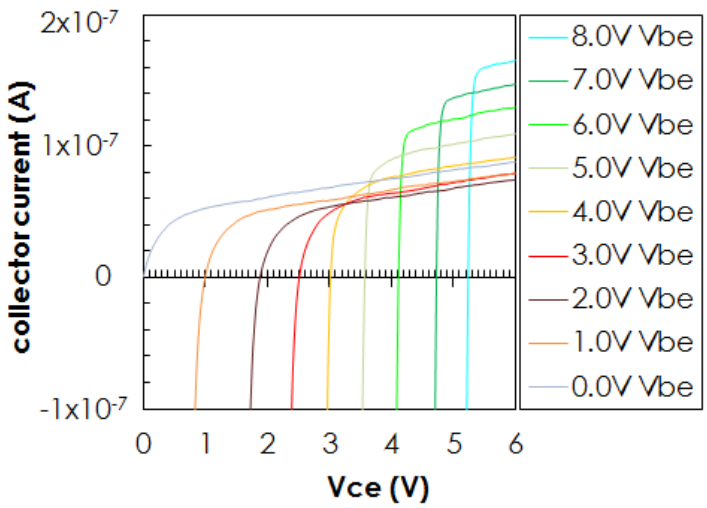
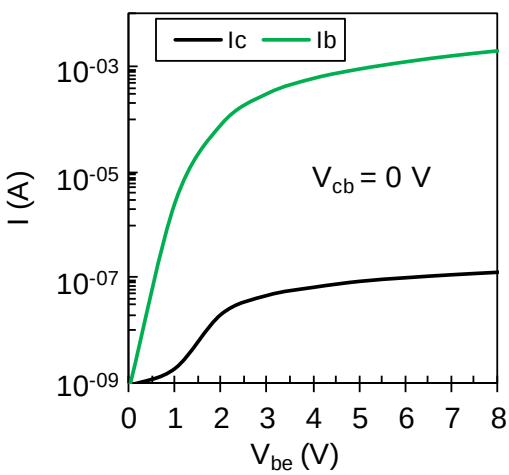
Graphical Abstract









Abstract

The graphene-base heterojunction transistor (GBHT [**1**], see Fig. above) is an attractive device concept to reach THz operation frequencies. The novel transistor consists of two n-doped silicon layers with a graphene monolayer in between. The structure of the device is similar to an n-p-n bipolar transistor with the base being replaced by graphene. This innovative concept exhibits a vertical arrangement of the emitter (E), base (B) and collector (C). Due to the very low base-transit time the device potentially allows for very high cut-off frequencies (f_T). Only recently, first attempts were made to put the GBHT into practice by means of amorphous silicon emitter and collector layers [**2**]. Here we demonstrate improved device performance with current saturation in the transistor's output characteristics. A clear modulation of the collector current by the applied graphene base voltage can be observed (see Figure above). The vertical transfer current from the emitter via graphene to the collector is much lower than expected from device simulations. A comparison of the graphene-base transistor and a reference silicon n-p-n bipolar transistor is performed with respect to the main DC transistor characteristics. A common-emitter gain of larger than one has been achieved for the reference device while the graphene-base transistor so far exhibits a much lower gain.

Limitations of the GBHT technology and optimization routes to improve gain of the GBHT will be discussed (e.g., permeable base transistor design, alternative 2D base materials, high-low work function materials for the emitter and collector semiconductor etc.). Especially, the permeable base transistor design seems promising and is realized by nanoimprint lithography.

Keywords: Graphene; heterojunction; transistor; current saturation.

Acknowledgements

Financial support by the German Research Foundation in the framework of the Priority Program SPP FFlexCom (BA 2009/6-1 and WE 3594/5-1) is gratefully acknowledged.

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IAAM Committment to High Quality Collaborative R&I

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Graphical Abstract

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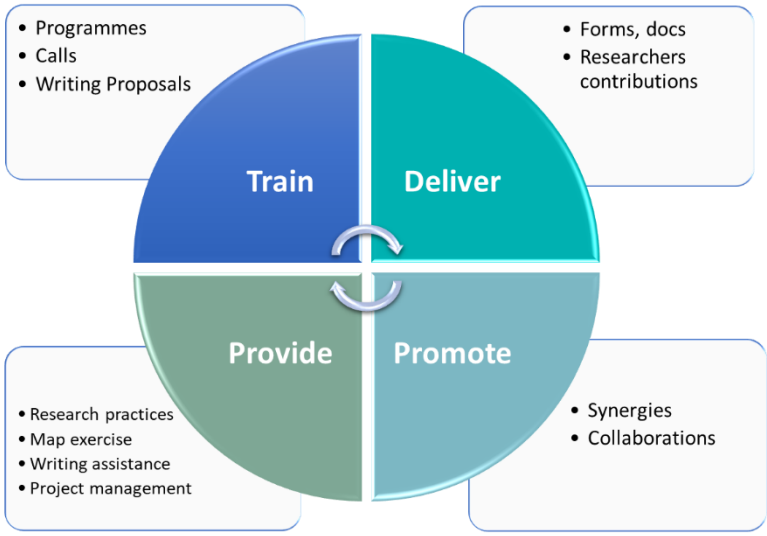

Abstract

Institute of Advanced Materials works in different fields and offers a wide range of services to support businesses and solve challenges that the business communities around the world face right now. Our services like global consultancy, Research & Development, Industrial Training, Technology Transfer, and innovations are targeted to help our clients enhance their business process and improve. Our Work Primarily Spans Over Three Major Areas: Energy, Environment, and Health.

IAAM is committed to high quality collaborative research and innovation that deliver advanced materials and technologies. Its scientific knowledge, extensive research experience, immense network, and effective project coordination and support mechanism enhance participation in R&I programmes and foster close partnerships across the globe. It elaborates dedicated services and promotion mechanism of researchers and consortium members, while synchronizing its policy with EU and UN towards cutting-edge safe, effective and green products through various technology readiness levels. It also boosts success rate in proposals, management and outputs of projects.

Keywords: Advanced materials, consortium, research, innovation, collaboration.

Smart Piezoelectric Scaffold for Nerve Regeneration

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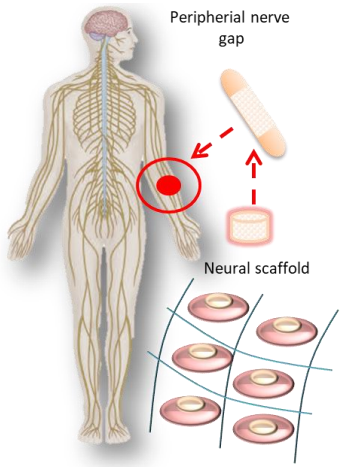

Schematic representation of the application of tissue engineered nerve graft in repairing injured peripheral nerve.

Abstract

As regards the field of biomedical engineering, in recent decades, there may be observed an increasing scientific and technical interest in research related to the development of Smart Materials (SM). Such materials are generally designed to react in response to external stimuli (physical, chemical, mechanical), behaving similarly to natural body tissues. One important type of such SMs is a piezoelectric scaffold, which can generate electrical signals in response to the applied stress [**1,2**]. This research aims to efficiently support the re-growth and reconstruction of the diseased or damaged tissues by designing a three-dimensional smart scaffold, which is essential from the perspective of society in terms of treating spinal cord injuries, degenerative brain diseases, etc. The overall objective is devoted to designing and developing of a novel smart piezoelectric scaffold belonging to the type of conducting and stimuli-responsive scaffolds dedicated to neural engineering applications. The smart scaffold will significantly improve the effectiveness and safety of the medical nerve reconstruction procedures [**3,4**]

Polyvinylidene fluoride (PVDF, Mw = 530 000 g/mol) nanofibers were electrospun from 15% solution of dimethylformamide and acetone (DMF/Ac 4:1 weight ratio) at feed rate 0.2 mL/h (3 mm needle) and collected on drum collector (diameter 40 mm) at a distance between the needle and collector 180 mm. Human adipose-derived stromal cells (ADSCs) were cultured in osteogenic medium on the piezoelectric PVDF scaffolds electrospun with different collector rotational speed

(200, 1000 and 2000 rpm) and subjected to ultrasound stimulation (power 80 mW, frequency 1.7 MHz) for 30 minutes every 24 hours. ADSCs seeded on piezoelectric PVDF scaffolds without ultrasonic stimulation were used as a control for each group. In order to confirm the piezoelectric effect on ADSCs viability, PrestoBlue cell viability test was performed on day 3, 14 and 21. Results were statistically analyzed using the Student's t-test. The observations of fibres and cell morphology were conducted using Scanning Electron Microscopy (SEM), Fourier-transform Infrared Spectroscopy (FTIR) and Differential Scanning Calorimetry (DSC).

PVDF nonwovens as piezoelectric polymers stimulated by ultrasounds are advantageous for cells viability. The obtained preliminary results are promising from the perspective of tissue engineering applications.

Keywords: Piezo-nerve; scaffold, nanofibers; tissue engineering; stem cells.

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Fragmentation of Bioactive Electrospun PLLA Fibers

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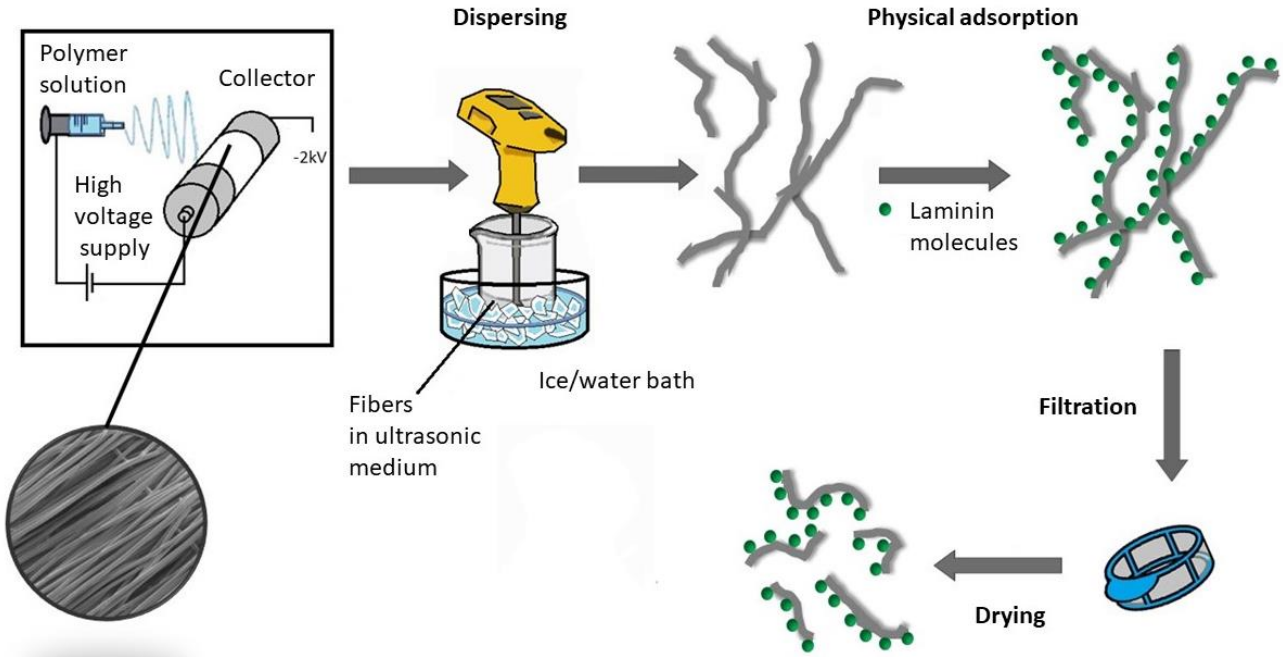
Graphical Abstract



Abstract

The aim of this research was obtaining short electrospun nanofibers which in future studies could serve as a supportive and bioactive component loaded into the hydrogel system. A poly(l-lactide) acid (PLLA) is biocompatible and characterizes relative brittleness, which enables effective mechanical fragmentation [**1**]. In these studies, PLLA nanofibers were fragmented using ultrasonication, which effectiveness was thoroughly studied and optimized. Such parameters as the type of sonication medium, processing time, and various PLLA molecular weights were investigated. A post-fragmentation of short fibers was carried out to narrow down the nanofibers length distribution. Additionally, short PLLA nanofibers were modified with laminin by physical adsorption. That functionalization allowed to overcome hydrophilicity and biochemical inertia of PLLA, providing IKVAV (Ile-Lys-Val-Ala-Val) effective sites for cell adhesion [**2,3,4**]. Laminin, as one of the ECM components, contains protein receptors, which are decent especially from the

perspective of neural cells. In this regards especially important is the IKVAV sequence, responsible for effective neuron differentiation [**2**]. This protein is essential especially for nerve regeneration - it effectively binds Schwann cells and regeneration of axons takes place only in the laminin presence [**2,5**].

In the future studies short bioactive nanofibers might be loaded into the injectable hydrogel for neural tissue engineering applications. Such an approach might provide nanofibers dispersion in the liquid media, injectability of hydrogel system, an appropriate mechanical and biological properties, that mimic native extracellular matrix (ECM).

In these studies scanning electron microscopy (SEM) was used to determine fiber length, and hence the effectiveness of shortening depending on the used sonication medium, the duration of the process as well as PLLA molecular weight. A gel permeation chromatography (GPC) was used to check if ultrasonic treatment decreases PLLA molecular weight. A water contact angle (WCA) was measured to evaluate the surface wettability after physical adsorption. A bicinchoninic acid assay (BCA) was carried out to detect and quantify the amount of laminin adsorbed to the fibers.

The ultrasonic fragmentation was successfully optimized by choosing isopropanol as a sonication medium, relevant fragmentation time of 60 min and selection of appropriate polymeric material with the highest molecular weight, which among others showed the highest level of fragmentation. The post-fragmentation filtration through 40 um filters removed the fraction of long fibers reducing fiber length distribution to c.a. 50 µm. The GPC results showed that the molecular weight distribution of PLLA is not affected by both electrospinning and subsequent fragmentation. The WCA showed an increase of hydrophilicity on modified surface, while BCA assay performed effective laminin immobilization to the PLLA fibers.

These studies show that such classic and simple methods as ultrasonication and physical adsorption effectively provide a macroscopic and bioactive change of PLLA oriented electrospun fibers enabling their further use as fillers for injectable hydrogels for regenerative medicine applications.

Keywords: Electrospinning; ultrasonication; short fibers, polymers; scaffold.

Acknowledgements

The authors acknowledge the funding provided by the Polish National Science Center (NCN), grant number 2018/29/N/ST8/00780.

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Electrospun Fibers made of Polyacrylonitrile and Polyethersulfone with Laccase Immobilized for Biodegradation of Estrogen

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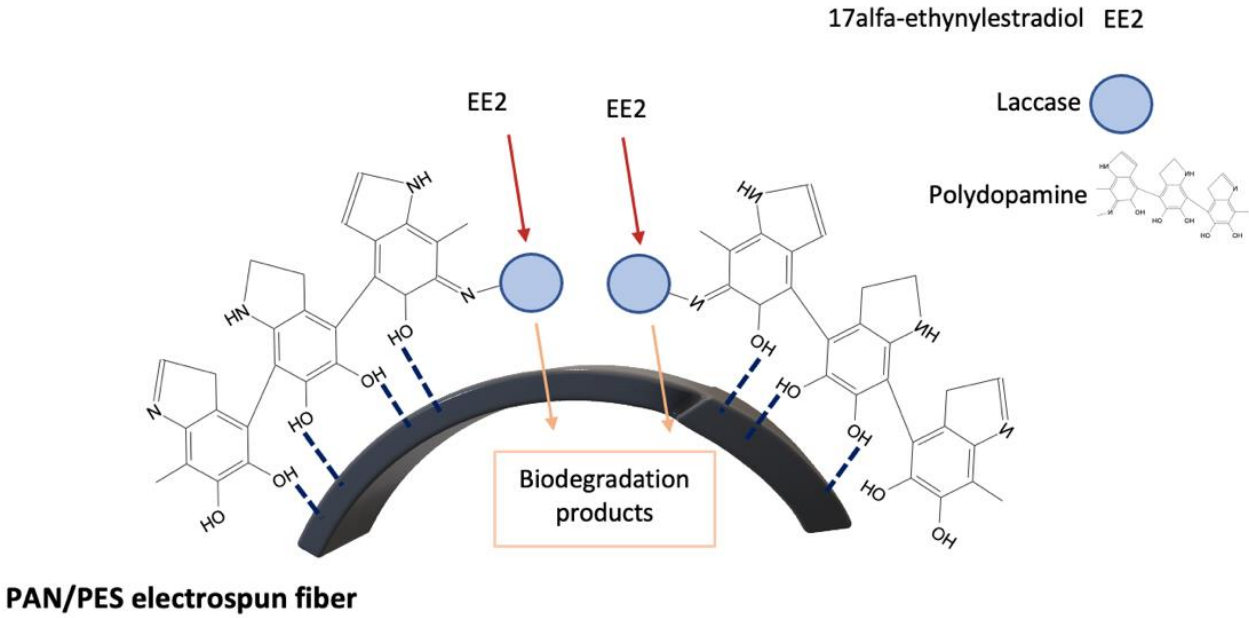

Abstract

Nowadays increasing amount of phenolic pollutants, especially pharmaceuticals, in waters is a big problem, which needs to be resolved. One of the most dangerous compounds, which could be get through into wastewaters and surface waters is 17alfa-ethynyloestradiol (EE2). This estrogen is a synthetic hormone and derivative of the estradiol (E2), naturally produced by human body. Despite that 17alfa-ethynyloestradiol is important component in birth control pills, their presence in drinking water could strongly affects human health causing reproductive problems or even disorders in circulatory or immune systems [**1,2**]. Therefore, it is very important to produce systems, which could degrade estrogens from waters. In our work we proposed production of new biocatalytic system made of polyacrylonitrile/polyethersulfone fibers (PAN/PES) and laccase immobilized by covalent binding

via polydopamine and its application for effective degradation of EE2 from model aqueous solutions. The fabricated electrospun fibers were deeply characterized before and after enzyme immobilization in terms of the average diameter of single fiber and the presence of specific functional groups. The results show that laccase immobilized onto PAN/PES fibers possesses around 70% of its initial activity after 30 days of storage. Moreover, the selection of degradation conditions was made, and it was found that EE2 is fully degraded at pH 5 and 25 °C from concentration even 5 mg L^{-1} for 24 h. What is more, even after 10 catalytic cycles it was possible to remove over 50% of EE2 from water solution. The obtained results show that laccase immobilized onto PAN/PES electrospun material modified by polydopamine could be an effective tool for removal of estrogens from waters. It should be stated that application of this type of heterogeneous biocatalyst with immobilized laccase in removal of phenolic compounds, such as pesticides, bisphenols or dyes is a future-proof way of removal other dangerous compounds from wastewaters and even drinking waters.

Keywords: Electrospun fibers; laccase; biodegradation; 17alfa-ethynylestradiol.

Acknowledgements

This work was supported by the National Science Centre, Poland under the research Grant number 2019/35/D/ST8/02087.

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Developing Acoustical Absorbers made from used Cigarette Butts

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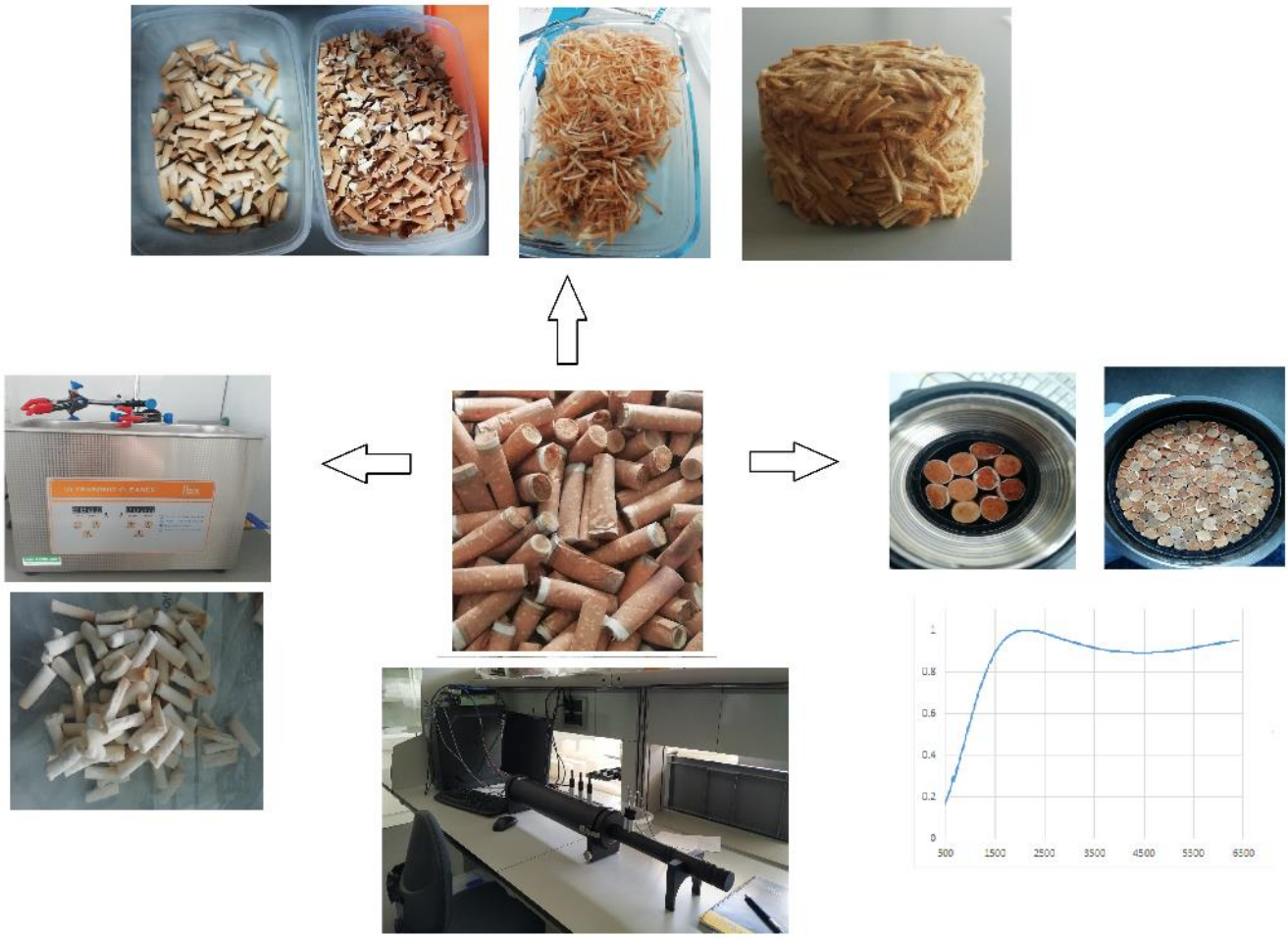
Graphical Abstract



Abstract

Although cigarette butts are a major component of our debris, both in appropriate disposal sites (i.e., bins, containers, etc.) or in unappropriated ones (streets, beaches, rivers, etc.), there are very few proposals to recycle them and new ones are necessary [**1,2**]. In this context, our research group is working in the use of this residue as acoustical absorbers [**3,4**]. Acoustical absorbers are used in construction both for adapting the acoustic conditions of a certain room to their use and, also, to improve the acoustical isolation characteristics of different constructions solutions.

In order to probe the acoustical behaviour of samples prepared from used cigarette butts, in this work, some studies in the development of these acoustical materials are presented. Acoustical behaviour of samples was characterized by the absorption coefficient measured using an impedance tube [Brüel & Kjær Impedance Tube Kit (Type 4206)] with two diameters, 29 mm and 100 mm (providing information in the 500-6400 Hz and 50-1600 Hz ranges, respectively). Measurements (based on the two-microphone transfer-function method) were performed according to the standard procedure detailed in the ISO 10534–2 standards.

Samples were prepared manually, placing a certain number of used cigarette butts in the impedance tube holder. In addition, some disaggregated samples were also prepared, considering different steps in the breaking-up of the samples.

Preliminary results concerning repeatability and reproducibility of preparation and measurements, influence of chemical cleaning in the acoustical behaviour, influence of breaking-up of the used cigarette butts, influence of density of samples will be presented in the poster.

The studies carried out show encouraging results showing a very good acoustical behaviour in mid and high frequencies. Comparison of acoustical results with other materials proposed for a similar use shows the potentiality of the prepared samples.

Nevertheless, there are still some questions to be addressed and further studies are proposed to solve some of them.

Keywords: Absorption coefficient; cigarette butts; impedance tube.

Acknowledgements

This work was partially supported by Altadis (Imperial Tobacco), by the European Regional Development Fund (ERDF) and also by Junta de Extremadura, Consejería de Economía, Ciencia y Agenda Digital (Project IB18033). This work was also supported by Consejería de Economía, Ciencia y Agenda Digital of Junta de Extremadura through grants for attracting and returning research talent to the R&D&I centers belonging to the Extremadura Science, Technology and Innovation System (TA18019); the University of Extremadura is the beneficiary entity

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Microstructural Evolution for Super304H Austenite Steel used in China Plants

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Graphical Abstract

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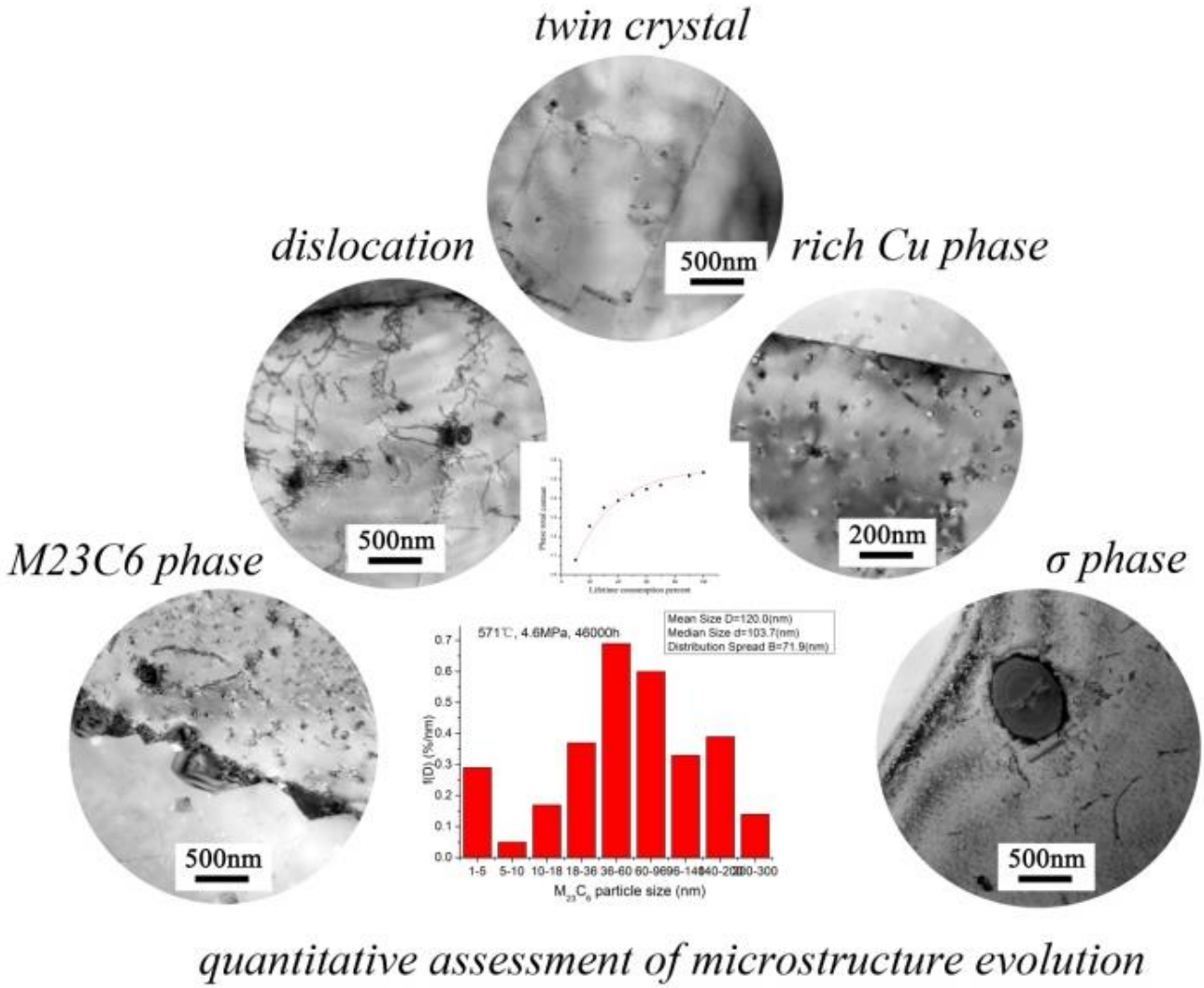

Abstract

Up to now, the amount of supercritical boilers in China has ranked number one in the world. Many supercritical boilers have run for more than 100,000 hours. Super304H (18Cr-9Ni-3Cu-Nb-N) austenite steel has high creep strength and has been used as the material of tubes in 600°C class USC power plants in China. The materials used in actual power plants are useful in estimating the changes of material properties caused by long-term aging and damage at low stress conditions, however, there are very few studies on Super304H steel actually used in power plants.

In this article, creep behavior of Super304H used in China plants was analyzed, microstructural evolution of Super304H tubes after different service conditions were studied involving in optical microscope, SEM, TEM and XRD. The results show, M23C6, Cu-rich particles, and σ phase were found to precipitate. A quantitative assessment of microstructure evolution was given during long-term creep, focusing on the dislocation density, particle size and number density of particles in Super304H steel.

Keywords: Microstructural evolution; austenite steel; supercritical boiler.

Acknowledgements

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Effect of Gamma Radiation on Mechanical Properties of Natural Fabric Reinforced Polyester Composites

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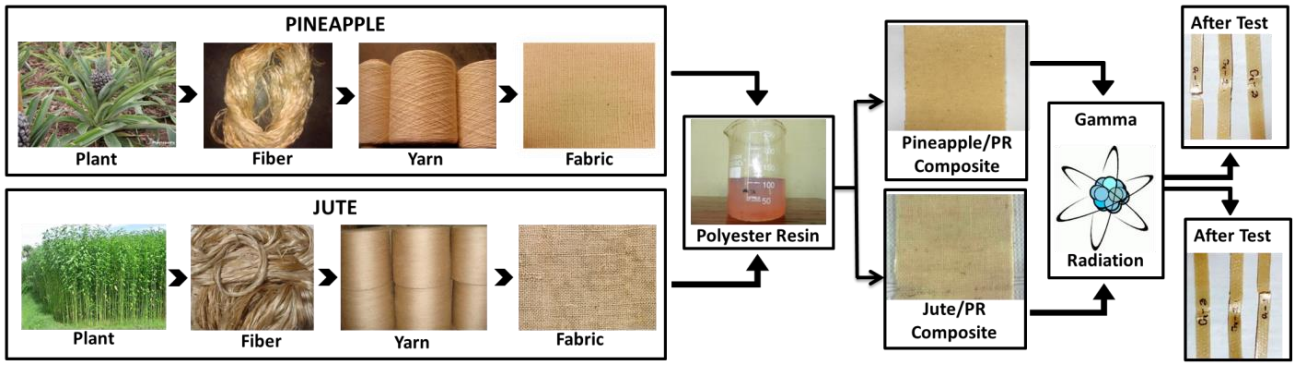

Abstract

Use of natural fibres in composite fabrication has drawn a great interest from the researchers due to its low density, low cost, environmental friendliness, biodegradability and high specific mechanical performance [**1**]. The main purpose of this research is to develop eco-friendly natural fabric reinforced polyester composite (NFRPC) materials with two different natural fabrics from pineapple and jute fibre; and their improvement of mechanical properties. One of the major drawbacks of NFRPC is its hydrophilic nature, responsible for moisture absorption which may cause swelling and maceration of the fibres, thus significantly decreasing its mechanical properties [**2**]. To overcome this problem, gamma radiation would be a great option due to its strong penetration power into the material that can change the internal structure of fibre and matrix. In this study, different doses of gamma radiation were applied to the composites and investigated their mechanical properties. Two types of bio-composites i.e., Pineapple fabric reinforced polyester resin (Pineapple/PR) and jute fabric reinforced polyester resin (Jute/PR) were prepared by hand lay-up method and irradiated with different gamma radiation dose by Co – 60 gamma source. The influence of gamma radiation on the mechanical properties i.e., tensile strength (TS), Young's modulus (YM), bending strength (BS), bending modulus (BM) and impact strength (IS) were investigated with five different gamma radiation doses i.e., 100, 200, 300, 400 and 500 krad. TS, YM, BS, BM of the composites were evaluated by a universal testing machine (H50KS-0404, HOUNSFIELD, series S, UK) according to

the ASTM D-638 and IS of the composite was evaluated by using an impact tester (HT-8041B IZOD, Pendulum type, Taiwan) according to the ASTM D-6110-97. It was found that, gamma radiation improved the mechanical properties to a certain limit over that of non-irradiated composites. In Pineapple/PR composite, a dose of 300 krad exhibited the best mechanical properties with an increase of 19% TS, 32% YM, 32% BS, 47% BM and 20% IS compare to the non-irradiated composite; and a gamma radiation dose of 200 krad showed the best mechanical properties for Jute/PR composite with an increase of 47% TS, 49% YM, 45% BS, 52% BM and 65% IS compare to the non-irradiated composite. This dramatic improvement is due to the cross-linking between fibre molecules, intra-chain bonding and the better adhesion of fibre and matrix obtained by gamma radiation. But further increasing of the gamma dose deteriorated the mechanical properties as overdoses may degrade the main polymer chain by breaking the molecules into small fragments **[3, 4**]. Hence, 300 krad for the pineapple/PR composite and 200 krad for the jute/PR composite are the optimum gamma radiation doses found in this experiment. In comparison, Jute/PR composites were influenced more than Pineapple/PR by gamma radiation in all the mechanical Properties. Therefore, the gamma radiation is recommended for improving the mechanical properties of NFRPCs but the optimum level of dose must be maintained.

Keywords: Fabric reinforced composites; pineapple fabric; jute fabric; polyester resin; gamma radiation; mechanical properties.

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Development of Advanced Composite Pressure Vessels for Hydrogen Storage

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Abstract

The shift from fossil fuels to fuel cells will increase the market demand on hydrogen. Efficient storage of hydrogen is crucial for the emerging hydrogen energy market. Storage is strongly connected to the performance and the safety of the car components. Currently, hydrogen is stored and transported in a compressed form to satisfy safety and weight regulations for high pressure gases and the traditional tanks that are used are made of stainless steel. Because of weight limitations these tanks are not suitable for automotive on-board applications. The weight of the tanks can however be considerably lowered, if composite materials can be used instead of stainless steel. At the same time the composite cylinders can offer high strength and safety. ADHERE is a project that aims at developing lightweight composite cylinders with improved mechanical and barriers properties for hydrogen using additive manufacturing (3D-printing). Furthermore, the motivation of the development of the cylinders are cost-competiveness. It is also important that future consumed hydrogen is produced by renewable energy and therefore the new storage cylinders will also be studied in energy systems using wind turbines. The project influences future prospects of advanced materials research and innovation for creating more utilization, impact in the society and sustainability.

Keywords: Advanced materials; energy materials; hydrogen; additive manufacturing.

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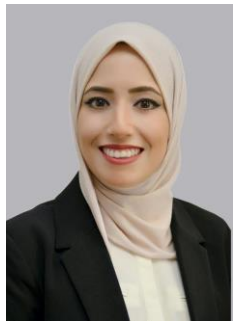
Anti-wettability of Chemically and Physically Modified Surfaces



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Abstract

The demand for new advanced functional materials has driven scientific work over the past decades. Nature has been inspiring in the creation of different types of self-cleaning and super repellent surfaces mimicking those of plants (lotus leaves), animals (shark skin) or insects (butterfly wings, water strider). To produce and maintain super repellent materials, chemical modification of the surface by using low surface energy materials such as siloxanes or fluoropolymers is necessary [**1**]. Also, physical modification of surface roughness enhances super-repellence against various liquids. The surface roughness can be achieved by the deposition of nano particles (NPs) using Liquid Flame Spray (LFS). Industrial applications like paper coatings [**2,3**], oil-water separation, and microfluidic devices have benefited from the fabrication of super-hydrophobic surfaces by LFS. In this work, substrates were silanated by chemical vapor deposition (CVD) method, and others were additionally pre-coated with silica NPS by LFS. The coated surfaces were characterized for their anti-wettability by measuring the contact angles of water and compare that to bare glass. The influence of the produced coatings on the wettability of surface with different liquids was examined through measuring advancing/receding dynamic contact angles as well as the roll off angle.

K**eywords:** Self-cleaning, silanization, nanoparticles, liquid flame spray.

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Perovskite Coatings on Ceria Foams and Membranes for Solar Fuel Production

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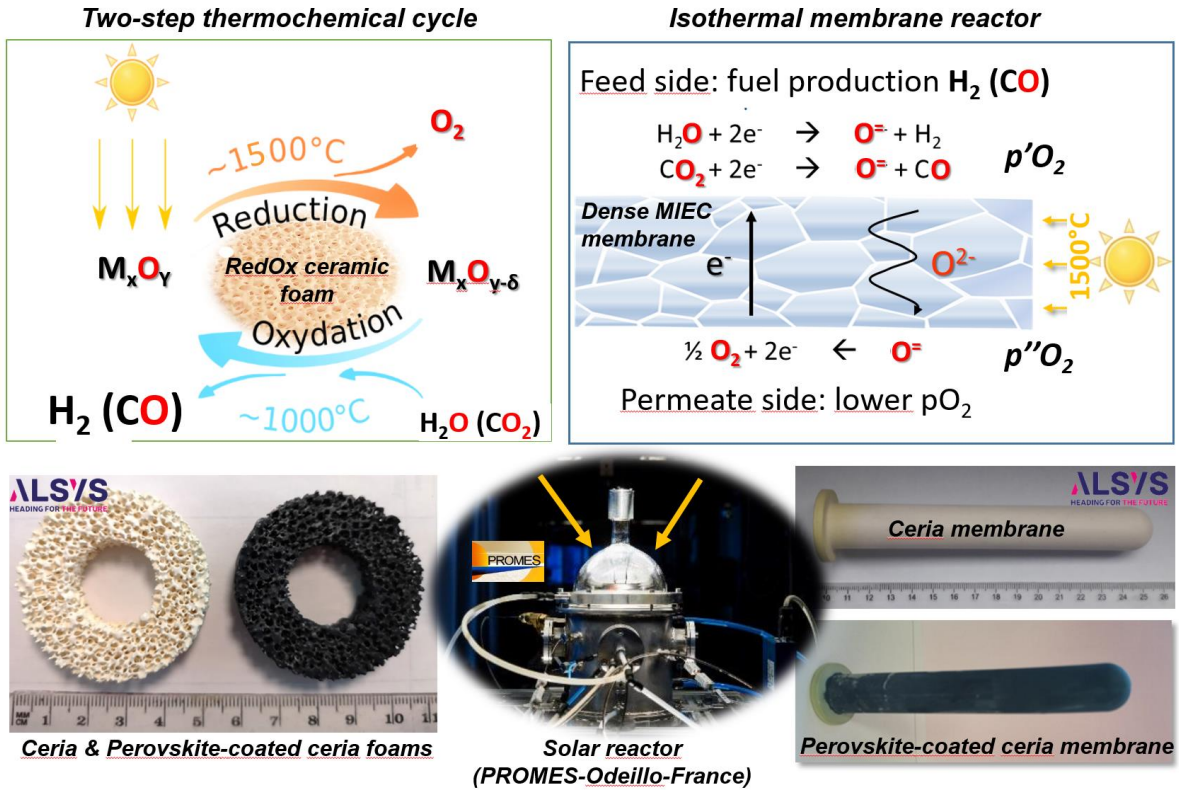
Graphical Abstract



Abstract

The production of renewable fuels is a major technological challenge to replace fossil fuels and fulfil the growing energy demand. In this context, the solar thermochemical splitting of CO_2 and H_2O by exploiting the redox properties of specific ceramic oxides is an attractive option for the production of synthetic fuels (CO and H_2) without greenhouse gas emission [**1**]. This work has been performed within the frame of a national project, coordinated by the PROMES-Odeillo CNRS laboratory, in collaboration

with the ceramic company ALSYS-CTI. The presentation will specifically focus on the development of a series of ion-conducting ceramic materials ($La_{1-x}Sr_xMnO_{3-\delta}$-based perovskites) meeting the criteria for application in solar reactors [**2**]. The large number of doping possibilities in perovskite materials offers great potential for tuning their thermodynamic properties. After the synthesis, characterization and selection of the most promising perovskite compositions [**3**], different shaping protocols were developed in order to prepare dense membranes and thin films coated on ceria foams [**4**] and tubes [**5**]. The performance of the optimized materials, tested in a solar reactor by PROMES-Odeillo, showed promising results for the production of CO and H_2 by thermochemical dissociation of CO_2 and H_2O. The ceria-coated foams were tested in two-step thermochemical cycles [**4**], while the dense oxygen-permeable tubes with mixed ion-electron conducting properties (MIEC membranes) were able to separate the reaction products (O_2/CO and O_2/H_2) in a single-step continuous isothermal process[5]. In both cases, perovskite coatings were found to enhance the fuel production yield of the pristine ceria materials, mainly by boosting the oxygen transfer rate. Perovskite-coated ceria membranes outperformed uncoated ceria membranes by yielding remarkable steady-state production of CO (>0.13 $\mu mol.s^{-1}.cm^{-2}$) at 1550°C[5]. The potential and limitations of the developed dual-phase materials and membranes for solar fuel production will be discussed.

Keywords: Ion-conducting ceramics, perovskites, membranes, thermochemical cycles, solar fuels.

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