

# **Book of Abstracts**

Faculty of Polymer Technology 24<sup>th</sup> – 25<sup>th</sup> September, 2020

Slovenj Gradec, Final meeting, September 2020

### **COST Action CA15107**

## MULTI-FUNCTIONAL NANO-CARBON COMPOSITE MATERIALS NETWORK (MULTICOMP)

Final Multicomp Meeting 2020

24th – 25th September, 2020 Slovenj Gradec, Slovenia

> Organized by Faculty of Polymer Technology

Slovenj Gradec, Final meeting, September 2020

### Zaključno Multicomp srečanje 2020

### Final Multicomp Meeting 2020

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COST Action CA15107 - Multi-Functional Nano-Carbon Composite Materials Network (MultiComp)

### Uredniki /Edited by:

Maja Mešl, Miroslav Huskić, Irena Pulko, Polona Umek

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### Foreword

MULTICOMP COST action was designed to bring together theorists, experimentalists and industrialists in the field of nanocarbon materials technology. In four years we achieved a lot and now it is time to come together for the last time, show, see and summarise results.

The final meeting will be held at the Faculty of Polymer Technology in Slovenj Gradec, Slovenia. Due to the unfortunate situation with the COVID 19, it will be different from all the other ones that we had before. The meeting is partially organised as an online meeting, and partially as a normal COST meeting. The security measurements have to be followed by participants who come to Slovenj Gradec. **Masks are now mandatory in closed public places, where social distance should also be obeyed.** 

The program of this meeting is shorter as usually. However, it is not less interesting. There will be 8 invited speakers, 19 flash presentations, and 7 posters. Some presentations will be given on-site, some online, using MS Teams. This is somewhat complicated but we believe it should not ruin scientific debate and experience exchange. Actually, it gives us even more opportunities to ask questions. Although the online audience should shut down their microphones, there is a "chat" they can use to ask questions during, or after the presentation. Therefore, even a 6-minutes presenter, can get, and later answer 10 questions or more. This is impossible during the normal COST meeting. However, the possibility of networking and exchange experiences will be hindered since most of the participants will be online.

We warmly welcome you all to the meeting, whether online or in Slovenj Gradec. We hope you will enjoy the programme and those who come to Slovenj Gradec, take your time and visit a small and beautiful city and its surroundings.

Local Organising committee Maja Mešl Miroslav Huskić Irena Pulko Polona Umek

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### **Conference chairs**

Assist. Prof. dr. Blaž Nardin
Faculty of Polymer technology, Slovenj Gradec
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### Scientific programme

### Thursday, September 24th

8:00 – 9:00	Registration	
9:00 9:00 – 9:15	Opening	Presentation Page
	Session 1 - chair Miroslav Huskić	
9:15 – 9:45	Invited lecture: Sharali Malik Nanotubes from Atlantis : Catalytic growth of Carbon Nanotubes	SG
9:45 — 10:15	Invited lecture: Silvia Marchesan Hybrid functional matter shaped by nanocarbon templates	SG
	FLASH Presentations (5 x 6 min talks)	
	Andraž Rešetič Thermomechanical functionalization of conventional silicone rubber – study and development of polymer dispersed liquid crystal elastomers	SG
10:15 –	Jacek Wychowaniec Unique cellular network formation guided by heterostructures based on reduced graphene oxide - Ti3C2Tx MXene hydrogels	online
10:45	Joanna Rymarczyk Carbon nanocomposite materials with gold nanoparticles - synthesis, characterization, applications	online
	Liutauras Marcinauskas Influence of the dopant type on the structure of amorphous carbon films	SG
	Maria Rybarczyk Coal Fly Ashes as a platform towards functional materials	online
10:45 – 11:15	Coffee break and Poster session	
	Session 2 - chair Sharali Malik	
11:15 – 11:45	Invited lecture: Aravind Vijayaraghavan High-grip and hard-wearing graphene reinforced polyurethane coatings	SG
44.45	FLASH Presentations (6x 6 min talks)	
	Alen Oseli Nano-mesh formation in single-walled carbon nanotube / polyethylene nanocomposites and its effect on their physical propertiesies	SG
11:45 – 12:25	Saide Umerova Rheology of thermomechanically active shape-programmable elastomer microparticles suspension in a viscous medium	SG
	Ana Barra Graphene-based sponges for water decontamination	online
	Tamas Szabó	online

Slovenj Gradec, Final meeting, September 2020

	Platelet size-effects in the colloidal stability of aqueous graphene oxide dispersions	
	Valentina Gargiulo Enhancing TiO2 photocatalytic activity: a survey on the effects of self-doping and of GRM-TiO2 interfacing	online
	Marjetka Conradi Stainless Steel Wettability And Friction In Different Environments Manipulated By Adsorption Of TiO <sub>2</sub> Nanoparticle Coatings	online
12:25 – 14:00	Lunch brake	
	Session 3 - chair Silvia Marchesan	
14:00 – 14:30	Invited lecture: Paola Ayala Working towards sensing at room temperature with carbon nanotubes	SG
	FLASH Presentations (3 x 6 min talks)	
	FLASH Presentations (3 x 6 min talks)Yasir Beeran PottatharaDielectric Films from Cellulose nanofibrils and Graphene Oxide	SG
14:30 – 14:50	Yasir Beeran Pottathara	SG online
	Yasir Beeran PottatharaDielectric Films from Cellulose nanofibrils and Graphene OxideZélia AlvesAntioxidant and electrically conductive starch-based films with	
14:50	Yasir Beeran Pottathara Dielectric Films from Cellulose nanofibrils and Graphene Oxide Zélia Alves Antioxidant and electrically conductive starch-based films with multiwalled carbon nanotubes: the effect of surfactant solution Roberto Di Capua Integration of conductive layers within the Eumelanin pigment: advanced spectroscopic and structural studies on EU/GL and	online
	Yasir Beeran Pottathara Dielectric Films from Cellulose nanofibrils and Graphene Oxide Zélia Alves Antioxidant and electrically conductive starch-based films with multiwalled carbon nanotubes: the effect of surfactant solution Roberto Di Capua Integration of conductive layers within the Eumelanin pigment: advanced spectroscopic and structural studies on EU/GL and	online

Slovenj Gradec, Final meeting, September 2020

### Friday, September 25<sup>th</sup>

8:30 – 9:00	Registration	
	Session 4 - chair Paola Ayala	
9:00 – 9:30	Invited lecture: Mitjan Kalin Lubrication of diamond-like carbon (DLC) coatings: challenges and opportunities	SG
9:30 – 10:00	Invited lecture: Milo Shaffer Incorporating nanotubes into next generation fibre reinforcements	online
	FLASH Presentations (5 x 6 min talks)	
	<b>Tjaša Kolar</b> Thermo-physiological and mechanical properties of textile, screen-printed with SWCNT-based printing pastes	SG
	Raul Arenal In-situ TEM Studies on Carbon Nanomaterials	online
10:00 – 10:30	Michela Alfè Carbon Dots (CND) from carbon black: scalable top-down production and deposition in ultrathin film	online
	Christopher Ewels Bottom-up design and realisation of stable fullerene spin systems	online
	Maria Kandyla Functional surfaces of laser-microstructured silicon coated with polymer blends with reversible wettability upon heating	online
10:30 – 11:00	Coffie break and Poster session	
	Session 5 - chair Mitjan Kalin	
11:00 - 11:30	Invited lecture: Petra Pötschke Melt-mixed thermoplastic polymer-CNT composites as thermoelectric materials	online
11:30 – 12:00	Invited lecture: Jan Peters Diversity and inclusion: beyond numbers. Communication and Coaching in STEM Research	online
		online to SO
12:00 – 12:50	MC Meeting	and MC members
12:50 – 14:00	Lunch brake	
14:00 – 15:00	MC Meeting concluded	online to SO and MC members
15:00 – 18:00	WGs Meetings and WGs Leaders/Representatves Reporting	SG

	Posters
P1	Tamara Rozman
11	Kinetic of crystallization of HDPE/SWCNT determined by Fast Scanning Chip Calorimetry
	Jaroslav Otta
P2	Thin Metal Layers as DRLs for High-Resolution CW-LIFT of Phthalocyanine-Fullerene
	Heterojunctions
	Aleksandras Iljinas
Р3	Formation of titanium doped diamond-like carbon films by magnetron sputtering
	technique
	Subramanian Lakshmanan
Ρ4	Temperature dependent electrical conductive properties of films prepared from
	differently dispersed single-walled carbon nanotubes and cellulose nanofibrils
P5	Polona Umek
PD	The role of cerium in $H_2Ti_3O_7$ nanoribbons in transformation to $TiO_2$ -B nanoribbons
P6	Ivan Radović
FU	Wake effect in interactions of ions with graphene-sapphire-graphene structure
P7	Ivan Brnardić
г7	Influence of Mg on Al alloy / MWCNT nanocomposites

### INDEX

1.	Invited lectures:
	Nanotubes from Atlantis : Catalytic growth of Carbon Nanotubes1
	Hybrid functional matter shaped by nanocarbon templates2
	High-grip and hard-wearing graphene reinforced polyurethane coatings
	Working towards sensing at room temperature with carbon nanotubes 4
	Lubrication of diamond-like carbon (DLC) coatings: challenges and opportunities
	Incorporating nanotubes into next generation fibre reinforcements
	Melt-mixed thermoplastic polymer-CNT composites as thermoelectric materials7
	Diversity and inclusion: beyond numbers, Communication and Coaching in STEM Research
2.	Flash presentations9
	Thermomechanical functionalization of conventional silicone rubber – study and development of polymer dispersed liquid crystal elastomers
	Unique cellular network formation guided by heterostructures based on reduced graphene oxide - $Ti_3C_2T_x$ MXene hydrogels
	Carbon nanocomposite materials with gold nanoparticles - synthesis, characterization, applications
	Influence of the dopant type on the structure of amorphous carbon films
	Coal Fly Ashes as a platform towards functional materials13
	Nano-mesh formation in single-walled carbon nanotube / polyethylene nanocomposites and its effect on their physical properties
	Rheology of thermomechanically active shape-programmable elastomer microparticles suspension in a viscous medium
	Graphene-based sponges for water decontamination16
	Platelet size-effects in the colloidal stability of aqueous graphene oxide dispersions
	Enhancing $TiO_2$ photocatalytic activity: a survey on the effects of self-doping and of GRM-TiO <sub>2</sub> interfacing
	Stainless Steel Wettability And Friction In Different Environments Manipulated By Adsorption Of TiO2 Nanoparticle Coatings
	Dielectric Films from Cellulose nanofibrils and Graphene Oxide 20
	Antioxidant and electrically conductive starch-based films with multiwalled carbon nanotubes: the effect of surfactant solution
	Integration of conductive layers within the Eumelanin pigment: advanced spectroscopic and structural studies on EU/GL and EU/GO hybrid materials

### Slovenj Gradec, Final meeting, September 2020

	Thermo-physiological and mechanical properties of textile, screen-printed with SWCNT-based printing pastes
	In-situ TEM Studies on Carbon Nanomaterials
	Carbon Dots (CND) from carbon black: scalable top-down production and deposition in ultrathin film
	Bottom-up design and realisation of stable fullerene spin systems
	Functional surfaces of laser-microstructured silicon coated with polymer blends with reversible wettability upon heating
3	. Posters
	Kinetic of crystallization of HDPE/SWCNT determined by Fast Scanning Chip Calorimetry
	Thin Metal Layers as DRLs for High-Resolution CW-LIFT of Phthalocyanine-Fullerene Heterojunctions
	Formation of titanium doped diamond-like carbon films by magnetron sputtering technique 30
	Temperature dependent electrical conductive properties of films prepared from differently dispersed single-walled carbon nanotubes and cellulose nanofibrils
	The role of cerium in $H_2Ti_3O_7$ nanoribbons in transformation to $TiO_2$ -B nanoribbons
	Wake effect in interactions of ions with graphene-sapphire-graphene structure
	Influence of Mg on Al alloy / MWCNT nanocomposites



Slovenj Gradec, Final meeting, September 2020

#### 1. Invited lectures:

### Nanotubes from Atlantis : Catalytic growth of Carbon Nanotubes

#### Sharali Malik

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Nanosized carbon materials such as Carbon nanotubes (CNTs) provide the possibility to achieve, in terms of tensile strength and Young's modulus, incredibly strong materials. Therefore, the fabrication of nanocomposites with CNTs offers the potential for applications in electronics, medicine, defense and aerospace. Furthermore, it has been shown that having branched CNT structures is a promising way forward in terms of providing structures with enhanced mechanical properties. However, in order to realize this, mass production techniques at reasonable costs are needed. One possibility is the chemical vapor deposition (CVD) method which involves the decomposited on or inside a support such as silica, alumina or titania. Here we report a simple and industrially scalable CVD process to manufacture long single-walled carbon nanotubes (SWNTs), branched multi-walled carbon nanotubes (b-MWNTs) and multi-walled carbon nanotubes (MWNTs) using the abundant pumice from the Akrotiri volcanoes on the Greek island of Santorini to catalyze the transformation of the carbon in methane (CH<sub>4</sub>) into CNT materials [1].

Acknowledgement S. M. acknowledges support by the Helmholtz Society through program Science and Technology of Nanosystems (STN). It is a pleasure to thank Valeriu Mereacre for the Mößbauer measurement and Annie Powell for many helpful discussions. The networking support by the COST Action MultiComp (CA15107) supported by the COST Association (European Cooperation in Science and Technology) is acknowledged.

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Slovenj Gradec, Final meeting, September 2020

### Hybrid functional matter shaped by nanocarbon templates

Silvia Marchesan

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Carbon nanostructures come in different morphology and size, which are well-known to affect their chemical reactivity. Yet it is still unclear how such properties affect nanocarbon behavior in composite or hybrid systems, and especially which nanocarbon is best suited for a higher performance of the final, multicomponent material. For instance, comparison between carbon nanotubes, few-layered graphene, and carbon nanohorns have revealed remarkable differences when used as scaffolds for the growth in situ of inorganic metal oxide nanoparticles, and thus in the resulting organic-inorganic hybrids, for applications in water, in areas as diverse as catalysis and phosphoproteomics. Another case of particular interest is the combination of nanocarbons and self-assembling tripeptides, whereby the latter can act as surfactants to disperse the former in aqueous buffer and still successfully self-organize, even in the presence of large amounts of nanocarbons. Interestingly, the similarity between the anisotropic morphology of carbon nanotubes and peptide fibrils can lead to the emergence of new properties such as self-healing behavior.

The lessons learnt from unexpected properties that arise in multi-component materials featuring one or another carbon nanostructure will be discussed to gain insights for the design of the next-generation advanced materials for applications in polar solvents such as water.

### High-grip and hard-wearing graphene reinforced polyurethane coatings

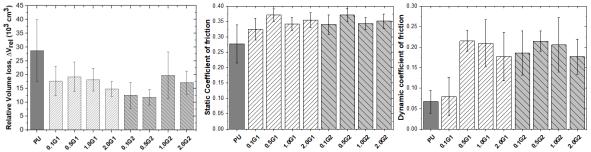
Monica Alberto, Maria Iliut, Mohan Pitchan, and **Aravind Vijayaraghavan**\* Department of Materials and National Graphene Institute, The University of Manchester, Oxford Road, Manchester M13 9PL, UK \* aravind@manchester.ac.uk

Graphene has significant potential to improve the mechanical properties of elastomers such as rubbers and polyurethane. We have shown that graphene-reinforced natural rubber can deliver significantly enhanced strength, elasticity and abrasion resistance, and this can be used in applications such as footwear outsoles.

In this talk, I will present other examples of ongoing work in my group involving the behaviour of graphene dispersions and graphene-enhanced composite materials.

In particular, I will focus on one example of a follow-on work, based on liquid polyurethane (PU) resins [1]. These are used to form anti-slip surface coatings either on their own or mixed with recycled rubber particles. In this work, we reinforce PU resin films with few-layer graphene (FLG) nanoparticles from two commercial sources (G1 and G2). The FLGs are incorporated by high-shear mixing, which gives good dispersion as evidenced by optical tomography. The FLG does not appreciably change the tensile strength or Shore hardness of the PU, but we report modest increase of 10% in tear strength and Young's modulus, accompanied by a similar decrease in elongation to failure. However, significant improvements of over 100% are observed in the abrasion resistance (Fig 1b). At the same time, we report a 25% increase in the coefficient of static friction (Fig 1c) and 200% increase in the Coefficient of dynamic friction (Fig 1d). We attribute this to corresponding decrease that we observe in the PU surface energy and increase in the water contact angle.

These results, taken together, suggests that graphene can significantly improve the grip and durability of PU anti-slip coatings, without significantly affecting the other mechanical properties of the coating.



**Figure 1.** Improvements in (a) abrasion resistance, (b) coefficient of static friction and (c) coefficient of dynamic friction of polyurethane coatings with two types of few-layer graphene flakes, G1 and G2.

Acknowledgement MA and AV acknowledge InnovateUK Knowledge Transfer Partnership grant KTP10967 and Let's Play Everywhere Ltd. for supporting this work.

**References** [1] Alberto, M. et al., High-grip and hard-wearing graphene reinforced polyurethane coatings. In press, 2020.

#### Working towards sensing at room temperature with carbon nanotubes

Paola Ayala paola.ayala@univie.ac.at

The electronic and optical properties of carbon nanotubes are very sensitive to the chemical environments. It is therefore inferable why they are so attractive as sensing objects. These onedimensional nanostructured materials have been the focus of intensive research but it is important to keep in mind that practical difficulties to produce them ultra-clean and nearly defect-free have constantly appeared as stumbling blocks for their use in applications controllably and reproducibly. One of our pilot experiments -to understand how the intrinsic properties of single-walled carbon nanotubes vary when they are exposed to gases- was to investigate the adsorption of O2, NO and NO2 molecules. We performed experiments on ultra-pure nanotube material and then tested the influence of molecular fillers. Strikingly, we figured out that many of the sensing effects that had been reported previously were produced in great part by the presence of impurities and defects. This affects tremendously the reproducibility of the experiments. We have also shed light on the nature of adsorption and its effect on their electronic properties of the tubes. Metallicity-sorting and the further use of carbon nanotube hybrids are able to unfold two major challenges: tuning the gas-tube interaction and achieving desorption of gases at ambient temperature. A result to highlight was that using time resolved photoemission we observed that in semiconducting nanotube hosts the chemical potential is pinned inside their energy gap shifted to the onset of the conduction band when nanotubes filled with nanoclusters are used. This remarkably reveals that having a metal cluster filling could represent a key to high sensitivity with a very effective desorption at ambient temperature. I will present an overview and a progress report of my group's related research.

#### Acknowledgement

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Slovenj Gradec, Final meeting, September 2020

# Lubrication of diamond-like carbon (DLC) coatings: challenges and opportunities

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Diamond-like-carbon (DLC) coatings are an amorphous material consisting mainly of carbon atoms in the sp<sup>2</sup> and sp<sup>3</sup> hybridization, typically with some hydrogen content, with many doping strategies being employed to tailor their properties [1, 2]. In the search for the best surface solutions under tribological conditions, DLC coatings are becoming very attractive due to their inherent low-wear and low-friction properties. However, the key benefit, but also a challenge with DLC coatings and so with their lubrication, is their low reactivity. They exhibit very low adhesion [3], which gives them a low-friction property, but on the other hand this means that their interactions with lubricants are weak, and difficult to control or predict. So, DLC coatings rise chalanges and opportunities at the same time, and thus a great potential for innovative lubrication solutions. While their use in boundary lubrication has been explored for almost two decades and is well documented [4,5], their use in full film lubrication is still very new and broadly unknown [6,7]. The above aspects will be discussed in this work.

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Slovenj Gradec, Final meeting, September 2020

#### Incorporating nanotubes into next generation fibre reinforcements

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Nanostructured materials offer the possibility to improve the performance and functionality of existing structural fibres. There are broadly two strategies: One involves the incorporation of the nanomaterial into existing state of the art fibres, in order to address critical weaknesses and/or introduce new functions. The second, which is more challenging but potentially more transformative, relies on the development of entirely new fibre systems from the nanostructured or nanocomposite constituents.

Examples of the first approach include the development of nanostructured interphases on existing carbon and glass fibres. Here, the nanomaterial can improve load transfer between the fibre and the matrix and reduce stress concentration. Surface grafting of carbon nanotubes (CNTs) by direct CVD provides a hierarchical fibre with two differing reinforcement length scales. The advantages of this approach are well known, but typically limited by damage to the substrate fibres, and difficulties with scale-up. Recently, we have developed a continuous spool-to-spool process with exploits a local electric field to ensure a homogeneous growth process and maintain the performance of the primary fibres<sup>1</sup>. The products show excellent single fibre interfacial characteristics and allow the preparation of composite coupons. The high surface area may be relevant to multifunctional electrochemical applications as well as structural composites, as illustrated by recent work on structural energy storage, and structural heath monitoring.

On the other hand, entirely new fibre systems require processes to assemble and orient the constituent nanostructures. Individual perfect nanocarbon structures have exceptional properties; the challenge is often how to exploit their potential in real macroscopic systems. Whilst dry spinning approaches may be attractive, wet spinning is more obviously scalable and applicable. However, the formation of individualized solutions of functionalised single wall nanotubes (SWNTs) and graphenes is a particular challenge. We exploit reductive charging to form pure nanotubides (nanotube anions) which can be redissolved, purified, or optionally functionalised, whist avoiding the damage typically associated with sonication and oxidation based processing<sup>2,3</sup>. The reaction mechanism can be understood in more detail using in situ open circuit measurements during the chemical reactions.<sup>4</sup> This simple system is effective for a host of nanocarbon materials including MWCNTs, ultralong SWCNTs, carbon blacks, and graphenes (as reviewed here<sup>5</sup>). The resulting nanocarbon ions can be readily chemically grafted for a variety of applications. Nanotubide solutions can be spun directly into coagulant baths in order to prepare functionalised SWCNT fibres directly in situ<sup>6</sup>. Grafting of suitable polymer constituents can increase dispersibility of both nanotubes and graphenes<sup>7-9</sup>, and hence help to produce nanocomposite fibres will high strength and strain to failure. Other non-carbon based analogues of nanotubes offer opportunities for greener fibre systems<sup>10</sup> and additional functions. In particular, recent work on inorganic nanotubes has produced healable structural fibres, with exceptionally high performance compared to existing alternative approaches. Spinning nanotubes filled with 1D phases of other allotropes (such as phosphorous or arsenic), may provide an interesting means of manipulation.<sup>11</sup>

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Slovenj Gradec, Final meeting, September 2020

### Melt-mixed thermoplastic polymer-CNT composites as thermoelectric materials

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Electrically conductive polymer composites (CPCs) based on insulating polymer matrices filled with carbon nanotubes (CNTs) can also be used as potential thermoelectric (TE) materials to convert waste heat into electrical energy. The advantages of polymer-based TE materials over typically used metal oxides such as bismuth tellurides are not only their better availability and cost efficiency, but also their ease of processing, flexibility, lower density and low thermal conductivity.

Based on previous work on PC with MWCNTs [1] and PP with SWCNTs [2], the aim of this study was to show the influences of the CNT and polymer type and the CNT content on the electrical conductivity, the Seebeck coefficient (S) and the resulting power factor. Different commercially available CNTs were used to produce melt-mixed composites of different thermoplastic polymers on a small scale using an Xplore 15 ccm microcompounder [3]. CNTs are typically reported to result in p-type composites with positive S values, which means that the charge carriers are holes.

The different CNT materials lead to different dispersion states, which strongly influence the electrical conductivity. When comparing two MWCNT materials at constant filler content, the composites with higher electrical conductivity also show a higher Seebeck coefficient, which leads to higher power factors. The selected SWCNT material with a content of 2 wt.% gives the highest S-values among all CNTs and reaches values up to 60 microV/K (in PBT). The type of polymer matrix also influences the electrical conductivity and the Seebeck coefficient. At a constant CNT load of 2 wt% MWCNT, PVDF-based composites always showed higher values than those based on PP, PBT and PC. For SWCNTs the highest S-values were achieved with PBT. Interestingly, MWCNTs in polymers such as ABS behave differently than SWCNTs. SWCNTs are able to produce n-type composites with negative Seebeck coefficients, which means that the charge carriers are electrons. The magnitude of these negative S-values depends on the type and quantity of SWCNTs. A common feature of such matrix polymers is the presence of amide and nitrile groups that can dope SWCNTs by inserting electrons to make them n-type. The maximum Seebeck coefficients achieved were 66.4 microV/K for PBT with 7 wt% SWCNTs and -51.5 microV/K for ABS with 0.5 wt% SWCNTs.

Thus, by varying the matrix and the CNT type, it is possible to produce melt-mixed p- and n-type polymer-based materials and even to obtain p- and n-type materials based on the same polymer matrix.

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Slovenj Gradec, Final meeting, September 2020

# Diversity and inclusion: beyond numbers, Communication and Coaching in STEM Research

### Jan Peters MBE PhD

Finally the conversation about diversity has shifted from being just about women. But we still tend to think of women in science as the main Big Issue. And many of the European level programmes and initiatives still focus on representation and statistics. While having the data is undoubtedly important there are other reasons for addressing diversity. Not least because it is about doing excellent science that stands the test of scrutiny and time.

Jan will talk about the need to focus on excellence and innovation. How we address this by building an inclusive lab culture; one that is founded on better communication and how a coaching approach can help each person be their best. Also, how having an open conversation about difference can improve the quality of research.

Slovenj Gradec, Final meeting, September 2020

### 2. Flash presentations

### Thermomechanical functionalization of conventional silicone rubber – study and development of polymer dispersed liquid crystal elastomers

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The method of dispersing additional material into a polymer network can enhance or introduce new properties to elastic materials, thus broadening its applicability and adaptability to various industrial needs. We have adopted this idea to introduce a novel method of thermomechanically functionalizing conventional silicone rubber. By producing a composite material consisting of magnetically oriented liquid crystal elastomer particles incorporated in a cured PDMS matrix, we have transferred thermomechanical properties from the particles onto the composite, meaning that the material experiences reversible contraction in the particle's alignment direction upon thermal activation. Such composites, termed polymer-dispersed liquid crystal elastomers or PDLCE's [1] can be molded into arbitrary shapes and sizes. By spatially modulating the particle's director orientation throughout the specimen using an external magnetic field, it is possible to achieve complex reversible thermomechanical deformations (Fig 1). The lack of mechanical manipulation of the specimen and the liquid nature of the pre-polymerized PDLCD melt makes the material well suited for implementation into additive manufacturing techniques.

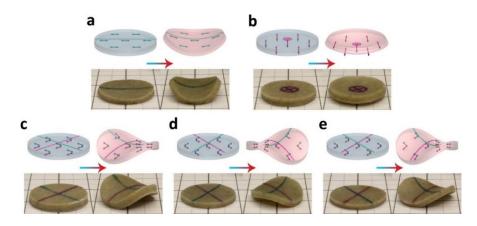


Fig. 1: Five basic morphing configurations made from differently ordered functionalized and non/functionalized PDLCE bilayers.

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Slovenj Gradec, Final meeting, September 2020

# Unique cellular network formation guided by heterostructures based on reduced graphene oxide - Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene hydrogels

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Two-dimensional (2D) materials remain highly interesting for assembling three-dimensional (3D) structures, among others, in the form of macroscopic hydrogels [1]. Herein, we present a novel approach for inducing chemical inter-sheet crosslinks via an ethylenediamine mediated reaction between  $Ti_3C_2T_x$  and graphene oxide in order to obtain a reduced graphene oxide-MXene (rGO-MXene) hydrogel (Fig 1.). The composite hydrogels are hydrophilic with a stiffness of ~20 kPa. They also possess a unique inter-connected porous architecture, which led to a hitherto unprecedented ability of human cells across three different types, epithelial adenocarcinoma, neuroblastoma and fibroblasts, to form inter-connected three-dimensional networks [2]. The attachments of the cells to the rGO-MXene hydrogels were superior to those of the sole rGO-control gels. This phenomenon stems from the strong affinity of cellular protrusions (neurites, lamellipodia and filopodia) to grow and connect along architectural network paths within the rGO-MXene hydrogel, which could lead to advanced control over macroscopic formations of cellular networks for technologically relevant bioengineering applications, including tissue engineering and personalized diagnostic networks-on-chip.



Figure 1: Scheme showing the reaction between the ethylenediamine (EDA), GO and MXene flakes.

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# Carbon nanocomposite materials with gold nanoparticles - synthesis, characterization, applications

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The type of nanoparticles (metallic, carbon, ceramic), their size and shape, the degree of surface development, surface energy and the distribution of nanoparticles in the matrix have a significant impact on the properties of the nanocomposite material. The method of obtaining new type of carbon-based composite film with gold nanoparticles (C-Au film) has been developed in the Łukasiewicz Research Network - Tele and Radio Research Institute. Gold nanoparticles, due to their different properties on the nano scale compared to the macro scale, are widely used in many fields of science, including electronics, catalysis, medicine, photovoltaics, biological sensors and others. C-Au films were prepared by the PVD method at different technological process parameters. In this method, C-Au films can be applied directly to various substrates, which enable many types of electrical connections. The amount and size of Au nanoparticles in the nanocomposite can be also investigated. Such films could be applied as sensors or in chemical reaction enabling glucose oxidase.

The research carried out under the STSM grant contributed to the developed application of new multifunctional carbon-gold nanocomposite material.

The characterization and potential application of these films based on their photoelectric and / or photothermal properties will be shown. The results of topography studies obtained by using scanning electron microscopy (Fig. 1a), , morphology properties obtained through ultra-high resolution scanning transmission electron microscopy(Fig. 1b), elemental analysis - energy dispersive X-ray spectroscopy, crystal structure – X-ray diffraction and electron structure - visible and near ultraviolet spectroscopy will be discussed.

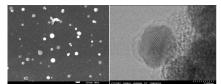


Fig. 1 a) SEM image of topography of C-Au film, b) UHR TEM image of C-Au film

#### Acknowledgement

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### Influence of the dopant type on the structure of amorphous carbon films

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Metal and oxygen containing amorphous diamond-like carbon films were deposited using layer by layer magnetron sputtering technique. Thin films were deposited by sputtering graphite and various metal (chromium, titanium, and nickel) targets in low pressure environment. The influence of metal concentration and type on the amorphous carbon films surface morphology, structure and properties were investigated. The surface morphology and elemental composition of the amorphous carbon films were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM) and energy dispersive X-ray (EDX) spectroscopy. Nanoindentation tests were performed by MTS-Agilent G200 nanoindenter. The optical properties were determined using UV-VIS-NIR spectrophotometer (Shimadzu UV-3600). 1.5 µm diameter spherical tip was use to measure force of friction of several coatings. The influence of metal-oxygen doping on the structure of carbons films were investigated using multiple (458 nm, 488 nm, 514 nm and 633 nm) wavelength excitation Raman spectroscopy. Dispersive behaviour of D and G peaks and I<sub>D</sub>/I<sub>G</sub> ratios of the films were analysed. The results showed that the increase of metal concentration reduced the sp<sup>3</sup> sites fraction and enhanced oxygen fraction in the films. It was obtained that the addition of the metal content in the amorphous carbon films increased the surface roughness values. Meanwhile, the increase of the metal (from 2 at.% to ~12 at.%) concentration slightly reduced the roughness of the films. The optical measurements indicated that films were highly transparent in near infrared range, however only Cr and Ti doped carbon films were transparent in visible light range. Tribology tests revealed that doping DLC films with titanium decreases friction coefficient. It was determined that the type of dopant metal had insignificant influence on the microhardness and Young's modulus values of films.

#### Acknowledgements

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### Coal Fly Ashes as a platform towards functional materials

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Coal fly ashes (CFA) as industrial by-products are generated in coal-fired power plants after coal combustion. Only up to 30% are fully used in the soil amelioration, construction industry as well as geopolymer or zeolite synthesis [1-2]. The balance is disposed of in controlled landfills causing serious environmental concern. Thus, there is a need to develop new recycling methods.

In this work, we have reviewed selected CFA applications, including synthesis of zeolites. As an example the sub-pilot scale process of synthesis of Na-P1 zeolite from the coal fly ash is presented (Fig. 1). After establishing the synthesis conditions (20 kg of fly ash, 12 kg of NaOH, 90 dm<sup>3</sup> of water, the reaction temperature: 80 °C, and the reaction time: 36 h), the high-purity (81 wt%) Na-P1 zeolite product was fabricated [3].

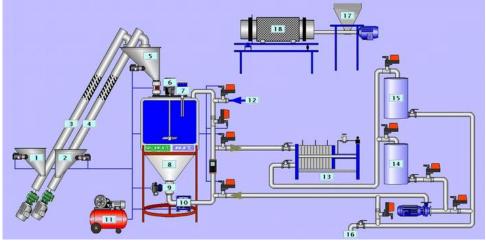


Figure 1: Technological scheme of the prototype line for the synthesis of zeolites [3], where: 1 NaOH storage tank with the vibrator, 2 fly ash storage tank with the vibrator, 3 screw conveyor transporting NaOH, 4 screw conveyor transporting fly ash, 5 weighting tank suspended on three-strain gauge weight sensors with the vibrator, 6 mechanical stirrer, 7 heater with the control system of the reactants level and reaction temperature, 8 reaction vessel, 9 pneumatic membrane valve, 10 membrane pump, 11 compressor, 12 water supply with the control volume by means of flowmeter, 13 hydraulic press, 14 NaOH aqueous solution of the synthesis reaction, 15 water solution from flushing of zeolite material in the press, 16 waste for disposal, 17 feed to the calciner, 18 calciner

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M.K. Rybarczyk would acknowledge the financial support from COST Action CA15107.

L. Bandura was supported by the Foundation for Polish Science (FNP).

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# Nano-mesh formation in single-walled carbon nanotube / polyethylene nanocomposites and its effect on their physical properties

Alen Oseli<sup>1</sup>, Alenka Vesel<sup>2</sup>, Miran Mozetič<sup>2</sup>, Ema Žagar<sup>3</sup>, Miroslav Huskić<sup>4</sup>, Lidija Slemenik Perše<sup>1\*</sup>

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The mesh formation of single-walled carbon nanotube (SWCNT) superstructure, i.e., nano-mesh, in lowand high-density polyethylene (LDPE and HDPE) matrices was observed by using plasma etching technique and SEM analysis, Figure 1 [1]. Nano-mesh was established by two mechanisms: i) alignment of SWCNT bundles (forming network backbone) and ii) shish-kebab induced crystallization (forming network net). The network was formed at low SWCNT content, due to the high aspect ratio of nanofiller. SWCNT acted as a nucleating agent; however, formed network caused confinement effect, disrupting crystallization and melting kinetics, i.e., shifting of peak crystallization temperature to lower values, peak melting temperature to higher values and reducing the degree of crystallinity, which directly affected mechanical properties. With the addition of SWCNTs, mechanical properties of LDPE and HDPE nanocomposites profoundly improved, i.e., in Young's modulus 230% and 30% respectively at 1 wt.% of SWCNTs. However, LDPE nanocomposites exhibited no confinement; thus, effective reinforcement remained unchanged. Unlike LDPE, HDPE nanocomposites showed visible confinement that reduced effective reinforcement for ~3x within observed SWCNT content (from 0 to 1 wt.% of SWCNTs). It seems that certain types of semi-crystalline polymers, such as HDPE, cannot achieve full reinforcing potential since confinement effect induced by superstructure restricts the crystal growth, which gradually reduces effective reinforcement already in the semi-dilute regime.

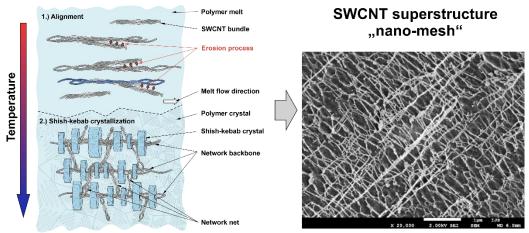


Figure 1: Mechanisms of nano-mesh superstructure formation in SWCNT/PE nanocomposites [1].

Acknowledgement The authors acknowledge the financial support from the Slovenian Research Agency (research core funding No. P2-0264 and No. P2-0145) and the Ministry of Education, Science and Sport (Project CoSiMa, Contract No. C3330-18-952020).

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# Rheology of thermomechanically active shape-programmable elastomer microparticles suspension in a viscous medium

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Thermomechanically active shape-programmable elastomer microparticles are very promising for developing particulate composites of different configurations, with unique operational properties attractive for various applications, e.g., in 3D printing. In this regard, one of the best candidates are liquid crystal elastomers due to their remarkable spontaneous shape changes response. We discuss a simple way of producing the suspension of a monodomain-like liquid crystal elastomers microparticles (µLCEs) with unconventional rheological properties. We demonstrate, that shear stress can be effectively used to manipulate the nematic order-driven morphology of µLCEs and assume the role of external orienting field. Specifically, by simultaneous exploiting the soft-elasticity character of the material and control of shear amplitude time-profile, the alignment of nematic director is switched along the flow providing for effective means of orienting the microparticles. Therefore, at room temperature, the suspension is now found in the state of well-aligned, thermomechanically deformed nematic microdomain µLCEs, formed during shear stress-assisted cooling. Despite the gradual loss of particles spatial orientation over time, the aligned state can be achieved instantaneously by switching on the flow. We attribute this to the stability of frozen-in deformations to locking-in of the soft elasticity driven nematic director reorientations, assisted by elastic hardening, making such a suspension ready for applications in additive manufacturing.

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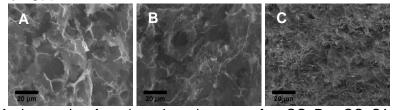
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### Graphene-based sponges for water decontamination

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Mercury (Hg) is a toxic heavy metal commonly present in wastewater. Therefore, it is necessary to adopt efficient methods to keep this metal at low concentrations and guarantee the water quality.1 Graphene-based materials, such as reduced graphene oxide (rGO), are promising candidates for water decontamination due to their high specific surface area, negative surface charge and remaining oxygen containing groups.<sup>2</sup> Herein, we report a simple methodology to prepare graphene-based sponges and their application for Hg(II) removal from water. Graphene oxide was synthesized by the improved Hummers method<sup>3</sup> and reduced by hydrothermal carbonization, obtaining the rGO. Another sample was prepared by hydrothermal treatment in presence of caffeic acid (CA) as reducing agent (rGO\_CA). A third sample was produced by immersion of the rGO\_CA sample into a chitosan (CS) solution (rGO CA CS). At the end all three materials were freeze-dried to obtain the sponges. The reduction of graphene oxide was confirmed by XRD and Raman spectroscopy. The sponges' morphology and textural properties were analysed by SEM, Figure 1, and by -196 °C nitrogen adsorption-desorption isotherms. The Hg(II) removal from water by the sponges was studied in function of pH, being observed an optimal pH range between 4 and 6. The rGO\_CA sample had the best performance for Hg(II) removal. The minimum amount of this sponge to achieve a Hg(II) removal superior to 80% was 25 mg/L. The equilibrium isotherm showed a sigmoidal shape and the Sips model was the one that best described the equilibrium data. These simple graphene-based sponges are promising materials for environmental remediation, namely Hg(II) removal from water.



**Figure 1:** SEM micrographs of graphene-based sponges **A** – rGO; **B** – rGO\_CA; **C** – rGO\_CA\_CS. Acknowledgment: This work was developed within the scope of the project CICECO - Aveiro Institute of Materials, UIDB/50011/2020 & UIDP/50011/2020. AB and PF are thankful to FCT for grant SFRH/BD/148856/2019 and the Investigator FCT. CN and CL are grateful to Portuguese national funds (OE), through FCT, I.P., in the scope of the framework contract foreseen in the numbers 4, 5 and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19. COST action 15107, Grant No. 101016-080937 is also acknowledged. ERH gratefully acknowledges the financial support from MINECO (Spain) and FEDER (EU), project MAT2015-71117-R.

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Slovenj Gradec, Final meeting, September 2020

## Platelet size-effects in the colloidal stability of aqueous graphene oxide dispersions

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Aqueous-phase exfoliation (individual separation of elementary layers) of multilayered graphite oxide to single-layer graphene oxide (GO) is a promising strategy to prepare bulk amounts of graphene based materials. A crucial point to the reproducible fabrication of solution-processed graphene materials (thin films, nanocomposites, etc.) is the knowledge and possible control of the dispersion stability of MLGO and SLGO. While this issue has largely been overlooked until several years ago, Chowdhury et al.<sup>1</sup> presented first results on the aggregation of GO's, revealing that their aggregation and stability in the aqueous environment followed colloidal theory (DLVO and Schulze-Hardy rule), even though GO's shape is not spherical. Following, Wu et al. presented somewhat contradictory results pointing out a significant pH-dependence in the colloidal stability of GO samples prepared by the same (Hummers-Offeman) method.<sup>2</sup>

Herein, we present new quantitative results of the charging and aggregation of graphene oxide dispersions. Particularly, we clarify the effect of pH on the colloidal stability in light of the previously published contradictory results. We shall explore the size dependence of the colloidal aggregation by demonstrating stability plots of GO fractionated into three size intervals. Our findings<sup>3</sup> demonstrate that the platelet size variation of GO results in highly different coagulation kinetics in the presence of a simple monovalent salt. This result may find important use in the formulation of GO dispersions allowing for a simple way towards hindering their aggregation by the decrease of particle size.

The financial support by the Ministry of Human Capacities, Hungary through grants 20391-3/2018/FEKUSTRAT and ÚNKP-20-5 New National Excellence Program is gratefully acknowledged. Projects no. 124851 has been implemented with the support provided from the National Research, Development and Innovation Fund of Hungary, financed under the FK funding scheme. T. S. also acknowledges the support by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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Slovenj Gradec, Final meeting, September 2020

### Enhancing TiO<sub>2</sub> photocatalytic activity: a survey on the effects of self-doping and of GRM-TiO<sub>2</sub> interfacing

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The superior intrinsic photocatalytic activity, the easy availability, the low cost, the low toxicity and the long-term stability against photo and chemical corrosion make TiO<sub>2</sub> a candidate of choice for the photoassisted removal of environmental pollutants and for chemicals and fuels production [1]. The TiO2 energy bandgaps (between 3.0-3.2 eV), which correspond to an optical absorption edge in the ultraviolet (UV) range, limits the actual TiO<sub>2</sub> performances since it cannot be activated by visible light and thus by solar light [1]. The development and the optimization of modified forms of TiO<sub>2</sub> that can be efficiently activated by visible light thus represent an important technological issue. The broadening of the optical absorption spectrum of  $TiO_2$  can be achieved by several approaches as doping (and/or co-doping) with foreign elements, formation of intrinsic defects (self-doping) as oxygen vacancies (OVs), synthesis of TiO<sub>2</sub>-based composite materials. In this work we investigate the effects of the latter two routes by considering specific TiO<sub>2</sub> surface modifications. As concerns the TiO<sub>2</sub> self-doping by OVs generation. we show that a simple and non-expensive thermal treatment of TiO<sub>2</sub> in ethanol (EtOH) reflux allows the production of a blue-colored TiO<sub>2</sub> powder characterized by surface oxygen vacancies, additional optical absorption in the visible range, unusual photoluminescence (PL) behaviors and enhanced VIS photocatalytic activity [2]. The broadening of the TiO<sub>2</sub> optical absorption is also achieved by interfacing TiO<sub>2</sub> with materials belonging to graphene family. In particular, graphene related materials GRM/TiO<sub>2</sub> hybrids are purposely produced to shed light on the peculiar charge-transfer processes activated by two GRMs, differing in chemo-physical and morphological features, in their interaction with the TiO<sub>2</sub> surface [3]. In both cases, the experimental campaign is carried out by combining standard characterization techniques, excitation-resolved photoluminescence (PLE) spectroscopy and photodegradation tests carried out using methylene blue as probe molecule in aqueous solution.

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### Stainless Steel Wettability And Friction In Different Environments Manipulated By Adsorption Of TiO2 Nanoparticle Coatings

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We present functionalization of AISI 316L surface by adsorption of hydrophilic epoxy and epoxy/TiO2/epoxy coatings and hydrophobic epoxy/fluoroalkylsilane functionalized, FAS-TiO2/epoxy coatings. Besides different wettability, the coatings differ also in morphology and average surface roughness. This enables a study of the combined effect of surface wettability and morphology on the friction coefficient and wear resistance. Experiments were performed in dry and distilled water environments as well as in simulated physiological solution (Hank's solution). In the case of dry friction, lower coefficient of friction is achieved for both TiO2 coatings compared to pure epoxy coating. In water environment the same level of friction is shown for all three coatings, indicating that friction level is defined by water itself. In Hank's solution, however, the wettability and implementation of TiO2 nanoparticles regulate the friction level through the reactions between the elements of the coating. Friction is reduced for hydrophilic epoxy/TiO2/epoxy coating, increased for hydrophobic epoxy/FAS-TiO2/epoxy and has no effect on pure epoxy coating. Finally, results show that coatings reinforced with TiO2 nanoparticles provide better protection of the steel surface as well as better resistance to mechanical and tribological loading provided by the formation of patches of coating material rich in Ti.

### **Dielectric Films from Cellulose nanofibrils and Graphene Oxide**

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Dielectric materials are, used to control and store dielectric energy, the basic components of film capacitors, which are in almost every sort of electronic devices. Polymer composites have been extensively utilized as dielectric materials than metals and ceramics due to their significant characteristics such as flexibility, low cost, lightweight nature, easy processability, etc. Due to the biodegradable and renewable nature, biopolymers like cellulose overcomes the existing nonrenewable polymer-based dielectric materials [1-3]. Here we investigate the dielectric performance of films based on cellulose nanofibrils (CNF) and graphene oxide (GO) where the GO was reduced via UV irradiation in-situ [1]. The resulting CNF-reduced GO composite films remain flexible and show improved dielectric properties. In such a composite system, the charge accumulated at the interface acts as a large electric dipole and using the Maxwell-Wagner polarization, the dielectric constant of composite system has been increased significantly. In addition, the UV induced reduction of GO, dispersed into the CNF network, is seen as a promising alternative dry method to hazardous wet chemical processes.

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# Antioxidant and electrically conductive starch-based films with multiwalled carbon nanotubes: the effect of surfactant solution

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The use of carbon-based materials is delivering new functional polysaccharide-based materials with an over broad range of application. The aim of this work was to develop starch films filled with multiwalled carbon nanotubes (MWNTs) non-covalently functionalized with surfactants. Before films formulation, MWNTs were dispersed and stabilized in aqueous media using surfactants with diverse chemical structures, such as sodium dodecyl sulphate (SDS), cetyl trimethylammonium bromide (CTAB), and sodium cholate (SC), under well-controlled conditions [1]. The starch-based films were produced by solvent casting, using glycerol as a plasticizer and MWNTs dispersion in three concentrations (1, 2 and 5 wt.% of starch). Films with SC show a better MWNT dispersion and mechanical properties than films with SDS and CTAB, since the last two surfactants turns the starch films less resistant and stiff. Antioxidant activity and electrical conductivity imparted to the starch matrix showed to be dependent of the amount of MWNTs and the type of surfactant, with CTAB being the most promising surfactant to functionalize MWNTs. Although the higher dispersion of MWNTs with SC, the strongest adsorption of SC on the MWNT surface and/or its good interfacial interaction with the starch molecules work out as a block effect on the MWNT performance for both antioxidant and electrical conductive properties. These films have potential applications in the packaging industry, particularly for food packaged sterilization by pulse electric field technology.

#### Acknowledgement

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# Integration of conductive layers within the Eumelanin pigment: advanced spectroscopic and structural studies on EU/GL and EU/GO hybrid materials

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Eumelanin (EU)-based blends obtained integrating this natural pigment with organic conducting materials are gaining increasing interest in the field of bioelectronics. Among these, hybrid materials obtained from EU and graphene-like (GL) layers revealed intriguing features concerning biocompatibility and transport properties [1-2].

Recent photoemission and nuclear magnetic resonances measurements [3] indicated the occurrence of peculiar packing features at a supramolecular scale in EU/GL hybrid materials (EUGLs), and their possible role on the enhancement of electrical conductivity in EUGLs. We performed a deeper investigation of the properties of these hybrids by: Small Angle X-ray Scattering (SAXS), High Resolution - Scanning Transmission Electron Microscopy (HR-STEM) and conductive Atomic Force Microscopy (C-AFM). Hybrid materials were prepared by in situ polymerization of the EU precursor 5,6dihydroxyindole (DHI) in presence of various amounts of GL layers, and carefully characterized by several standard laboratory techniques. Commercial Graphene-Oxide (GO) was also employed to realize analogous hybrids with EU (EUGOs) and used for comparison in our study. HR-STEM and SAXS confirmed the strong tendency of both EUGLs and EUGOs to organize themselves in aggregates much larger than in precursors EU, GL, and GO. First quantitative evaluations of SAXS data seem to indicate a bigger size of EUGL aggregates compared to EUGO ones; however, a more ordered arrangement in the latter hybrids, revealed by STEM images, is probably at the origin of the stronger electrical conductivity on a microscopic scale detected in the conductive AFM maps. Ongoing analyses should provide answers to some open questions concerning the fundamental mechanisms in the aggregation of EU with carbonaceous conducting materials.

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# Thermo-physiological and mechanical properties of textile, screen-printed with SWCNT-based printing pastes

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High thermal conductivity, stability and hardness of single-walled carbon nanotubes (SWCNT) [1, 2] are properties, that are important in improving thermo-physiological properties of textiles. Heat and water vapour transmission through fabric are two of the most important factors affecting the comfortable feeling when worn, since they control the transfer of excessive heat and water away from the body [3, 4].

The conventional screen printing method was used to apply SWCNT, dispersed in an acrylic-based paste or in a phosphorylated cellulose nanofibrils (PCNF) on a textile fabric using different printing methods (screen opening, one/two phase, single/double sided), thus to improve its thermo-physiological properties without affecting on its air permeability. The samples were dried after each printing step, fixated at higher temperatures and laundry washed. As prepared samples were analyzed by microscopy to identify the distribution of applied nanomaterials, as well as related to the mechanical, dimensional, heat and moisture resistance properties, air permeability and hydrophilicity (by contact angle).

Both SWCNT and PCNF have been shown to reduce resistance to heat transfer (up to 22%) and water vapor (up to 18%), and when printed double-sides using SWCNT-acrylic paste on one side and PCNF on the other, it results in the hydrophobic (outside turned when wearing) and hydrophilic (skin turned) surface, respectively, without significant reduction of air permeability. Features that all contribute to better wearing comfort, as body heat is easily transferred through the fabric and water vapor from the body. In addition, the mechanical properties are slightly increased.

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### In-situ TEM Studies on Carbon Nanomaterials

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In-situ transmission electron microscopy (TEM) is a very powerful and useful technique to investigate the properties of nanomaterials, even to modify them. Importantly, the structural information at the subnanometer scale (even at the atomic level) can be obtained during the measurements in parallel [1-6].

In this contribution, I will present the TEM in-situ possibilities that we have via some examples going from the thermal reduction of the graphene oxide (GO) [4], the transport measurements of this material [5] and the transformation of different nanotube-fullerene systems [6]. These works illustrate the rich information that can be obtained via this kind of experiments and their interest for studying such nanomaterials.

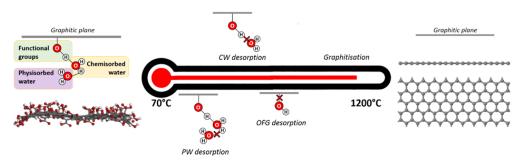


Figure 1: In-situ TEM thermal reduction of GO [4].

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the EU H2020 & APCIN-MICINN Spain (JTC-2017 Flag-ERA GATES project, PCI2018-093137) and the EU H2020 programs "Graphene Flagship" (Grant Agreements 785219, 881603), Marie Sklodowska-Curie "Enabling Excellence" (Grant agreement 642742) and "ESTEEM3" (Grant Agreement 823717).

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# Carbon Dots (CND) from carbon black: scalable top-down production and deposition in ultrathin film

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An extensive experimentation has been conducted since many years in our group aiming at exploring the potentiality of carbons blacks (CB) as starting material for the production of a highly varied array of advanced materials [1-2]. Our goal is to apply feasible approaches specifically designed to meet the continuous need of low cost and scalable protocols for tuning easily the relevant chemico-physical properties of carbon-based materials. Our recent work has succeeded in fabrication of water-stable yellow - green fluorescent carbon nanodots (CNDs) through a top-down demolition of a nanostructured CB (CB N110 type, furnace black) by a scalable wet chemistry approach.

In this study we will report the CNDs structural and morphological characterization (UV-VIS, FTIR and fluorescence spectroscopy, AFM) and we will explore the CND work-up as ultra-thin film by Matrix Assisted Pulsed Laser Evaporation (MAPLE) deposition technique. MAPLE technique provides a gentle deposition process specifically designed for fabricating thin layers of organic compounds, from the condensed phase (frozen water suspension), into the vapor phase using infrared laser radiation [3]. The MAPLE technique is particularly suitable for obtaining homogeneous, ultra-thin, well adherent coatings over the desired substrate with accurate thickness control by maintaining the chemical structure and the physiochemical properties of the deposited organic or polymer molecules. Structural characterization (UV-VIS, FTIR and fluorescence spectroscopy) confirms that the deposited CND films maintain the characteristics of the pristine CNDs. This circumstance opens to the large-scale production of next generation flexible electronic devices, passivation coatings, organic sensors and opto-electronic components.

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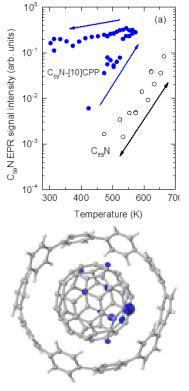
### Bottom-up design and realisation of stable fullerene spin systems

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Discrete energy levels of quantum spins at the molecular level are a promising platform for realising qubits. The major challenge remains how to build complex circuits from such molecular spin entities with sufficiently long decoherence times in order to conduct quantum computation algorithms. A major handicap towards exploitation of radicals is their inherently instability. In paramagnetic azafullerenyl radical C<sub>59</sub>N• the unpaired electron is strongly localized neighbouring the nitrogen and induces dimerization to diamagnetic bisazafullerene (C<sub>59</sub>N)<sub>2</sub>. We develop an innovative radical shielding approach using supramolecular complexation, exploiting the protection offered by a [10]cycloparaphenylene ([10]CPP) nanobelt ('the shortest carbon nanotube') encircling the C<sub>59</sub>N•. Photo-induced radical generation is increased 300 times. The characteristic triplet signal of C<sub>59</sub>N•@[10]CPP is traced even after several weeks, a lifetime increase of >10<sup>8</sup>, and in the solid phase produced via thermolysis, currently for several years.

This talk will focus on the role of DFT calculations in guiding this nanocarbon molecular design, and explore future possibilities for bottom-up design in fullerenes and ultra-short nanotubes.



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We acknowledge regional "Pari Scientifique" funding NEWTUBE for financial support, and the CCIPL (centre de calculs intensif pays de la loire) where many of these calculations were performed. We also thank COST CA15107 MultiComp and the MultiComp organisers for STSM exchange funding, many interesting meetings, and all their hard work planning and running MultiComp.

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Slovenj Gradec, Final meeting, September 2020

# Functional surfaces of laser-microstructured silicon coated with polymer blends with reversible wettability upon heating

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We develop functional surfaces of laser-microstructured Si, spin-coated with thermoresponsive PS/PNIPAM polymer blends and we study their switchable wetting behavior between hydrophilicity and hydrophobicity upon heating. PNIPAM is a thermoresponsive polymer, which is hydrophilic below 32°C and hydrophobic above 32°C. We take advantage of the large specific area and roughness of the micro-Si substrate to enhance the PS/PNIPAM film thermoresponsiveness.

Microstructured Si substrates were fabricated by ns laser irradiation in SF<sub>6</sub> gas. PS/PNIPAM blends, of various blend ratios, in THF were spin-casted onto flat and micro-Si substrates, with or without a native SiO<sub>2</sub> layer. The wetting state of PS/PNIPAM films was determined by water contact angle measurements. The morphology of the surfaces was mapped by SEM and the chemical composition by EDS and micro-Raman spectroscopy. The depth-resolved chemical composition of the polymer films was provided by XPS.

Upon heating, films on micro-Si switch from hydrophilic to hydrophobic. The transition is reversible for multiple heating/cooling cycles. Films casted on flat silicon do not undergo switching of their wetting behavior, even though they respond moderately to temperature. When films are casted on silicon with native SiO<sub>2</sub>, they show higher thermoresponsiveness, compared to substrates without SiO<sub>2</sub>. XPS reveals this is due to the arrangement of PS and PNIPAM in the films, depending on the presence or absence of the underlying SiO<sub>2</sub>.

#### Acknowledgement

We acknowledge support of this work by the project "Advanced Materials and Devices" (MIS 5002409) which is implemented under the "Action for the Strategic Development on the Research and Technological Sector", funded by the Operational Programme "Competitiveness, Entrepreneurship and Innovation" (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

Slovenj Gradec, Final meeting, September 2020

Multi**Comp** 

3. Posters

### Kinetic of crystallization of HDPE/SWCNT determined by Fast Scanning Chip Calorimetry

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The mechanical properties of polymers depend a lot on the degree of crystallisation, which depends on the processing conditions. The degree of crystallisation as well as the kinetics of crystallisation are usually determined by differential scanning calorimetry (DSC). However, the technique is slow and the kinetic of crystallisation can only be obtained at low supercoolings. Fast scanning chip calorimetry (FSC) is a tool to establish crystallization kinetics at high supercoolings, usually a few thousand degrees Celsius per second, which are usually observed during the polymer processing. Therefore, FSC is not only a good tool to determine the influence of processing condition on the degree of crystallisation [1], but also to simulate the development of the crystallinity during various processing condition.

Nanocomposites were prepared by using Haake MiniLab twin screw extruder, equipped with MiniJet injection moulding machine in a concentration of SWCNT of 0.1%, 0.2%, 0.3%, 0,4% 0.5%, 1%, 2%, 3%, 4% and 5%. The SWCNT were added in a form of masterbatch having 10% of SWCNT in paraffin. The temperature was 220 °C and the screw rotation was set to 100 rpm for 1 min (dosing) and 200 rpm for 9 min.

Kinetic of crystallisation was determined under dynamic conditions, The sample was heated to  $185 \,^{\circ}$ C at the heating rate 100 K/s and cooled to 0  $^{\circ}$ C at the cooling rates of 50 K/s, 100 K/s, 200 K/s, 500 K/s, 1000 K/s, 2000 K/s, 3000 K/s and 4000 K/s. However, due to very fast crystallization of the HDPE and nucleating effect of SWCNT the results obtained at 3000 K/s and 4000 K/s could not be properly evaluated.

The addition of SWCNT increased the temperature of the beginning of crystallization for 5-7 °C, which means that the nanotubes acted as a nucleating agent. The peak crystallisation temperature was also increasing with the increasing SWCNT concentration up to 0.5%, above that the results scattered. It seems that at lower content of SWCNT the crystallisation proceeded faster, while at the higher content (above 0.5%) the crystallisation rate was reduced, which is in agreement with classical DSC measurements.[2] The Avrami constants, obtained at various cooling rates were in the range of 2.0-2.7 for pure HDPE and mostly above 3.0 for composites. However, no correlations were observed according to the heating rate or nanotubes concentration. The scattering might be a consequence of the small sample size (nanograms) needed for FSC and non-homogenous particle distribution on such a small scale.

#### Acknowledgement

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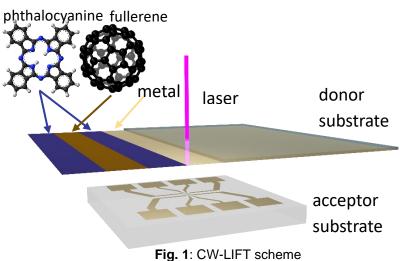
### Thin Metal Layers as DRLs for High-Resolution CW-LIFT of Phthalocyanine-Fullerene Heterojunctions

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Phthalocyanine-fullerene thin films, a promising material for solar cell technology, are typically formed by vacuum co-evaporation<sup>1</sup>. However, such deposition technique requires vacuum system and do not offer high-resolution. Here, we investigate the use of continuous-wave laser-induced forward transfer (CW-LIFT) as a suitable deposition technique for the formation of zinc phthalocyanine-fullerene nanocomposites. Continuous lasers enable the transferred materials to be designed into more precise patterns.

Thus far, CW-LIFT has only been used to deposit inorganic materials such as silver inks<sup>2</sup>, carbon nanofibers<sup>3</sup> and graphene<sup>4</sup>. However, we believe that it has considerable potential for the deposition of nanocomposite and organic materials when used with a metal dynamic release layer (DRL). In particular, we seek to determine the laser energy range at which nanocomposites are formed with suitable morphology and composition. The laser deposition system consisted of a CW laser with a 405 nm operating wavelength, 50 mW power source and 4x microscope objective. The laser energy was controlled by altering the laser scan speed in the range of 0.05 - 5 mm/s. Gold DRL was used to absorb the laser energy for the local thermal transfer of thin phthalocyanine and/or fullerene films to a receiver substrate. SEM scans showed that microcrystals were formed in a wide laser scan speed range. Our results suggest that CW-LIFT is a suitable deposition technique when operated with the appropriate laser scan speed.



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# Formation of titanium doped diamond-like carbon films by magnetron sputtering technique

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Titanium and oxygen doped amorphous carbon films were deposited using layer by layer magnetron sputtering technique. To obtain thin films graphite and titanium cathodes were sputtered at low pressure (2 Pa) argon atmosphere. During the experiments the graphite cathode sputtering power was kept constant (~ 1.0 kW), while the titanium cathode power varied (80 W, 175 W and 360 W). The influence of dopant concentration on the amorphous carbon films properties was examined. The elemental composition of the amorphous carbon films and surface morphology and were inspected using energy dispersive X-ray Quantax system with a XFlash 4030 detector (Bruker) attached to the field emission scanning electron microscope Quanta 200 FEG. To determine the surface roughness NT-206 atomic force microscope was used. Nanoindentation tests were performed by MTS-Agilent G200 nanoindenter. The optical properties were determined using UV–VIS–NIR spectrophotometer (Shimadzu UV-3600). The structure of titanium-oxygen doped carbons films was investigated using Horiba Jobin Yvon LabRAM HR micro-Raman spectrometer.

It was obtained that the increase of titanium sputtering power enhance the titanium concentration from  $\sim$ 2 at.% to  $\sim$ 12 at.%. Titanium has strong bonding affinity with oxygen, therefore, as the titanium content increased in the coatings, the oxygen concentration had risen from  $\sim$ 15 at.% to  $\sim$ 45 at.%. Raman spectroscopy results indicated that the increase of dopant concentration caused graphitization of the coatings. Incorporation of dopants resulted in a higher surface roughness values. However, the increase of titanium content reduced the surface roughness of the films. VIS - NIR spectroscopy results showed that the transparency of the films decreases with the decreasing wavelength. Microhardness test revealed that the hardness of the films was  $\sim$  4 GPa.

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# Temperature dependent electrical conductive properties of films prepared from differently dispersed single-walled carbon nanotubes and cellulose nanofibrils

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The effect of temperature and humidity on the electrical properties of thin films based on multiwalled carbon nanotubes (MWCNT) [1] and cellulose nanofibers (CNF) have been recently reported [2]. In order to get better inside into the effect of nanostructure of such a paper-based films on their el. conductivity and physico-mechanical properties, the films prepared from differently dispersed single-walled carbon nanotubes (SWCNT, including cellulose derivative/CD, polymeric carboxylic acid / PCA, and carboxymethyl cellulose / CMC) and different types of fibrillated cellulose (cellulose nanofibrils / CNF, cellulose microfibrils / MFC, and phosphorylated CNF) were investigated. The change in DC resistivity was measured using in situ electrical resistance measurement cell having four probe technique. The composite films were found remaining stable for most of the films up to 150°C with an average conductance of 0.645 S/cm, given the best result (1.89 S/cm) for the film prepared from 50 w/w% of SWCNTs dispersed in CMC. The SEM images obtained supported the study by showing homogenously dispersed SWCNTs in all nanocellulose matrices. The films mechanical properties and hydrophobicity was also improved.

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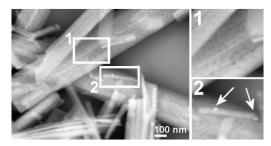
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# The role of cerium in H<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> nanoribbons in transformation to TiO<sub>2</sub>-B nanoribbons

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The presence of cerium in  $H_2Ti_3O_7$  nanoribbons in transformation to  $TiO_2$ -B nanoribbons was investigated. Pristine  $H_2Ti_3O_7$  nanoribbons were exposed to the aqueous solution of  $Ce(SO_4)_2 \cdot 4H_2O$ , followed by calcination of dried material at ~600 °C,  $TiO_2$ -B phase was still observed in X-ray diffractograms (XRD) of materials calcined above 700 °C. Typically pure  $TiO_2$ -B nanoribbons are obtained at calcination at 400 °C [1]. As expected, calcination in air did not affect the nanoribbon morphology of the product  $TiO_2$  nanoribbons, as can be seen from scanning electron images (SEM) of the sample calcined at 620 °C (Figure 1). However, upon this transformation, the nanoribbons became mesoporous, and pore diameter ranges from 2 to 10 nm, which is characteristic of less dense  $TiO_2$ -B phase [2]. The cerium oxidation state was determined by X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS). The results show that the oxidation state of cerium partially changed from 4+ to 3+ already during the first preparation step, i.e. adsorption and drying.



**Figure 1**: SEM image of Ce-TiO<sub>2</sub>-B nanoribbons taken with a backscattered detector. Inset 1 reveals mesoporous texture of the nanoribbons. Arrows in inset 2 are pointing toward bright CeO<sub>x</sub> particles.

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### Wake effect in interactions of ions with graphene-sapphire-graphene structure

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In our recent publication<sup>1</sup> we have studied the wake potential induced by an external charged particle that moves parallel to various  $sy_1$ -Al<sub>2</sub>O<sub>3</sub>- $sy_2$  composites, where  $sy_i$  (with i=1,2) may be vacuum, pristine graphene, or doped graphene. Several important parameters were fixed at their respective typical values: the distance of the charged particle from the closest surface, the thickness of the sapphire (aluminum oxide, Al<sub>2</sub>O<sub>3</sub>) layer, and the doping density (i.e., Fermi energy) of graphene.

In this work we present a detailed study of the effects due to variations of all those parameters in the case of the wake potential produced by charged particle moving parallel to the graphene-Al<sub>2</sub>O<sub>3</sub>-graphene composite system, by using the dynamic polarization function of graphene within the random phase approximation for its  $\pi$  electrons described as Dirac's fermions and by using a local dielectric function for the sapphire layer<sup>2</sup>.

For the velocity of the charged particle below the threshold for excitations of the Dirac plasmon in graphene, given by its Fermi velocity  $v_F$ , strong effects are observed due to variation of the particle distance, while for the velocity of the charged particle above  $v_F$  strong effects are observed due to variation of the particle varying the thickness of the Al<sub>2</sub>O<sub>3</sub> layer, as well as due to graphene doping.

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### Influence of Mg on Al alloy / MWCNT nanocomposites

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Lighter auto parts reduce the overall weight of the car, contributing to the reduced fuel consumption and decrease in carbon (IV) oxide (CO<sub>2</sub>) emissions. In order to achieve this, the scientists are focused on the research of new materials, nanocomposites based on a metal matrix and multi-walled carbon nanotubes (MWCNTs). MWCNT have been imposed as a reinforces because of their high strength, high active surface and good thermal-mechanical properties. In the auto parts manufacturing industry, the High Pressure Die Casting (HPDC) process is the most commonly used, which has not been sufficiently investigated in the literature as a possible process for a nanocomposite preparation.

The aim of this study was to investigate the possibility of an HPDC process for the production of AlSi9Cu3 (Fe) alloy nanocomposite material with the MWCNT and to investigate the effect of the Mg on the surface interaction between the Al alloy and the MWCNT. The results obtained by scanning electron and light microscope and energy dispersive X-ray spectroscopy showed the stability of the MWCNT and, with the results obtained by the mechanical testing through the small scattering of the results, the homogeneity of the nanocomposite samples with 0.05 wt% MWCNT was proven. With the addition of the Mg the most significant increase in the elongation, hardness and elasticity of the sample were achieved, what is attributed to the better wettability of the phases, i.e. Mg improved the interfacial bonding, which is in the line with the literature<sup>1,2</sup>.

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