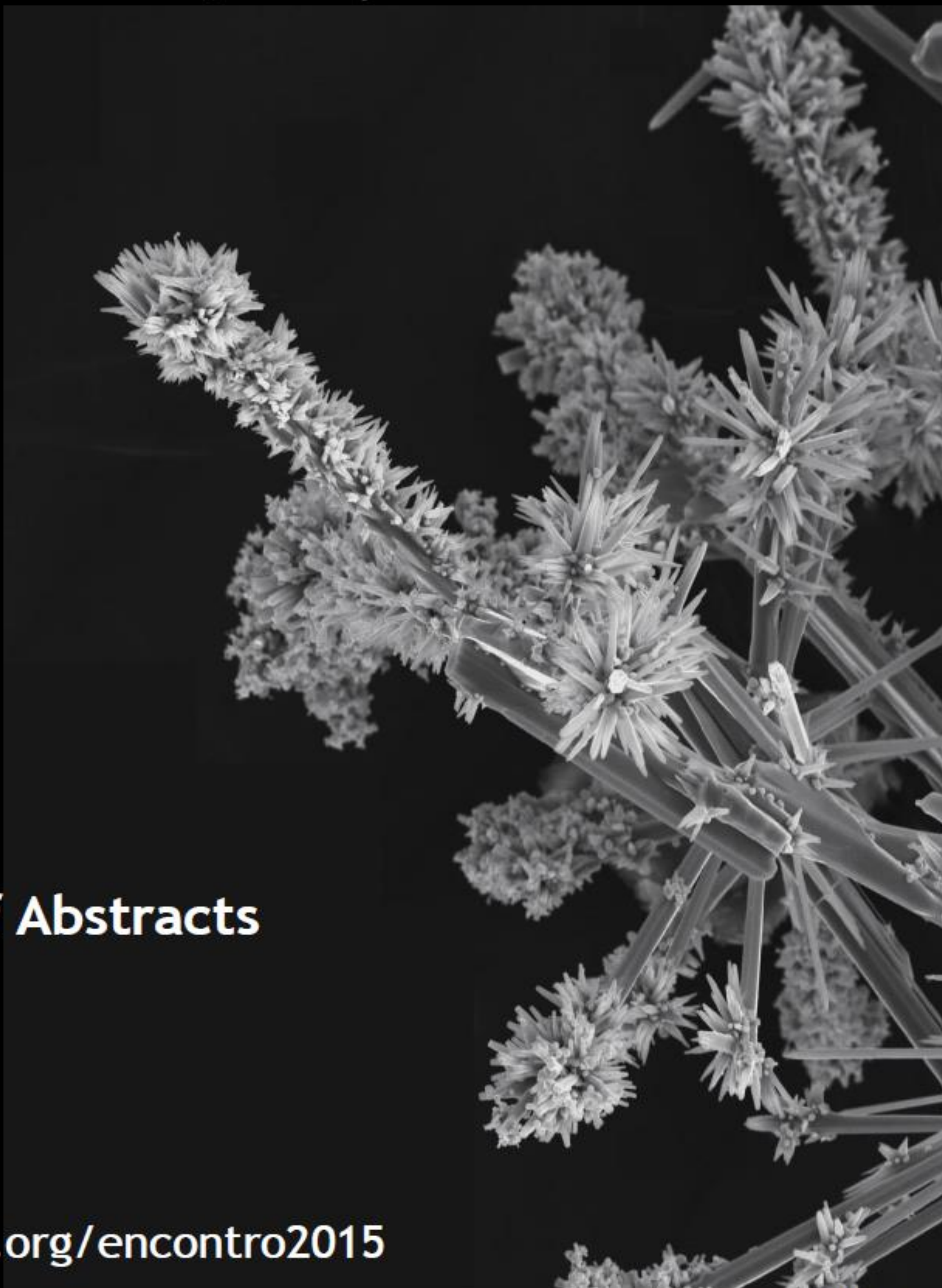
V Annual Meeting i3N

Aveiro, 10-11April 2015



ZnO/Ag Crystals
(Joana Rodrigues, I3N)

Book of Abstracts

www.i3n.org/encontro2015

i3N

Universidade do Minho
Escola de Engenharia

universidade
de aveiro

FCT FACULDADE DE CIÊNCIAS E TECNOLOGIA

Book of Abstracts

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Welcome to Aveiro

Nanosciences and Nanotechnology in strong relation with Advanced Materials, are key elements for today's society and at i3N we have now a great responsibility, since we have achieved the highest mark of "OUTSTANDING" from the recent evaluation done by FCT-MEC, which is placing now i3N as the leading Portuguese research unit in the areas of Nanotechnology and Advanced Materials.

At i3N we believe that the combined strengths of a collaborative team is by far, orders of magnitude greater than the sum of the individuals. In a multidisciplinary field such as Nanotechnology this is even truer.

i3N is organized into 9 research groups with a strong interaction under 3 main thematic lines:

- Micro/Nano Integration into Demonstrator Systems
- Theoretical and Computational Studies on Materials and Devices/Systems behaviour
- Advanced Micro/Nano Materials and Technologies

This year we would like to thank again all the authors and a special thank to Prof. Lars Montelius, INL Director and Prof. Ehrenfried Zschech, Director Dresden Center for Nanoanalysis.

With the state-of-the art tools for micro/nanotechnology fabrication, advanced materials production, and device characterization available at i3N, the sky is the limit in terms of what one can achieve here!

Enjoy the meeting and your time in Aveiro.

Elvira Fortunato
I3N Director

Programme

Friday, 10 April

12h00 - Registration and Lunch at Castro – Building M

14h00 - Opening

14h05 - Invited Talk

Prof. Lars Montelius (NL Director)

15h00 - Group presentations I

15h00 Engineering Design and Technologies with Polymers and Composites, O. Carneiro

15h15 Nanomaterials and Novel Polymer Systems, Z. Denchev

15h30 Semiconductors Physics, A. Neves

15h45 Theoretical and Computational Physics, V. Torres

16h00 Novel Materials and Bio-Systems, M. Valente

16h15 Optics and Optoelectronics, J. Pinto

16h30 - Posters presentations and Coffee break

18h00 - Invited Talk

Prof. Ehrenfried Zschech (Dresden Center for Nanoanalysis)

19h00 - Group presentations II

19h00 Materials for Electronics, Optoelectronics and Nanotechnologies, R. Martins

19h15 Soft and Biofunctional Materials Group, M.H. Godinho

19h30 Structural Materials, Braz Fernandes

20h30 - Dinner

Saturday, 11 April

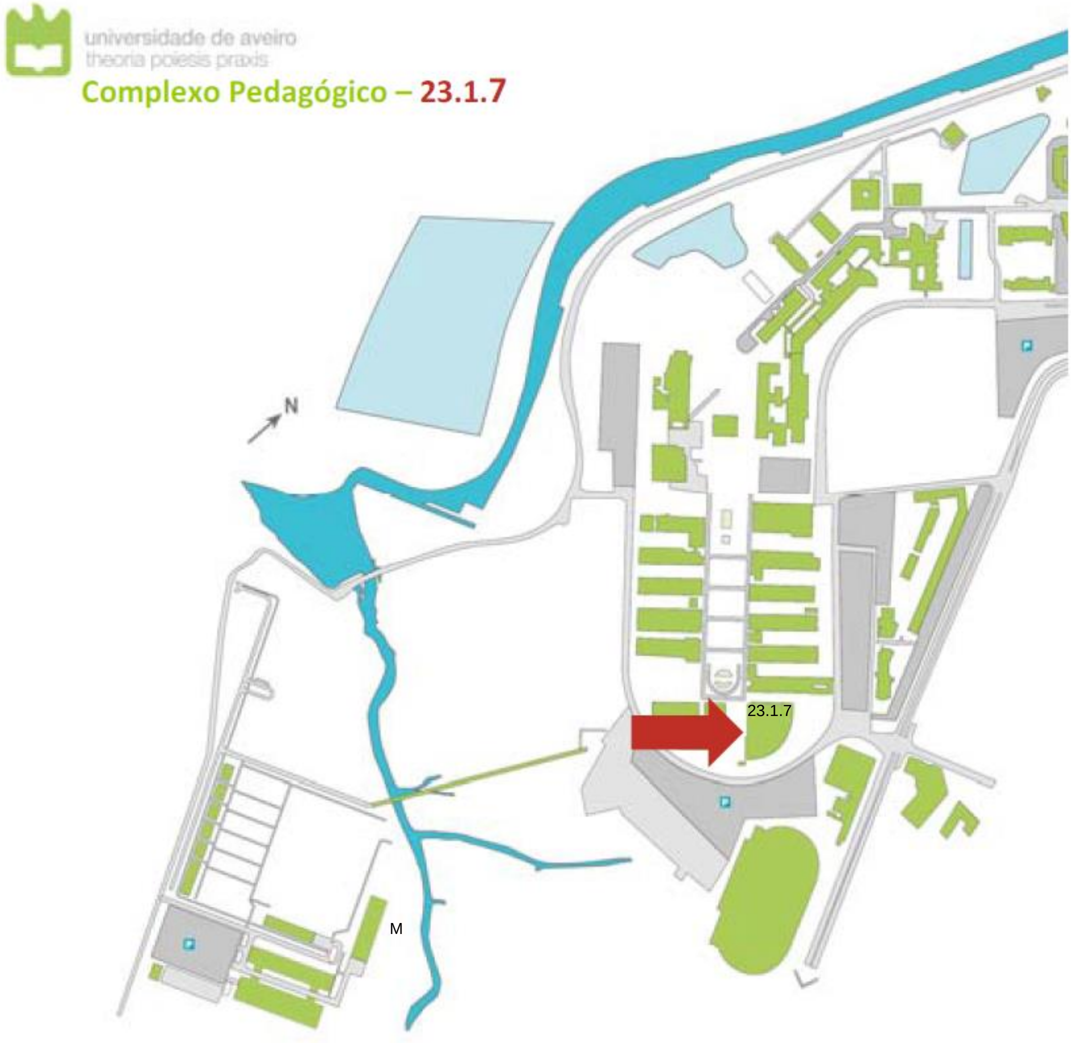
09h00 - General Meeting

11h00 – Closing and Coffee Break

General Information

Conference Venue

The Conference will be held at the Complexo Pedagógico building at the University of Aveiro, Aveiro, Portugal



About Aveiro

Aveiro is a city in Aveiro Municipality located in west-central Portugal, right by the Atlantic Ocean shore, with a total area of about 200 km² and a population close to 80,000 inhabitants. Inserted into a region of great industrial development, full of trades and services, Aveiro is annually visited by more than 100,000 tourists, being a reference centre for culture and leisure and offering a high quality of life.

The New Art (an architectural and decorative style that marked the late 19th and early 20th century) and all the several city museums, the salt flats, the famous Ria de Aveiro, its typical boats called Moliceiros and channels that cross the city (making it known as the "Venice of Portugal"), the beautiful extensive beaches just minutes away, the refreshing green spaces scattered all over town, the delicious local gastronomy (like Ovos Moles, a well-known delicacy made of egg yolks and sugar) and its vicinity to well-known wine caves (Porto, Bairrada, Dão, etc), all of these are just a few of the hallmarks of a young and dynamic city with plenty to offer to visitors.

University of Aveiro

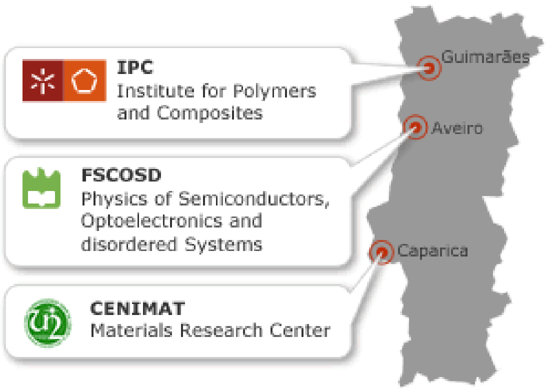
Created in 1973, the University of Aveiro quickly became one of the most dynamic and innovative universities in Portugal. Now a public foundation under private law, the UA's mission is to create knowledge and expand access to knowledge through research, education and cooperation for the benefit of people and society, to undertake the project of global development of the individual, to be active in the construction of a European research and education community and to promote a model of regional development based on innovation as well as scientific and technological knowledge.

Attended by about 15,000 students on undergraduate and postgraduate programmes, the UA has achieved a significant position amongst higher education institutions in Portugal, being one of the top universities regarding the quality of its infrastructures, the strength of its research and the excellence of its staff. More information available on the website: http://www.ua.pt

i3N

i3N, the Institute of Nanostructures, Nanomodelling and Nanofabrication was granted the status of Associated Laboratory on November 16th 2006, by the Portuguese minister of Science, Technology and Higher Education, José Mariano Gago.
i3N is one of the major portuguese institutions in the area of nanosciences and nanotechnologies.
i3N is a partnership between three leading research units in fundamental and applied science: IPC (Institute for Polymers and Composites, hosted by University of Minho), CENIMAT (Materials Research Center, hosted by the New University of Lisbon) and FSCOSD (Physics of Semiconductors, Optoelectronics and disordered Systems, hosted by the University of Aveiro). Over one hundred researchers are currently involved in multidisciplinary fundamental and applied research projects in three thematic lines:

- Micro/Nano Integration into Demonstrator Systems
- Theoretical and Computational Studies on Materials and Devices/Systems behaviour
- Advanced Micro/Nano Materials and Technologies



Invited Talks Presenters

	Prof. Lars Montelius	Director of Iberian Nanotechnology Laboratory, INL

Lars Montelius defended his thesis in 1987 at Lund University and during 1988-89 he spent a Post-doc year at IBM, Yorktown Heights working with Scanning Probe Microscopy. In 1989 he was appointed as Head of the Nanometer Laboratory at Lund University. His 25+ years of work in nanotechnology has centered around scanning probe microscopy & spectroscopy & luminescence & imaging & manipulation of low-D structures, electron & ion beam and nanoimprint lithography & processing applied to single electron tunneling, quantized conductance and various bio and NEMS-devices. Lars Montelius H-index is 32 and he has given more than 70 personally invited talks, filed 22 patent applications and published more than 170 publications giving rise to 3.639 citations, with ≈250 citations per year over last 5 years. (Data from ISI Web of Knowledge 2014-03-29).
Currently he is the President Elect for IUVSTA: The International Union for Vacuum Science, Technique and Applications iuvsta-us.org/ and he is Working Group Chair of the two European Technology Platforms NANOFutures: The European initiative for sustainable development by Nanotechnologies www.nanofutures.eu and EuMat: The European Technology Platform for Advanced Engineering Materials and Technologies: eumat.eu.
(source: http://inl.int/members/115)

Scientific Coordinator of the Dresden Center for Nanoanalysis at TU Dresden	Prof. Ehrenfried Zschech

Prof. Ehrenfried Zschech is Division Director at Fraunhofer Institute for Nondestructive Testing in Dresden, which he joint in 2009. His responsibilities include micro- and nano-analysis as well as R&D in the field of test systems.

He received his diploma degree in solid-state physics and his Dr. rer. nat. degree from Dresden University of Technology. After hav-ing spent four years as a project leader in the field of metal physics and reliability of micro-electronics interconnects at Research Institute of Nonferrous Metals in Freiberg, he was ap-pointed as a university teacher for ceramic materials at Freiberg University of Technology.

In 1992, he joined the development department at Airbus in Bremen. There he managed the metal physics group and worked on laser-joining metallurgy of light metals. From 1997 to 2009, Ehrenfried Zschech ma-naged the Materials Analysis Department and the Center for Complex Analysis at AMD in Dresden. In this position, he was responsible for the analytical support for process control and technology development, as well as physical failure analysis.

His current research interests are in the areas nanomaterials and nanoanalysis, with the focus on thin film technology and nanotechnology. He has published three books and more than 170 papers in scientific journals in the areas of solid-state physics and materials science. He is honorary professor for nanomaterials at the Brandenburg University of Technology in Cottbus, Germany. Ehrenfried Zschech was elected as President of the Federation of European Materials Societies (FEMS) for 2011/2012.

(source: http://www.mfd-dresden.com)

Groups Presentations

Engineering Design and Technologies with Polymers and Composites	Olga S. Carneiro	
	Zlatan Denchev	Nanomaterials and Novel Polymer Systems
Semiconductors Physics	Armando Neves	
	Vítor B. Torres	Theoretical and Computational Physics
Novel Materials and Bio-Systems	Manuel A. Valente	
	João L. Pinto	Optics and Optoelectronics
Materials for Electronics, Optoelectronics and Nanotechnologies	Rodrigo Martins	
	Mª Helena Godinho	Soft and Biofunctional Materials Group
Structural Materials	Francisco Braz Fernandes	

ENGINEERING DESIGN AND TECHNOLOGIES WITH POLYMERS AND COMPOSITES (EDTPC)

O. S. Carneiro

Institute for Polymers and Composites, IPC/i3N, Department of Polymer Engineering, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal

The main objectives of the EDTPC group are the following:

- to foster new knowledge through research in relevant areas promoting advanced design, optimized processing, high value manufacturing and innovative products, from concept to production phase, addressing the entire value chain of advanced materials knowledge;
- to improve the capabilities to design, to manufacture and to market high-value products and integrated systems, in order to support the competitiveness of the industrial tissue;
- to develop a multidisciplinary and integrated approach to engineering design and technologies with advanced material systems;
- to contribute towards fulfilment of major social needs and solving important industrial problems with a strategic relevance for the society and the industry, reinforcing national competences and sustainable environment.

Targeting these objectives, the EDTPC ongoing research activity is organized in four research lines (RL), where several research topics are addressed, according to:

- (RL2.1) Processing: modelling, monitoring and optimization (Process monitoring and visualization, Process modelling and optimization, Melt mixing methods, Processing of advanced polymer systems);
- (RL2.2) Development of advanced manufacturing processes, forming tools and products (New intelligent and integrated manufacturing processes, Microfabrication);
- (RL2.3) Processing-structure-properties relationships (Establishing relationships between processing, structure and properties, Structure development analysis, Deformation mechanisms, Multi-scale modelling);
- (RL2.4) Engineering Design and Sustainability Studies (Advanced methodologies and tools for engineering design, Methodologies for systems integration design, Design of multifunctional products and structures, Life-cycle thinking of polymer systems).

NANOMATERIALS AND NOVEL POLYMER SYSTEMS (NNPS)

Z. Z. Denchev

Institute for Polymers and Composites, IPC/i3N, Department of Polymer Engineering, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal

The main objectives of the NNPS group are:

- To perform innovative and internationally recognized fundamental and applied research related to various aspects of the synthesis, chemical modification, application and advanced characterization of polymer-based materials.
- Collaborating actively with the other entities of IPC and i3N, NNPS will carry out investigation in emerging interdisciplinary areas assisting the development of know-how for sustainable innovative materials, manufacturing techniques and devices related to polymer composites.
- To promote practical application of the R&D results fostering their transfer to industry and educating relevantly prepared workforce.

Targeting these objectives, the ongoing research activity of NNPS is organized in four research lines (RL), each of which having several research topics, namely:

RL1. Development of new polymer-based functional and active systems including: micro- and nanostructured composites with multiple stimuli response; polymer materials for energy production and storage; biodegradable and bioactive polymer systems for advanced industrial and environmental applications.

RL2. Functionalization and compatibilization in multicomponent polymer systems including: new synthetic routes towards functionalized carbon allotropes and their use in advanced composites; compatibiization in synthetic, bio- and bioderived nanostructured polymer systems.

RL3. Synthesis of new polymer and copolymer systems with controlled architecture involving: covalent and non-covalent interactions; organic/inorganic hybrids by advanced polymerization techniques; polymer micro- and nanocapsules with different payloads; micro- and nanoporous polymers and copolymers with medical and environmental application; self-healing polymer-based materials.

RL4. Advanced characterization of multicomponent polymer systems and developing of new methodologies for: in-situ characterization of flowing complex fluids, static and in-line optical and spectral characterization in various processing environments, advanced structural measurements including synchrotron X-ray and neutron scattering measurements.

SEMICONDUCTORS PHYSICS GROUP

Armando Neves

Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal

The Semiconductor Physics group develops its research activities in the preparation and characterization of semiconductor materials of different dimensionality, micro- and nano-structured, for applications in the areas of electronics and optoelectronics, energy and bio-medical. We aim to achieve a deep understanding of the physical properties (optical, electric, magnetic) relevant to the electronic behavior of the materials and their intended applications.

In the area of energy we explore new materials and novel architectures to enhance state-of-the-art solar cells; we identify suitable optical centres in doped wide band gap oxides and nitrides for efficient lightning; and develop light emission devices based on organic semiconductors. We produce and dope semiconductor nanoparticles and study their optical and electronic transport properties and the physical properties of their assemblies. In the bio-medical area we work on the development of bio-compatible nano-carbon structures for biosensors and for bone tissue reparation. The group nurtures a team that develops micro-structured gas detectors for dosimetry/tomography applications and for high-energy physics.

In this presentation the recent achievements of the group will be given, and the present and future work will be discussed.

THEORETICAL AND COMPUTATIONAL STUDIES AT I3N-AVEIRO

Vítor J.B. Torres[1] and José Fernando Mendes[1]

[1]Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal

The theoretical and computational group carry out studies on condensed matter, including nanocrystals, and on complex network systems.
Electronic and vibrational properties of defects in semicondutors and their alloys, as well in nanocrystal and nanosystems, are calculated using Density Functional Theory Codes. High electronic correlated materials and phase transitions are investigated using Monte Carlo and Molecular Dynamics methods. Figure 1 illustrated how we can achieve charge transfer (doping) between a molecule and Si nanocrystals of different sizes. Few more examples will be presented in the talk.
Complex network systems comprises non equilibrium systems, multiplex and neural networks.

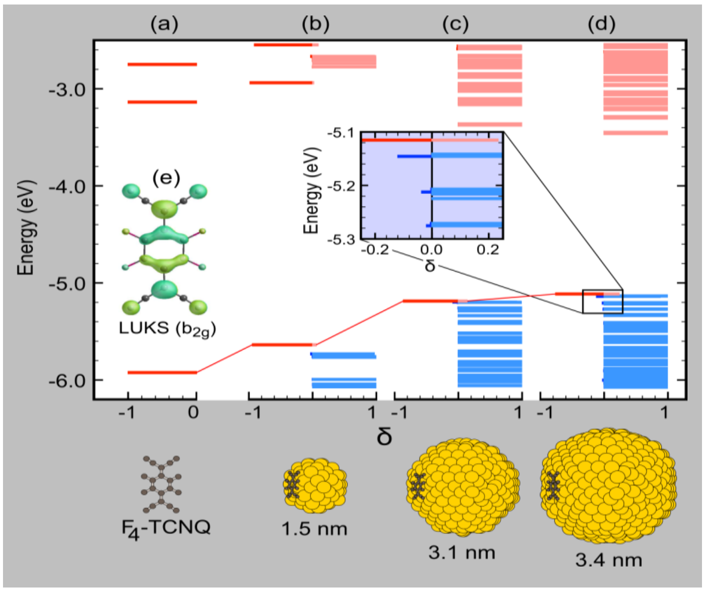


Figure 1 – Eletronic energy levels of a F4-TCNQ molecule and a Si nanocrystal.

BRIEF NOTES ABOUT THE RESEARCH DONE BY "NOVEL MATERIALS AND BIO-SYSTEMS" GROUP

M.A. Valente[1], L.C. Costa[1], F.M. Costa[1], S.K. Mendiratta[1], M.P.F. Graça[1], N. M. Ferreira[1], F. Amaral[2] , E.V. Ramana[1], J. Suresh Kumar[1], K. Pavani[1]

[1]Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal
[2]Polytecnic Institute of Coimbra, 3000-271 Coimbra, Portugal

The "Novel Materials and Bio-systems Group" is devoted to the materials processing as well as dielectric, electrical, magnetic and optical characterization of materials for electronic, optoelectronic and energy applications. The group is focused on: **1**-Development of techniques for preparation of materials: a) Laser floating zone for superconductors, thermoelectric and large dielectric constant materials, b) microwave processing for porcelain synthesis (T=1450ºC) and "cure cork" (a low temperature). **2**-Development of novel materials prepared by sol-gel, auto-combustion, spin-coating, high energy ball milling, sintering, their structural, electrical, magnetic and optical characterizations: a) polymer composites with carbon nanotubes and nanoparticles, graphene, b) magnetic nanoparticles and ferrites for microwave absorption, c) glasses and glass-ceramics with dielectric, magnetic, and/or optical properties, glasses and phosphors for photoluminescence, d) ferroelectrics and multiferroics**,** e) materials with colossal dielectric constant, f) hydroxyapatite-based materials for bio applications. **3 -** Advanced characterization techniques: a) VSM platform to characterize: a) magnetic nanoparticles, glasses with magnetic oxides, multiferroics, crystals, manganites, hydroxyapatite. **4-** Effect of electromagnetic field in living organisms. **5 -** Projects with industrial deliverables. The group led or participated in projects promoted by industry.

MATERIALS FOR ELECTRONICS, OPTOELECTRONICS AND NANOTECHNOLOGIES (MEON)

R. Martins

Department of Materials Science/i3N, FCT-UNL, Campus de Caparica, 2829-516 Caparica, Portugal

The MEON group is involved in developing, design, modelling and fabrication of advanced multifunctional oxides at a micro and nanoscale levels processed via chemical and physical routes, followed by a proper heat treatment, for a broad range of applications, such as: transparent and flexible electronics; electrochromic materials; thermoelectric materials; solar cells; thin film transistors; CMOS; ring oscillators; power controllers; logic gate circuits; amplifiers; memories; sensors; among others, combined or not with organic materials, aiming to develop a new generation of devices away from silicon, where are included the hybrid devices to boost to excellency the potential of the materials involved.

The paper electronics, is one of the key areas where activity related to paper selection; fibers, surface and bulk functionalization are ongoing activities aiming to produce test vehicles targeting sustainable and low cost systems of great relevancy for our future such as intelligent packaging, smart labels for food and pharmaceutics industry; full disposable active and passive bio-detection platforms for a broad range of applications, all full recyclable. Here the main target is to promote a paper electronic pilot line to serve the Country and Europe.

The group is also developing thin silicon solar and their components using nanostructured, plasmonics, nanocrystalline and microcrystalline silicon materials, processed by plasma enhanced chemical vapour deposition with higher sunlight to-electricity conversion efficiency and reduced costs. Another relevant area concerns the development of biosensors, including microfluidic platform for a broad range of analysis, as DNA via colorimetric methods based on gold nanoparticles plasmonics, using different configurations and substrates, as paper.

SOFT AND BIOFUNCTIONAL MATERIALS GROUP

M.H. Godinho

Department of Materials Science, CENIMAT/I3N, FCT-UNL, Campus de Caparica, 2829-516 Caparica, Portugal

The Soft and Biofunctional Materials group (SBMG) is much involved in the study of soft materials, which are easily deformable by external stresses, magnetic, electric fields, or even by thermal fluctuations. The SBMG is directing its activities in three main research lines, in order to intensify the collaboration across different groups in I3N: i. Nanostructures, nanodevices and microsystems, ii. Structural functional and smart materials, and iii. Flexible electronics and photonics. The materials in which we are interested on include liquid crystalline-based soft systems, colloids, macromolecular, namely cellulose based materials, biological systems and elastomeric Janus particles. The structure of those materials as well as their dynamics at the mesoscopic scales determines their physical properties. The goal of our research has been dedicated to probe and understand this relationship. The techniques we use include rheology (Rheo), nuclear magnetic resonance (NMR), Rheo-NMR, magnetic resonance imaging (MRI), light scattering, optical microscopy, electrospinning, microfluidics and tensile and wettability measurements. In this presentation an overall view of the more recent achievements of the group will be given. We very much expect that this brief and full of images talk will encourage for deeper discussions and future collaborations between the I3N groups.

STRUCTURAL MATERIALS RESEARCH GROUP - OVERVIEW

Francisco Manuel Braz Fernandes

Department of Materials Science, CENIMAT/I3N, FCT-UNL, Campus de Caparica,
2829-516 Caparica, Portugal

The presentation will cover a general overview of recent results obtained by the Structural Materials Research Group (SMRG) in the field of the production of nanostructured materials (metals, ceramics and composites), as well as on techniques of micro/ nano-characterization:

- Shape memory alloys (processing and joining techniques, as well as applications in biomedical engineering),
- Friction Stir Processing (FSP) of Al alloys,
- Archaeometallurgy studies on micro/nano characterization (μ-XRF, OM, SEMEDS and μ-XRD),
- Novel low temperature sinterable glasses and glass/nanoceramic particle composites,
- Innovative optical microsensors based on rare-earth doped phosphate glass,
- Micro/nano characterization through X-ray absorption spectroscopy techniques using synchrotron radiation,
- Perspectives for new trends of micro/nano characterization based on 3D X-ray diffraction.

These results will be complemented by information about the national / international collaborations, as well as some figures illustrating the scientific productivity of the group.

Posters Presentations

N.º	Author	Title
P1	Neto, Joana	Validating devices for recording neural activity
P2	Rodrigues, Joana	ZnO micro/nanocrystals grown by Laser Assisted Flow Deposition
P3	Nunes, Daniela	Design of new functional materials for electronics applications
P4	Botas, Alexandre	Core-shell and core-host interaction effects on the optoelectronic properties of functional silicon nanoparticles
P5	Soares, Rosa	Luminescence in Ln^{3+} doped YSZ Phosphors
P6	Falcão, Bruno	Structural and optical properties of Mg-doped wurtzite-rich GaAs nanowires
P7	Santos, N.F.	Nanocarbon hybrids for biosensors and microelectronics
P8	Cunha, Eunice	Preparation of graphene nanoribons and few-layer graphene in solution
P9	Echeverria, Coro	A Cellulosic Liquid Crystal under shear: Rheo-NMR study
P10	Lima, Ana Luísa	Novel Organic Materials for Optoelectronics
P11	Costa, R.A.	Solution of the explosive percolation quest
P12	Oliveira, Tiago	Metadopants for Semiconductor Nanocrystal Superlattices
P13	Nico, Cláudia	Fundamental Studies on the Physical properties of Niobium Oxides
P14	Mould, Sacha	Multiscale modelling of polymer nanocomposites
P15	Dencheva, Nadya	Polyamide Microcapsules and Composites Thereof for Technical and Biotechnological Applications
P16	Sepúlveda, Alexandra	Use of Nanocomposites for Flexible Pressure Sensors
P17	Fernandes, Célio	Computational Rheology
P18	Teixeira, Paulo	A small-scale experimental set-up for processing-related materials characterization
P19	Araújo, Andreia	Metal Nanoparticles for Plasmon-Enhancement in SI Solar Cells and Raman Spectroscopy
P20	Sousa, M.G.	Effect of the sulphurization conditions on the properties of Cu2ZnSnS4 thin films and solar cell performance
P21	Teixeira, J.P.	Identification of radiative and non-radiative channels in Cu-poor $Cu_2ZnSn(S,Se)_4$ solar cells
P22	Krishnapuram, Pavani	Spectral converters to enhance the efficiency of solar cells
P23	Deuermeier, Jonas	Transparent p-type transistors based on Cu2O – Understanding material properties to enhance device performance
P24	João, Carlos	Liquid Crystalline Inverse Opals - New Bone like Assemblies for Tissue Engineering
P25	Salgueir, Daneila	Ink-jet printing of amorphous oxide semiconductors for high performance TFTs
P26	Wojcik, Pawel	Printable organic and inorganic materials for flexible electrochromic devices
P27	Gaspar, Diana	Cellulose based substrates for application in electronic devices
P28	Wojcik, Bernacka	Design and development of a microfluidic platform for use with colorimetric gold nanoprobe assays
P29	Ferrás, Luís	Studies on dispersion efficiency of polymer nanocomposites
P30	Santos, Raquel	The effect of surface functionalization of graphite nanoplates on the dispersion in polypropylene melts

P31	Lopes, M.A.	Forecasting epileptic seizures in neuronal networks
P32	Holz, Tiago	Diamond and stiff diamond/buckypaper carbon hybrids for MEMS
P33	Castro, I.F.C.	Nuclear medical imaging devices based on solid-state materials
P34	Vieira, Tânia	Development of a new nanostructured scaffold for neural stem/progenitor cell transplantation
P35	Fernandes, Susete	Structural colours in cellulose: Sculpting the flow of light
P36	Triandade, Ana Catarina	Janus Particles
P37	Olievira, João	Laser welding of shape memory alloys
P38	Silva, A.M.L.	Micropattern structures for gaseous detectors –large radiation detection at micro-scale resolution
P39	Kumar, J.S:	Photoluminescence studies on sodium niobium tellurite glass-ceramics for optical sensor applications
P40	Pereira, Filipa	Early metallurgical steps in the Prehistoric Portuguese Estremadura
P41	Figueiredo, Elin	From Ores to Metal: investigating ancient bronze production
P42	Sendrine, N.B.	Raman spectroscopy of MBE-grown INGAAS/ALP ultra-short period superlattices
P43	Ferreira, N.M.	Assessment of a free CO2 iron making method
P44	Almeida, A.J.	Electronic doping and magnetic anisotropy in nanocrystal quantum dot systems
P45	Rodrigues, S.M.G.	Nonlinear optical phenomena in microstructured optical fibers
P46	Santos. Lídia	Nanostructured Metal Oxides for Application in Electrochemical devices
P47	Costa, Mafalda	Lab-on-Paper Platforms for Assembling Inexpensive Diagnostic Assays
P48	Martins, Jorge	Transparent Electronics: Implementation of Process/Physical Device Simulation Tools and Analog Circuit Fabrication with Oxide TFTS
P49	Ramana, F.V.	Lead-free multifunctional magnetoelectric materials for device applications
P50	Santos, P.	Hydrogen passivation of titanium impurities in silicon: effect of doping conditions
P51	Baxter, G.	Weak percolation on multiplex networks
P52	Pimentel, Ana	Study and Development of Multifunctional ZNO:1D Nanostructures to te used in Electronics Devices
P53	Vicente, António	Development of Nanomorphous Silicon Solar Cells on Ceramic Substrates with Biomedical Application
P54	Leitão, C.	Optical fiber sensors in non-invasive cardiovascular monitoring
P55	Santo,s T.	Modelization and development of microwave sintering cavities
P56	Teixeira, S.S	Development of new materials for energy storage based on alkali ferrites
P57	Mendes, Manuel	Light Trapping in Thin Film Solar Cells With Self-Organized Plasmonic Nanospheres

P1

VALIDATING DEVICES FOR RECORDING NEURAL ACTIVITY

J. P. Neto[1,2], G. Lopes[2] , J. Frazão[2], J. Nogueira[2], P. Lacerda[2], P. Baião[1], P. Barquinha[1], A. R. Kampff[2]

[1] CENIMAT/I3N, Departamento de Ciências dos Materiais, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa and CEMOP/Uninova, Caparica, Portugal

[2] Champalimaud Neuroscience Programme, Champalimaud Centre for the Unknown, Lisbon, Portugal

Considerable progress is still necessary to reliably understand and increase the number of neurons that are recorded and identified simultaneously during extracellular recordings. This project aims to deliver ‘ground truth’ data that can be used to validate existing, and future, large and dense extracellular recordings. Therefore, we developed a novel targeting system that will be vital for characterizing new electrode materials/designs, the development of new algorithms for automatically sorting single-units, and resolving nagging questions regarding the origin and nature of the extracellular signal.

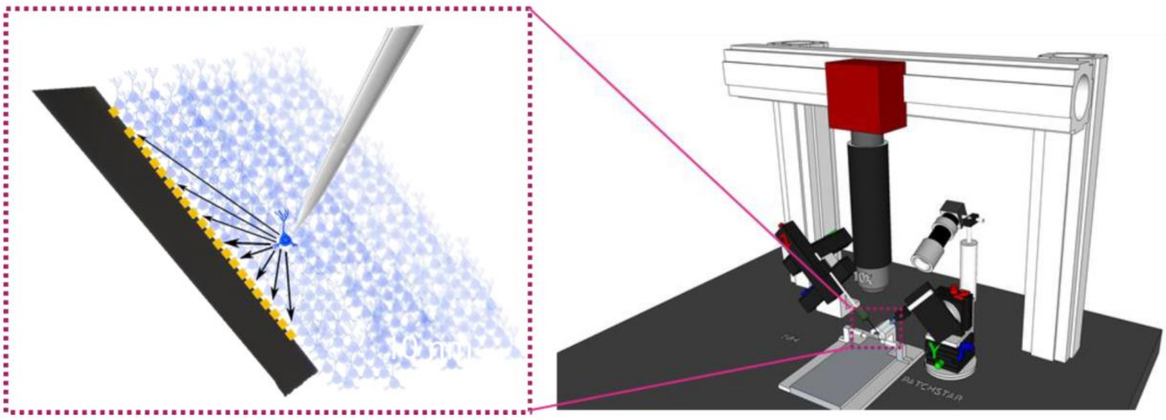


Figure 1 – Setup for acquiring “dual-recordings” where the spiking activity of a neuron is monitored with both a dense extracellular polytrode and a juxtacellular micro-pipette. Our setup allows for efficient, reliable and automated targeting of both probes to the same neural structure with micron

P2

ZnO MICRO/NANOCRYSTALS GROWN BY LASER ASSISTED FLOW DEPOSITION

J. Rodrigues, T. Monteiro, F. M. Costa

Department of Physics/I3N, University of Aveiro, Campus Santiago, 3810-193 Aveiro, Portugal

ZnO is one of the most widely studied materials due to its high potential for applications in several fields, such as optoelectronics, energy conversion or biomedicine. The high vapor pressure of ZnO and the fact that the material decomposes into its atomic components at the melting temperature (1977ºC) at atmospheric pressure, makes ZnO a suitable candidate for the Laser Assisted Flow Deposition (LAFD) growth. This method is a high yield technique that takes advantage of the mentioned properties combined with the local heating generated by a high power laser [1,2]. The LAFD technique leads to different ZnO morphologies depending on the region of the growth chamber where the products are formed, mainly nanoparticles, tetrapods and microrods. These morphologies are formed during the same run of growth. Nonetheless, with an appropriate choice of the growth conditions, namely the laser power and the growth atmosphere, it is possible to control the growth and selected the morphology. The crystals grown by this process usually reveal high structural and optical quality.

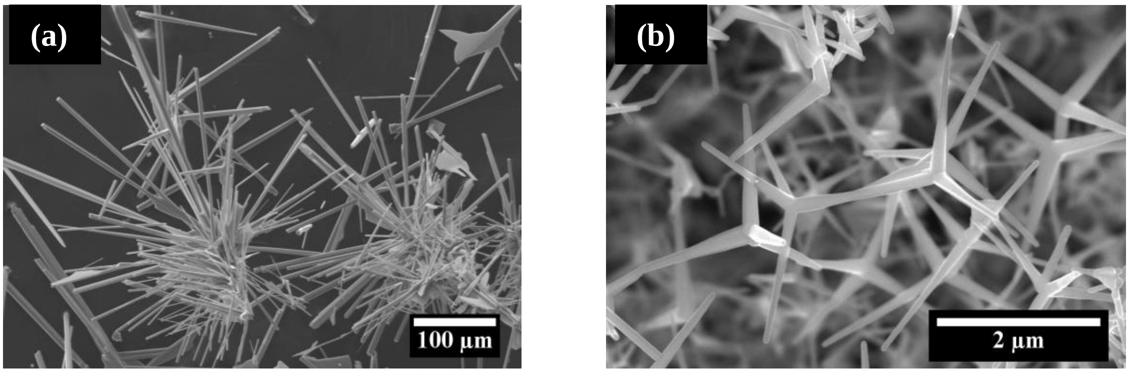


Figure 1 – ZnO (a) microrods and (b) tetrapods grown by LAFD.

[1] J. Rodrigues *et al.*, Thin Solid Films **520**, 4717–4721 (2012);
[2] J. Rodrigues *et al.*, Acta Materialia **60**, 5143–5150 (2012).

P3

DESIGN OF NEW FUNCTIONAL MATERIALS FOR ELECTRONICS APPLICATIONS

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The aim of my work is to develop and structurally characterize Cu and Cu oxide-based nanostructures. The study involves the synthesis of materials ranging from nanowires to nanospheres, and their morphology, as well as the effect of structural defects will be investigated. The as-synthesized Cu nanowires (Fig. 1 (a)) were further oxidized under microwave irradiation [1] or by furnace annealing in air, originating Cu2O and CuO nanowires, respectively. The nanowires oxidized by furnace annealing displayed aggregates of nanoparticles with about 30 nm in size (Fig. 1 (b)), while the nanowires oxidized via microwave irradiation consisted of larger Cu2O polyhedral nanocrystals (Fig. 1 (c)). EFM showed that Cu nanowires displayed different energy levels of trap charges along their body associated to structural defects and native oxide islands. Cu2O nanospheres consisted of aggregates of nanocrystals, which displayed distinct cathodoluminescence effects.

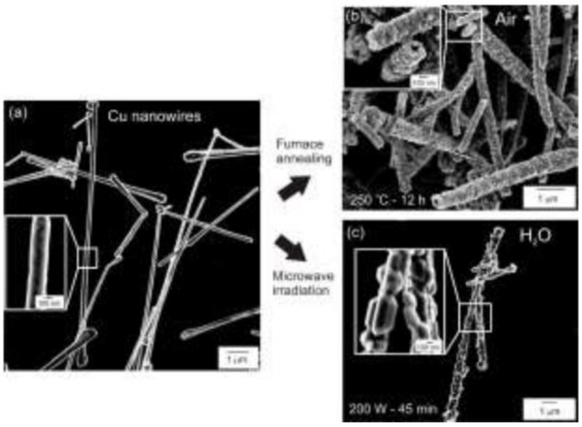

Figure 1 –- (a) SEM images of metallic Cu nanowires, (b) nanowires oxidized by annealing in air, and (c) nanowires oxidized with microwave irradiation.

[1] D. Nunes, A. Pimentel, P. Barquinha, P.A. Carvalho, E. Fortunato, R. Martins, Cu_2O polyhedral nanowires produced by microwave irradiation, Journal of Materials Chemistry C, **2**, 6097 (2014).

P4

CORE-SHELL AND CORE-HOST INTERACTION EFFECTS ON THE OPTOELECTRONIC PROPERTIES OF FUNCTIONAL SILICON NANOPARTICLES

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Crystalline silicon nanoparticles (SiNPs) are under intense investigation as they combine the unique features of Si at the nanoscale with the versatile and inexpensive device fabrication associated with nanoparticle processing. Due to the small dimensions, the large surface shell and species chemically/physically attached to the SiNP, interface- and surface-related phenomena eventually dominate the optical response of SiNPs. In this work, temperature-dependent steady-state and time-resolved photoluminescence and absolute quantum yield are used to study gas-phase grown SiNPs with different surface termination, such as Si-H bonds (SiNPs-H) and 1-dodecene (SiNPs-C12). The emission spectra of SiNPs-H and SiNPs-C12 display a broad band peaking at ~1.64 eV ascribed to the recombination of photogenerated excitons in the crystalline core of the SiNPs. After surface oxidation another component with a distinct lifetime and associated with surface/interface states of the oxide shell appears at higher energies [1]. The SiNPs-C12 have a high quantum yield value (~24%) when compared to that measured for SiNPs-H (~3%). The experimental results were interpreted considering the decrease in the probability of the exciton migration provided not only by the different terminal groups but also by the distinct separation distances induced by these groups.

[1] Botas, A. M. P., R. A. S. Ferreira, R. N. Pereira, R. J. Anthony, T. Moura, D. J. Rowe, U. Kortshagen, J. Phys. Chem. C **118,** 10375 (2014)

P5

LUMINESCENCE IN Ln^{3+} DOPED YSZ PHOSPHORS

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Yttria stabilized zirconia (YSZ), a wide band gap oxide, is a suitable host for the incorporation of optical activated lanthanide ions (Ln^{3+}). High quality YSZ single crystals doped with different Ln^{3+} ions were grown by laser floating zone (LFZ) technique. Under prompt excitation conditions, these single crystals show intense emission with different colors, depending on dopant ion and ion concentration, evidencing its viability as efficient phosphors for solid state lighting [1]. Moreover, this host also reveled to be very interesting for the incorporation of Ln^{3+} ions with efficient up-conversion (UC) luminescence. UC nanomaterials are of great importance for bio-application including biosensing and bio-imaging. Pulsed laser ablation in liquid (PLAL) was successfully used to produce Er^{3+} and Er^{3+}, Yb^{3+} doped YSZ NPs with spherical shape and highly crystalline. Under infra-red excitation the NPs show an intense green UC luminescence at room temperature that increase in the presence of the Yb^{3+} sensitizer, revealing high pottentialities to be used as efficient bioprobes [2].

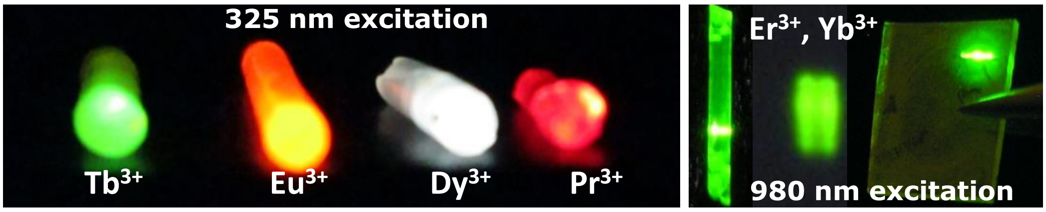

Figure 1 – Photos of the YSZ samples doped with different Ln^{3+} ions under UV (left) and infra-red excitation (right).

[1] M.R.N. Soares, M.J. Soares, A.J.S. Fernandes, L. Rino, F.M. Costa, T. Monteiro, YSZ:Dy^{3+} single crystal white emitter, J. Mater. Chem., **21**, 15262 (2011).
[2] M.R.N. Soares, T. Holz, F. Oliveira, F.M. Costa, T. Monteiro, Tunable green to red ZrO_2:Er nanophosphors, RSC Adv, **5**, 20138 (2015).

P6

STRUCTURAL AND OPTICAL PROPERTIES OF Mg-DOPED WURTZITE-RICH GaAs NANOWIRES

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GaAs nanowires (NWs) are promising building blocks for third-generation solar cells. In this work, we present a report on the photoluminescence of Mg-doped GaAs NWs and thin-films with different levels of doping. In the case of the thin-films, it is only observed a single radiative transition related to Mg acceptors that redshifts with the increase of concentration, due to the bandgap energy narrowing effect [1]. The photoluminescence from individual NWs and from a bunch of several hundreds of NWs is analyzed at several excitation power densities and over a wide temperature range, and is compared to that of the thin-films. It is found that in the NWs the radiative transitions are critically influenced by the staggered type II band alignment, due to the existence of polytypic regions along the NWs, and seems to be independent of the Mg concentration [1,2].

[1] B. P. Falcão et al., New insights on the temperature-dependent photoluminescence of Mg-doped GaAs nanowires and epilayers, J. Mater. Chem. C, **2**, 7104 (2014).
[2] B. P. Falcão et al., Structural and optical characterization of Mg-doped GaAs nanowires grown on GaAs and Si substrates, J. Appl. Phys., **114**, 183508 (2013).

P7

NANOCARBON HYBRIDS FOR BIOSENSORS AND MICROELECTRONICS

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Nanocarbon hybrids hold a high application potential, namely through the integration of sp^3 and sp^2 coordinated carbon forms and their properties. In this framework, microwave plasma CVD conditions for the growth of nanocarbon hybrids were studied. Using a single MPCVD run, nanocrystalline diamond (NCD) and carbon nanotube (CNT) hybrids were obtained using a continuous delivery of Fe catalyst. The films were characterized by SEM and µ-Raman spectroscopy, proving the coexistence of sp^2 and sp^3 phases, either in a dense multi-layer arrangement or in a porous 3-D like morphology, Fig.1a. Without catalyst, NCD nanoplatelets were also synthesised, Fig1b. High quality and well intercalated hybrid carbon forms were thus successfully obtained in a simultaneous growth procedure.

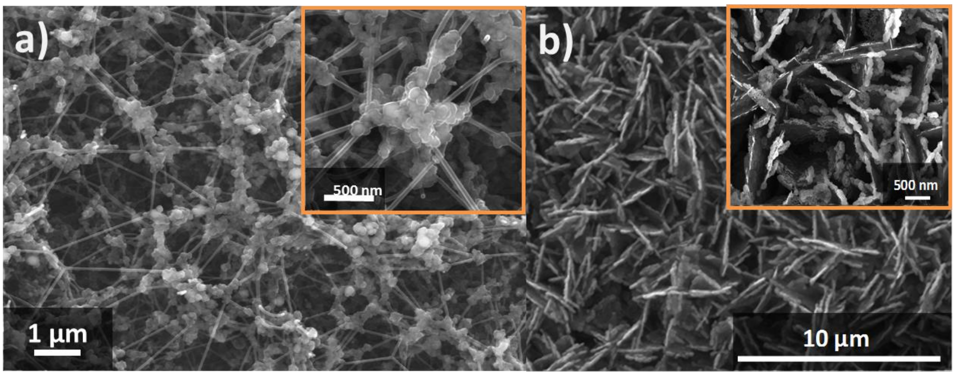

Figure 1 – a) neural-like network CNT/NCD hybrid and b) diamond nanoplatelets

The wide variety of biocompatible stable allotropes of carbon enables the development of new functional materials for biosensing and microelectronics.

[1] N.F. Santos, A.J.S. Fernandes, T. Holz, R.F. Silva, F.M. Costa, Simultaneous CVD Growth of Nanostructured Carbon Hybrids, *NATO SCIE PEACE SECU*, **39**, 111 (2015).

P8

PREPARATION OF GRAPHENE NANORIBONS AND FEW-LAYER GRAPHENE IN SOLUTION

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Two approaches to produce suspensions of graphene using non-oxidative routes were investigated at IPC. One of the approaches is based on the unzipping of functionalized carbon nanotubes in ethanol to form graphene nanoribbons (GNR), and the other concerns the exfoliation of graphite in water using pyrene derivatives, through a non-covalent functionalization approach, to produce few-layer graphene. The graphene produced was characterized by Raman spectroscopy and scanning tunneling microscopy (STM). Applications of these graphene under study comprise nanostructured multilayer films and electrochemical sensors.

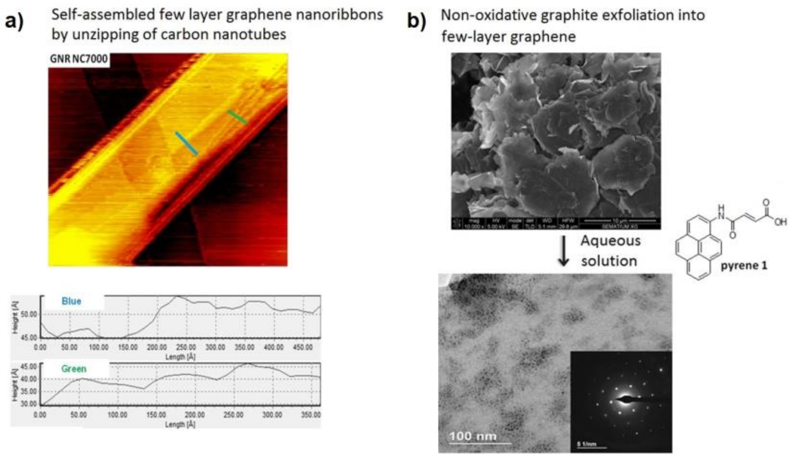

Figure 1 – A stacking of few layers of graphene nanoribbons observed by STM (a); graphene flakes obtained by exfoliations with functionalized pyrene (b).

P9

A CELLULOSIC LIQUID CRYSTAL UNDER SHEAR: RHEO-NMR STUDY

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Since long ago cellulosic lyotropic liquid crystals were thought as potential systems to produce fibers competitive with spiderwebs or Kevlar, yet the processing of high modulus materials from cellulose-based systems was hampered by their complex rheological behaviour. Cellulose and its derivatives such as hydroxypropylcellulose (HPC) can form networks similar to elastomers when produced from liquid crystalline (LC) solutions, that can be manipulated in order to produce helicoidal structures and spirals that respond to external stimuli producing bending, unbending and torsion motions similar to movements found in plants. The main objective of this work is to understand the structure-properties relationship and the mechanism behind the motion by means of a deep study of the cholesteric liquid crystal HPC/water system using Rotational rheology and Rheo-NMR in order to determine the structural changes induced by shear flow. [1]

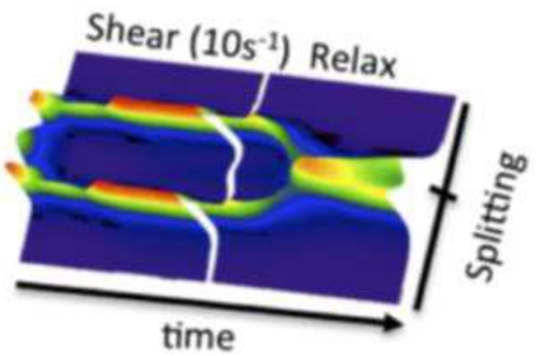

Figure 1 – Evolution with time of DNMR spectra of LC-HPC during shear and relaxation process.

[1] C. Echeverria, P.L. Almedia, G. Feio, J. L. Figueirinhas, A.D. Rey and M.H. Godinho., Rheo-NMR study of Water-Based Cellulose Liquid Crystal System at High Shear Rates, Polymer, DOI: 10.1016/j.polymer.2015.03.050 (2015).

P10

NOVEL CELLULOSE BASED MATERIALS FOR OPTOELECTRONICS

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Nowadays the intensive use of polymeric materials raised environmental problems related with waste management. To solve this problem some strategies were adapted, but were not applied to high performance materials. Cellulose acetate (CA) is a biodegradable polymer and is an alternative to cellulose, which is difficult to process [1]. In order to develop novel biodegradable materials with optical/conductive properties, it is necessary to incorporate some specific compounds into the biodegradable matrix [2]. These compounds should allow to conduct electricity, as carbon nanotubes and porphyrins. The last ones are intensely coloured and have also interesting optical properties. Therefore the main objectives of this work is to prepare materials based in cellulose acetate with optical/conductive properties by using a green approach in order to obtain environmental friendly materials.
The results showed that the incorporation of small amounts of CNTs delayed the polymer degradation induced by thermal-mechanical effects during processing, and also enhanced the polymer thermal stability. Melt compounding in the extruder showed less and smaller agglomerates and a better distribution of CNTs into the polymer matrix. The sample prepared with 0.5 wt% CNTs was the only that achieved both rheological and electrical percolation. Future work relies on the preparation of nanofibers by electrospinning of cellulose acetate and porphyrins already modified in this work.

[1] Y. Li, M. Wu, R. Liu, and Y. M. Huang, Solar Energy Materials and Solar Cells **93** (8), 1321 (2009).
[2] Z. Spitalsky, D. Tasis, K. Papagelis, and C. Galiotis, Progress in Polymer Science **35** (3), 357 (2010).

P11

SOLUTION OF THE EXPLOSIVE PERCOLATION QUEST

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Percolation refers to the emergence of a giant connected cluster in a disordered system when the number of connections between nodes exceeds a critical value. The percolation phase transitions were believed to be continuous until recently when in a new so-called “explosive percolation” problem for a competition driven process, a discontinuous phase transition was reported. The analysis of evolution equations for this process showed however that this transition is actually continuous though with surprisingly tiny critical exponents. For a wide class of representative models, we develop a strict scaling theory of this exotic transition which provides the full set of scaling functions and critical exponents. This theory indicates the relevant order parameter and susceptibility for the problem, and explains the continuous nature of this transition and its unusual properties.

[1] R. A. da Costa, S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, Explosive Percolation Transition is Actually Continuous, Phys. Rev. Lett., **105**, 255701 (2010).
[2] R. A. da Costa, S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, Solution of the explosive percolation quest: Scaling functions and critical exponents, Phys. Rev. E., **90**, 022145 (2014).
[3] R. A. da Costa, S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, Critical exponents of the explosive percolation transition, Phys. Rev. E., **89**, 042148 (2014).
[4] R. A. da Costa, S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, Solution of the explosive percolation quest. II. Infinite-order transition produced by the initial distributions of clusters, Phys. Rev. E., **91**, 032140 (2015).

P12

METADOPANTS FOR SEMICONDUCTOR NANOCRYSTAL SUPERLATTICES

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Deliberate introduction of foreign atomic species into materials lies at the heart of microelectronics. It has allowed the fabrication of doped structures tailored to perform with precise electrical, magnetic, optical and catalytic specifications. Analogously, doping of artificial solids or multi-modal devices made of wave-function engineered nanocrystals (NCs), is expected to play a crucial role in exciting and disruptive technologies like quantum computing, logical sensing, photovoltaics or biological tagging. Unfortunately, doping of electronic confined nanocrystals may not share many benefits of bulk doping like (1) the strong screening of the dopant ionic potential; (2) host bent bands with low carrier effective masses; (3) incommensurately high density of host states available for carrier promotion; (4) the extreme purity of materials; not to mention self-purification and segregation effects that may hinder dopant introduction. Based on inter-NC and core-shell heterostructures, we propose that nanocrystals can be engineered to become the actual dopants (i.e., metadopants) with virtually vanishing ionization energies to be used in NC superlattices, disordered networks and other ensembles. We employ density functional calculations of NC superlattices with several NCs per unit cell (including the metadopant) to explore this alternative doping route for the prototypical example of SiGe core-shell system.

P13

FUNDAMENTAL STUDIES ON THE PHYSICAL PROPERTIES OF NIOBIUM OXIDES

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Niobium oxides have been pointed as an alternative to tantalum in the production of solid electrolytic capacitors, with advantages regarding the dielectric constant, density and price. In this work, it is intended to create a new family of niobium oxides based capacitors, adapting the technology and production line currently used with tantalum. Despite the known potentialities of niobium oxides, and many types of niobates, in several technological applications, the understanding of these oxide systems is still noticeably insufficient. In this context, several fundamental studies on niobium oxides are presented, namely structural, microstructural, optical and electrical characterizations, which allow not only to contribute in an important way for the general knowledge of the physical properties of these materials, but also to advance to a sustained development of the niobium oxides based solid electrolytic capacitors. Several processing parameters were studied, which enables to point the direction to be followed in order to create a prototype.

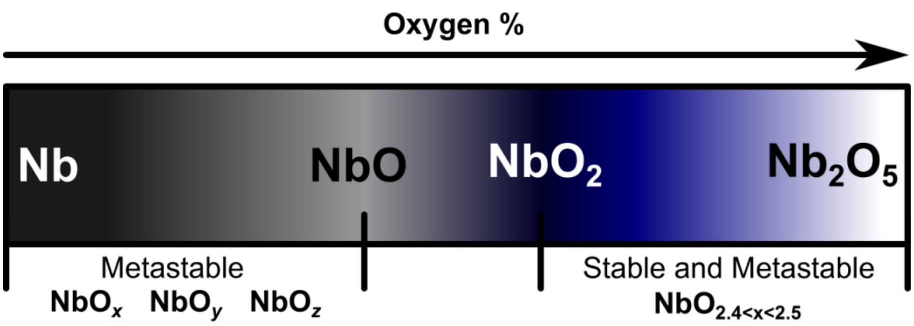

Figure 1 – Schematic illustration of the different oxidation states of Niobium.

P14

MULTISCALE MODELLING OF POLYMER NANOCOMPOSITES

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Tailoring the characteristics of polymer nanocomposites in order to obtain a specific behavior under service conditions requires a clear understanding of the link between their inherent many-scale features, the corresponding properties and the effects of manufacturing. Indeed, the hierarchical characteristics of these materials extend over a wide range of length and time scales, i.e., from the molecular scale (where the surface energetics between species dictate the miscibility), through the mesoscopic scale (where diffusion and solubility parameters influence the equilibrium morphology), and the macroscopic scale (where properties depend on the overall synergies betweem the components). Multiscale modelling combines models and simulation techniques intrinsic to each scale to predict relevant properties that cannot be handled with simulations at a single scale. This work presents an atomistic-to-mesoscopic multiscale procedure aiming to provide an insight into the range of length scales covered by the molecular structure and large-scale morphology of polymer nanocomposites. The link between scales is achieved following a coarse-graining strategy to estimate the effective free-energy terms for the mesoscopic model from atomistic simulations. A case study dealing with polymer/layered silicate nanocomposites is presented, providing good predictions of the interlayer morphology, basal spacing and particle dispersion state.

P15

POLYAMIDE MICROCAPSULES AND COMPOSITES THEREOF FOR TECHNICAL AND BIOTECHNOLOGICAL APPLICATIONS

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Polyamide microcapsules (PMC) were synthesized by an original one-pot method via activated anionic polymerization (AAP) of lactams [1]. The PMC contain in their cores a number of solid, finely divided materials: clays, metals or metal oxides, carbon allotropes, other polymer´s powders. These PMC were transformed through conventional melt-processing techniques into micro- and nanocomposites applicable in energy shielding or storage. Biotechnological applications for protein and enzyme immobilization or for stimuli-responsive microsystems sensitive to pH, magnetic fields and temperature were also studied. Functionalization of magnetic PMC for pH responsivenes with subsequent model proteine immobilization was studied envisaging applications in solid-phase diagnostics, biosensors, biocatalysts, in extracorporeal therapy and bioseparation.

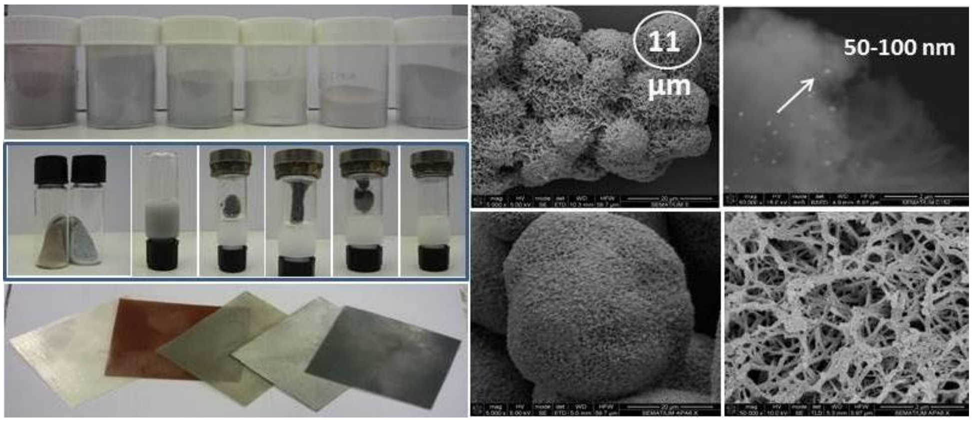

Figure 1 – PA6 hybrid microcapsules and hybrid composites thereof.

[
1] Z. Denchev, N. Dencheva, Polyamide microcapsules and method to produce the same, Patent Application No PT 107879 (2014)

P16

USE OF NANOCOMPOSITES FOR FLEXIBLE PRESSURE SENSORS

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This work presents a fabrication technique to produce conductive polymer nanocomposites (PNCs), which were used to produce flexible capacitive pressure sensors. The entire nanocomposite structure was fabricated using as-grown (1% V_f) vertically aligned carbon nanotubes (A-CNTs) embedded in a flexible substrate of polydimethylsiloxane (PDMS) through capillarity wetting. Mechanical characterization was performed in order to completely characterize the A-CNTs/PDMS nanocomposites. Its Young's modulus showed a 10 times increase (8.1 MPa) in the longitudinal direction in comparison to the unreinforced PDMS matrix (0.8 MPa).
The developed flexible capacitive pressure sensors are composed by three thin layers: top and bottom are A-CNTs/PDMS nanocomposites (electrodes) and the middle one is made of pure PDMS with a cavity with air defining the dielectric. Static results revealed reasonably good linearity in the range of 0 – 100 kPa, mainly in the region near to the atmospheric pressure. On the other hand, the response time of the sensor during a pressure decreasing step is lower than for a pressure increasing step, which is justified by the viscoelastic behaviour of the PDMS used for the nanocomposites fabrication.

(a)

$$\begin{bmatrix}\varepsilon_{xx}\\ \varepsilon_{yy}\\ \varepsilon_{zz}\\ \varepsilon_{yz}\\ \varepsilon_{zx}\\ \varepsilon_{xy}\end{bmatrix} = 10^{-6}\begin{bmatrix} 1/1.7 & -0.26/1.7 & -0.24/8.1 & 0 & 0 & 0 \\ -0.26/1.7 & 1/1.7 & -0.24/8.1 & 0 & 0 & 0 \\ -0.05/1.7 & -0.05/1.7 & -1/8.1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/0.48 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/0.48 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.26/1.7 \end{bmatrix}\begin{bmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{zz}\\ \sigma_{yz}\\ \sigma_{zx}\\ \sigma_{xy}\end{bmatrix}$$

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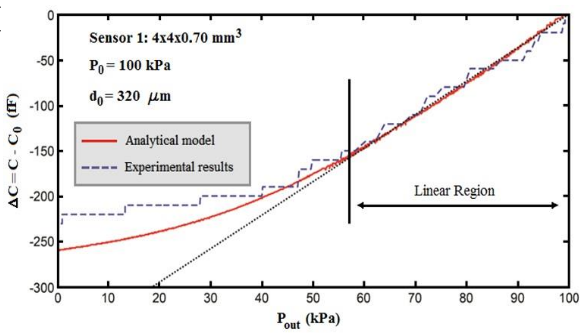

Figure 1 – a) First full constitutive law for transversely-isotropic nanocomposites and b) Capacity and pressure changes measurement.

P17

COMPUTATIONAL RHEOLOGY

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Understanding the behavior of complex rheology materials is a key issue in several industrial processes. Consequently, the availability of adequate numerical modelling tools is essential to increase process insight and support design activities.

The research in Computational Rheology comprises the development of numerical tools adequate to model the flow of complex rheology materials, with a special focus on polymer processing applications and motivated by topics with industrial/practical relevance. The developed routines are expected to aid the design of processing tools/equipment, in order to reduce the employed human, financial and material resources.

There are a number of applications where the developed codes have been successfully applied, e.g. design of profile extrusion forming tools (extrusion dies and cooling systems), study of mixing processes, particulate multiphase flows and modeling of complex rheology materials (differential, integral and fractional viscoelastic).

Due to its open nature and flexibility the OpenFOAM (Open source Field Operation and Manipulation) computational library was chosen as the framework for most of numerical developments performed.

P18

A SMALL-SCALE EXPERIMENTAL SET-UP FOR PROCESSING-RELATED MATERIALS CHARACTERIZATION

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[2]CENIMAT/I3N, Faculdade Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal.

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As polymers progressively meet more stringent requirements in terms of processing and performance, it is often necessary to developed complex material systems while minimizing costs and time-to-market. Thus, it seems useful to make available fast response characterization tools that although using small amounts of sample, are still capable of conveying adequate data on the correlations between rheological response, process-induced material structure and product properties. For this purpose, a prototype small-scale single / twin-screw extrusion system of modular construction, was coupled to a rheo-optical slit die designed to be able to measure shear viscosity and normal-stress differences, as well as performing rheo-optical experiments, namely small angle light scattering (SALS) and polarized optical microscopy (POM). The extruder is equipped with ports that allow sample collection, in order to subsequently evaluate the evolution of melting and mixing, morphology, or chemical conversion, whichever relevant. Also, downstream equipment is available, so that the engineering properties of the extrudate can be evaluated. As an example, processing of a PS/PMMA industrial blend and the properties of extruded sheets will be studied. Additionally the potential of the extrusion line with a liquid crystalline polymer is also investigated.

P19

METAL NANOPARTICLES FOR PLASMON-ENHANCEMENT IN SI SOLAR CELLS AND RAMAN SPECTROSCOPY

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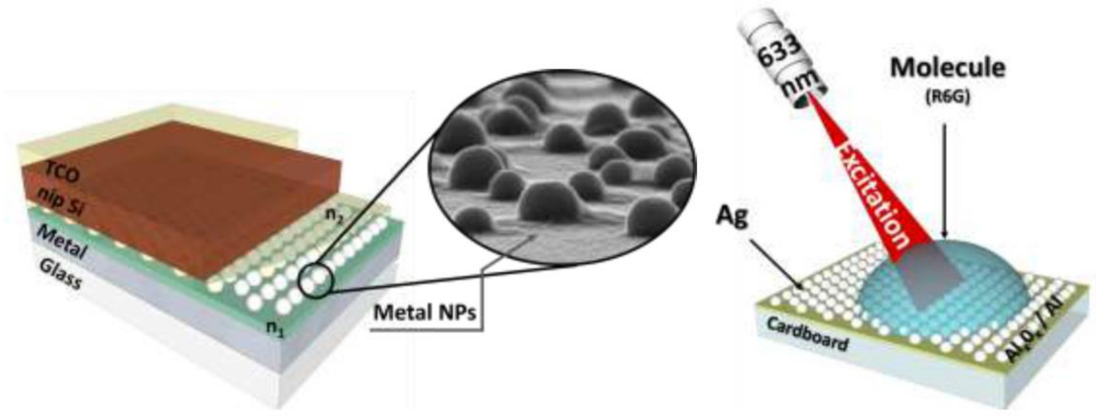
Metallic nanostructures supporting surface plasmons have been proposed as an alternative method to achieve enhancement in Si solar cells and also Surface Enhanced Raman Spectroscopy (SERS).
When metal nanoparticles (NPs) are excited by electromagnetic radiation of appropriate energy, their conduction electrons oscillate collectively exhibiting Localized Surface Plasmon Resonance (LSPR).The incident light near the resonance frequency can be resonantly absorbed or scattered by the nanoparticles, creating a propagating far-field localized near-field , depending on their physical parameters (size, shape and distance between them and the surrounding environment). In this work we explore the physical properties of silver (Ag) nanoparticles that can be best suited for each of these applications.



A. Araújo, C. Caro, MJ Mendes, D Nunes, E Fortunato, R Franco, H Águas, R Martins, Highly efficient nanoplasmonic SERS on cardboard packaging substrates, Nanotechnology, **25** (2014) 415202.

P20

EFFECT OF THE SULPHURIZATION CONDITIONS ON THE PROPERTIES OF Cu_2ZnSnS_4 THIN FILMS AND SOLAR CELL PERFORMANCE

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We studied the effect of several sulphurization conditions on the properties of Cu2ZnSnS4 thin films obtained through rapid thermal processing (RTP) of multiperiod precursors of Zn/SnS2/CuS. The heating rate, the maximum sulphurization, the time at maximum temperature and the amount of evaporated sulphur were varied. The morphological studies revealed that the samples sulphurized at higher temperatures, shorter times and higher amount of evaporated sulphur exhibited larger grain sizes. The structural analysis based on Raman scattering and XRD did not lead to a clear distinction between the samples. Photoluminescence spectroscopy studies showed an asymmetric broad band characteristic of CZTS, which occurs in the range of 1.0-1.4 eV and a second band, on the high energy side of the previous one, peaking at around 1.41 eV. The intensity of this latter band reveals substantial differences in the optical properties of the samples. The cell results hint toward a detrimental effect of long sulphurization times and a positive effect of higher sulphur vapour pressure and higher sulphurization temperature. Solar cell efficiencies improved with increased grain size in the absorber layer. The highest cell efficiency obtained in this study was 3.1% [1].

[1] M.G. Sousa, A.F. da Cunha, P.A. Fernandes, J.P. Teixeira, R.A. Sousa, J.P. Leitão, Effect of rapid thermal processing conditions on the properties of Cu2ZnSnS4 thin films and solar cell performance, Solar Energy Materials and Solar Cells, **126**, 101-106 (2014).

P21

IDENTIFICATION OF RADIATIVE AND NON-RADIATIVE CHANNELS IN CU-POOR CU2ZNSN(S,SE)4 SOLAR CELLS

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The improvement of the electrical performance of solar cells depends on the knowledge of fundamental physical properties, namely, the electronic levels' structure. In the literature, a few different models have been considered for the assignment of the radiative transitions in Cu(In,Ga)Se2 and Cu2ZnSnS4 (CZTS), namely: donor acceptor pair recombination (DAP), quasi-DAP recombination (QDAP) and radiative channels involving fluctuating potentials. In this work, we show that the radiative and non-radiative recombination channels are strongly influenced by electrostatic fluctuating potentials along the film due to the high doping level and strong compensation common in these materials. An acceptor level with an ionization energy of ~280 meV was identified for CZTS [1,2].

[1] J. P. Teixeira et al., Radiative transitions in highly doped and compensated chalcopyrites and kesterites: The case of Cu2ZnSnS4, Phys. Rev. B, **90**, 235202 (2014).

[2] J. P. Teixeira et al., Comparison of fluctuating potentials and donor-acceptor pair transitions in a Cu-poor Cu2ZnSnS4 based solar cell, Appl. Phys. Lett., **105**, 163901 (2014).

P22

SPECTRAL CONVERTERS TO ENHANCE THE EFFICIENCY OF SOLAR CELLS

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The efficiency of the solar cell would be increased by converting the high and low energy photons out of solar cell band gap into the photons within the band gap by using spectral converting mechanisms. In this context, phosphors of $BiGdWO_6$ (BGW) were prepared by solid state reaction and Pechini sol-gel techniques and characterised by X-Ray diffraction, Raman spectroscopy and photoluminescence spectroscopy. As observed in Fig.1 the diffraction peaks of the prepared samples matched the known structure for BGW, that is similar to the Bi_2WO_6 ferroelectric phase, the simplest member of the Aurivillius family of layered perovskites. The SEM image reveals the polycrystalline nature of the material with an average grain size in the micrometer range. When excited by UV radiation (325 nm) the emission spectrum consists of broad band (400 to 550 nm), which is ascribed to $^3P_1 \rightarrow {}^1S_0$ transition of Bi^{3+} ions in host lattice. This material can be useful to convert the UV photons into visible photons therefore increasing the efficiency of solar cells.

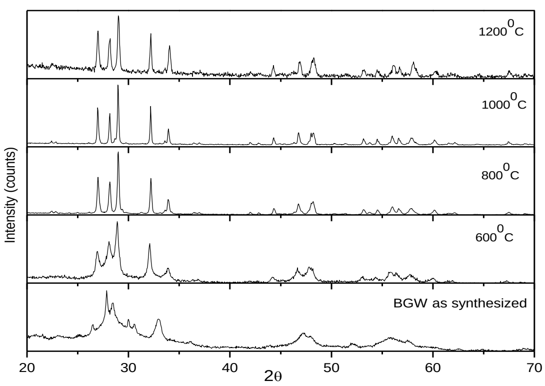

Fig. 1 - XRD patterns of BGW prepared by sol-gel method with different calcination temperatures.

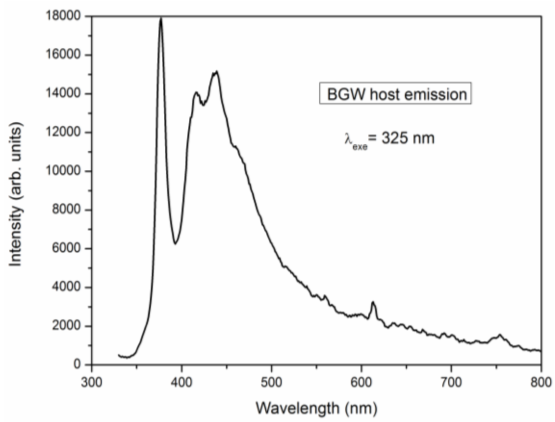

Fig. 2 – Photoluminescence of BGW powders with 325 nm excitation at room temperature.

BOUNDARY LAYERS IN CU_2O FOR P-TYPE THIN FILM TRANSISTORS

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Due to promising electrical characteristics as bulk material, Cu_2O is considered for application as p-type channel in thin film transistors. However, this material generally shows deteriorated performance in interface-driven devices. Consequently, the material has been investigated by in situ X-ray photoelectron spectroscopy and electrical characterization for boundary effects to top-gate and bottom-gate interfaces. A relative oxidation or reduction of Cu(I) has significant effect on electronic properties.

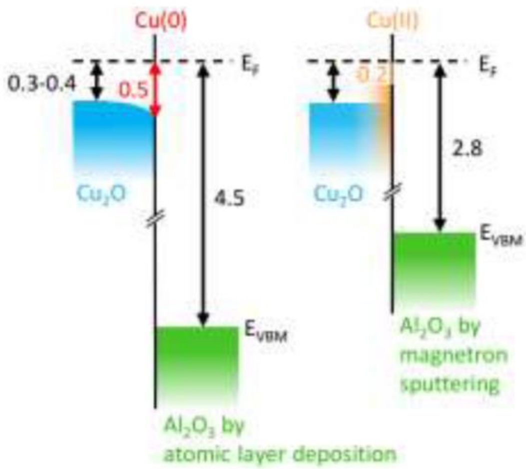

Figure 1 – Energy alignment at interface to Al_2O_3 under the influence of Cu(0) and Cu(II), respectively.

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LIQUID CRYSTALLINE INVERSE OPALS NEW BONE LIKE ASSEMBLIES FOR TISSUE ENGINEERING

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This work envisages the use of Inverted Colloidal Crystal (ICC), also known an Inverse Opals, to produce structures exhibiting a uniform pore size, interconnected network and a biodegradable matrix, essential for bone tissue engineering [1].

ICC scaffolds (Figure 1) – highly geometrically ordered structures that result from inverse replication of the structure of packed colloidal crystals (CC) – enhance oxygen and nutrient diffusion, providing optimum cellular development. For this purpose chitosan (CS) / chitin (CT) liquid crystalline solutions and gels (chiral nematic or cholesteric mesophases) will be used to produce the composite matrix of the scaffolds [2].

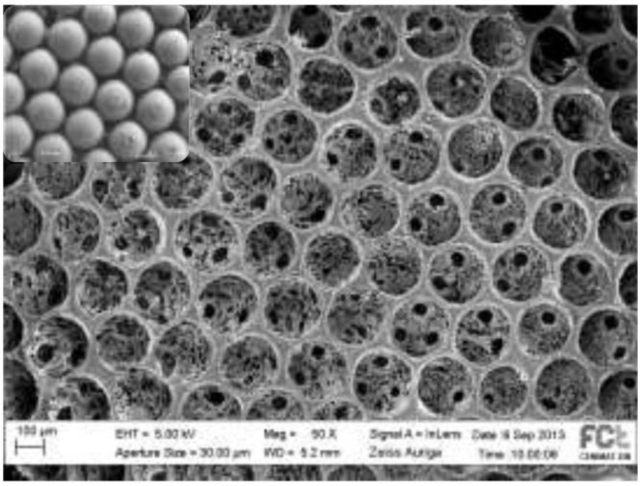

Figure 1 – SEM image of an ICC Chitosan/Hydroxyapatite Scaffold.

[1] João, C.; Vasconcelos, J.; Silva, J.; Borges, J. An Overview of Inverse Colloidal Crystal Systems for Tissue Engineering.Tissue Engineering - Part B, 2014.
[2] João, C.; Vasconcelos, J.; Silva, J.; Borges, J. Chitosan Based Inverse Colloidal Crystal Scaffolds. 25th European Conference on Biomaterials (ESB 2013). Madrid 8-12 September 2013.

P25

INKJET PRINTING OF AMORPHOUS OXIDE SEMICONDCUTORS FOR HIGH PERFORMANCE TFTS

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This work aims to combine two emerging technologies, inkjet printing and oxide thin film transistors (TFTs) developed by low temperature printable solutions.
Solution processing of indium free amorphous oxide semiconductors at low temperature will be developed using auto-combustion synthesis.
The oxide thin films (initially deposited by spin-coating [1][2]) will be characterized in detail and integrated in TFTs, aiming μFE>10 cm2/Vs. Precursor solutions will then be used for spray-coating, and finally adjusted to ink-jet printing. At the end, digital building blocks (e.g. inverters and ring oscillators) will be fabricated on flexible substrates with ink-jet printed oxide transistors as validation of low temperature solution processing.

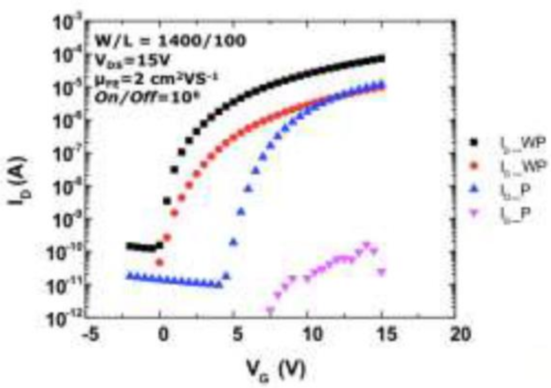

Figure 1 – Transfer characteristics of solution processed ZTO TFTs produced on top of Si/SiO2. WP - ZTO without pattern; P – ZTO patterned

[1] Salgueiro, D., Duarte, V., Sousa, C., Alves, M.J., Gil Fortes, A., "Diastereoselectivity in Diels–Alder Cycloadditions of Erythrose Benzylidene-acetal 1,3-Butadienes with Maleimides", Synlett, 2012, 23, 1765-1768.
[2] Salgueiro, D., Alves, M.J., Sousa C., Gil Fortes, A., "Diels-Alder Cycloaddition in the Synthesis of 1-Azafagomine, Analogues, and Derivatives as Glycosidase Inhibitors", Mini Reviews in Medicinal Chemistry, 2012, 12 (14), 1465-1476.

P26

PRINTABLE ORGANIC AND INORGANIC MATERIALS FOR FLEXIBLE ELECTROCHROMIC DEVICES

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The growing demand of consumer printed electronics such as smart cards, smart packaging, automotive displays, electronic paper and others led to the increased interest in fully printed electrochemical devices. The results presented here concern three main topics: (i) dual-phase inorganic electrochromic material processed at low temperature, (ii) enhancement in electrochromic performance *via* metal-oxide nanoparticles engineering and (iii) highly conductive and mechanically stable solid-state electrolyte. First two topics are related to crystallographic structure of metal-oxide films derived from sol-gel precursor, which is shown to be critical for electrochemical performance. The proposed method of microstructure control result in electrochromic (EC) films which outperform their amorphous or nanocrystalline analogues, leading to solid state EC devices exhibiting optical density on the level of 0.82 and switching time shorter than 3 seconds. Third topic concerns a new concept of solid state electrolyte based on plastic crystal doped with lithium salt, dispersed in a thermosetting polymer resin network. This printable electrolyte meets requirements for electrochromic applications, exhibiting ionic conductivities of 10^{-6} - 10^{-4} S cm^{-1} at ambient temperature, Young's Modulus in the range of 0.1 - 1.4 MPa and operational temperature up to 115 °C.

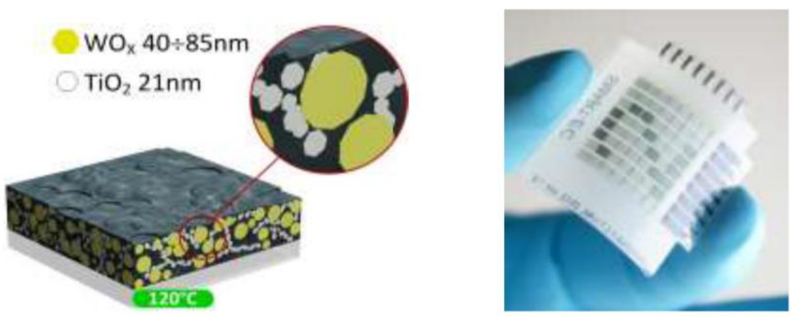

Figure 1 – Dual phase nanostructured EC layer and flexible printed solid state EC device.

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CELLULOSE BASED SUBSTRATES FOR APPLICATION IN ELECTRONIC DEVICES

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Paper electronics is a topic of huge interest due the possibility of having low cost, disposable and recyclable electronic devices. The final goal is to make paper itself an active part of such devices acting as the dielectric layer in file effect transistors (FETs), for instance. In this work we present new insights on paper substrates and devices' configuration engineering aiming the development of oxide based FETs. It was observed that paper planarization and impermeability can be improved using microfibers resulting in a very compact paper structure improving the stability of the FETs under variations in the environmental conditions. In this work it is successfully demonstrated that smooth and compact micro/nanofibrilated cellulose (MNFC) paper can be used as the dielectric in oxide based FETs processed at low temperatures with excellent electrical performances and remarkable stability under bending. [1-2]

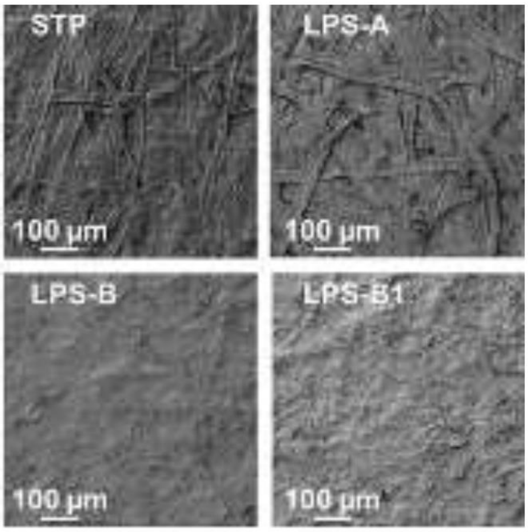

Figure 1 – SEM micrographs of micro/nano fibrillated cellulose (M-NFC).

[1] L. Pereira, *et al*., The influence of fibril composition and dimension on the performance of paper gated oxide transistors, Nanotechnology, **25,** (2014).
[2] D. Gaspar, *et al*., Nanocrystalline cellulose applied simultaneously as the gate dielectric and the substrate in flexible field effect transistors, Nanotechnology, **25,** (2014).

P28

DESIGN AND DEVELOPMENT OF A MICROFLUIDIC PLATFORM FOR USE WITH COLORIMETRIC GOLD NANOPROBE ASSAYS

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The objectives of the presented work are the development bio-microfluidic platform for colorimetric DNA detection based on non-cross-linking Au-nanoprobes hybridization to enable detection with much lower sample volume than in the state-of-the-art biosensor and to clearly distinguish between positive and negative assays of various DNA targets with single mismatch sensitivity and low detection limit. Besides that, micromixer channels were developed to enable reagents mixing on the chip.

The combination of the unique optical properties of gold nanoprobes with microfluidic platform resulted in sensitive and accurate sensor. Detection of single base mismatch using 10 × lower solution volume and target DNA concentration below the limit of the detection attained with a conventional microplate reader was achieved. Passive planar rhombic micromixer with obstacles were developed and optimised. A good fluid mixing with acceptable pressure drop values with a mixer length of 2.5 mm, being one of the shortest planar passive micromixers reported to date was achieved.

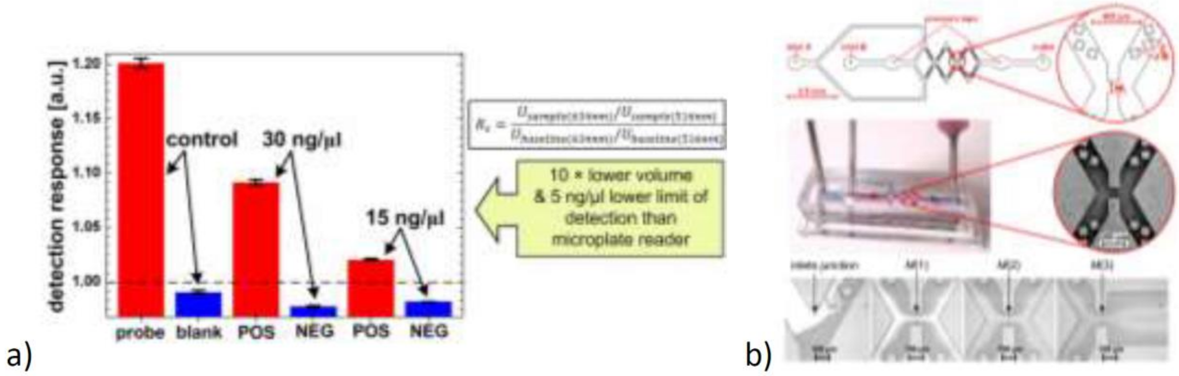

Figure 1 – a) Single base mismatch detection using Au NPs and the microfluidic platform with nanolenses, **b)** Micromixer schema, fabrication and characterization.

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P29

STUDIES ON DISPERSION EFFICIENCY OF POLYMER NANOCOMPOSITES

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In several industrial processes, highly complex materials are mixed using intricate mixing procedures. This is the case of the dispersion of fillers down to the nanoscale in molten polymer matrices by means of extruders, which create complex flow patterns. Since the performance of the resulting nanocomposites is highly dependent on the levels of dispersion attained, the availability of approaches to predict and/or improve mixing efficiency would be particularly relevant in practice.
In this work, a new Eulerian-Lagrangian numerical solver is developed in OpenFOAM® computational library, and used to better understand the mechanisms determining the dispersion of fillers in polymer matrices. Particular attention will be given to the effect of the rheological model used to represent the fluid behavior, on the level of dispersion obtained. For the Eulerian phase the averaged volume fraction governing equations (conservation of mass and linear momentum) are used to describe the fluid behavior. In the case of the Lagrangian phase, Newton's second law of motion is used to compute the particles trajectories and velocity. The gathered results are used to correlate the fluid and particle characteristics on the effectiveness of mixing and morphology obtained.

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THE EFFECT OF SURFACE FUNCTIONALIZATION OF GRAPHITE NANOPLATES ON THE DISPERSION IN POLYPROPYLENE MELTS

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Graphite, formed by stacks of 2-D layers of *sp*^{2} hybridized carbon atoms hexagonally bonded, is a promising low cost reinforcement for functional and smart nanocomposites[1]. However, the incorporation and dispersion of natural flaky graphite in polymer matrices is challenging due to the strong interaction, small spacing between graphene layers and lack of functional groups at the surface and edges. Chemical modification of graphite has been accomplished by covalent and non-covalent approaches to overcome the limitations associated to the efficient dispersion and interfacial bonding with polymers[2]. In this work, graphite nanoplates were chemically modified *via* 1,3 dipolar cycloaddition of azomethineylide and then grafted with polypropylene-graft-maleic anhydride. The effect of surface functionalization on the dispersion kinetics, re-agglomeration phenomenon and interface bonding with polymer is investigated. Nanocomposites with 2 or 10 wt. % of as-received and functionalized graphite nanoplates were prepared in a small-scale intensive mixer coupled to a capillary rheometer. The covalent attachment of pyrrolidine groups enhances the stability of dispersion, inhibiting efficiently the re-agglomeration.

[1] J. R. Potts, D. R. Dreyer, C. W. Bielawski and R. S. Ruoff, *Polymer*, **52**, 5-25 (2011).
[2] V. Georgakilas, M. Otyepka, A. B. Bourlinos, V. Chandra, N. Kim, K. C. Kemp, P. Hobza, R. Zboril and K. S. Kim, *Chemical Reviews*, **112**, 6156-6214 (2012).

FORECASTING EPILEPTIC SEIZURES IN NEURONAL NETWORKS

P31

M. A. Lopes, K.-E. Lee, J. F. F. Mendes , and A. V. Goltsev

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In the epileptic brain, EEG recordings reveal paroxysmal spikes. They emerge from low background with rapid onset, reach high voltage due to the synchronous discharge of many neurons, and then abruptly disappear. Seizures are highly correlated with this abnormal neuronal activity. Using a cortical model of neuronal networks composed by stochastic excitatory and inhibitory neurons in the presence of noise [1], we show that paroxysmal-like spikes appear as nonlinear excitations near a saddle-node bifurcation. This bifurcation is the mechanism of a second-order phase transition, which is accompanied by critical phenomena that allow us to propose a method to forecast epileptic seizures.

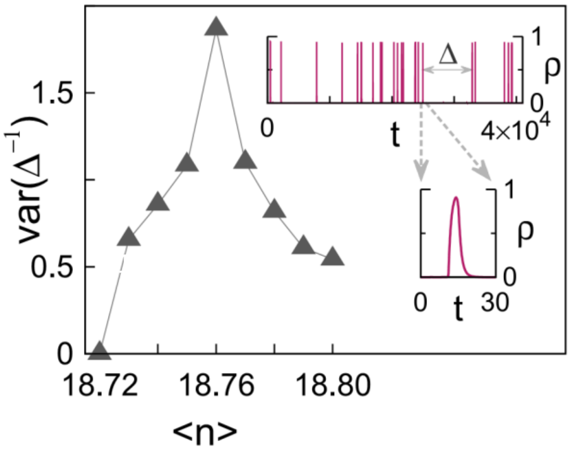

Figure 1 – Variance of the rate of paroxysmal-like spikes versus the noise. The peak signals the 2nd-order phase transition..

[1] K.-E. Lee, M. A. Lopes, J. F. F. Mendes, A. V. Goltsev, Critical phenomena and noise-induced phase transitions in neuronal networks. Physical Review E **89**: 012701 (2014).

P32

DIAMOND AND STIFF DIAMOND/BUCKYPAPER CARBON HYBRIDS FOR MEMS

T. Holz[1], D. Mata[1], N.F.Santos[1], A.J.S. Fernandes[1], J. T. Santos[2], V.Chu[2], J. P. Conde[2,3], F.M. Costa[1]

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MEMS are a well-established growing technology with high impact in bioscience, medicine, communications and inertial sensing. However, the emergent new high-tech applications require alternatives to the standard materials (Si, SiC, AlN). In this context, nano-crystalline diamond (NCD) films keep much of the overall intrinsic diamond outstanding properties relevant for applications in MEMS far exceeding those of the traditional materials. Therefore, in this work NCD films grown by microwave plasma CVD (MPCVD) were micro machined into basic MEMS structures. The vibrational analysis of the NCD resonators confirmed a high Young modulus of ~1000 GPa. Also, envisaging the integration of sp^2/sp^3 carbon phases, MWCNT buckypapers were produced and coated with NCD films. A strong interface was obtained under the NCD film, with fully preserved CNT embedded within the NCD matrix, Fig.1. Bending tests showed an increase of the Young's Modulus from 0.3 to 300 GPa after NCD growth[1].

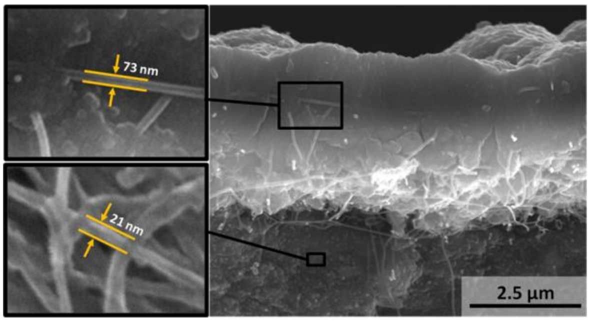

Figure 1 – SEM micrographs comparing the CNTs diameter of the pristine buckypaper with those mixed within de NCD matrix after MPCVD growth.

[1] T. Holz, D. Mata, N.F. Santos, I. Bdikin, A.J.S. Fernandes, F.M. Costa, Stiff diamond/buckypaper carbon hybrids, ACS Applied Materials & Interfaces, **6**, 22649 (2014).

P33

NUCLEAR MEDICAL IMAGING DEVICES BASED ON SOLID-STATE MATERIALS

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In this work we present some of the nuclear medical imaging and radiation dosimetry systems developed at DRIM (Radiation Detection and Medical Imaging) lab using solid-state materials, particularly scintillators (both innorganic and organic) and wavelength-shifters. These include a high-resolution gamma camera for breast and small animal scintigraphy [1], a high-resolution micro-PET scanner (Positron Emission Tomography) for small animal imaging and pre-clinical studies [2] and a high-sensitivity flexible optical fibre dosimeter for real-time dose measurement [3]. The latter will allow the optimization of procedures such as prostate brachytherapy, by providing a higher quality control and radiation safety, being also applicable to dosimetry of medical imaging exams using ionizing radiation (e.g. X-ray CT, PET).

[1] I.F.C. Castro et al., WSF Gamma Camera with SiPMs: First Small Animal Tests, IEEE Medical Imaging Conference Record (2013).
[2] P.M.M. Correia et al., Development of a micro PET system with improved spatial resolution through depth-of-interaction measurement, Proc SPIE 9286 (2014).
[3] L.M. Moutinho et al., Development of a scintillating optical fiber dosimeter with silicon photomultipliers, Nucl Instr Meth Phys Res A (2014).

P34

DEVELOPMENT OF A NEW NANOSTRUCTURED SCAFFOLD FOR NEURAL STEM/PROGENITOR CELL TRANSPLANTATION

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Disruption of nerve cells in spinal cord injury (SCI) is followed by glial scar and cyst formation that block regeneration. A scaffold to bridge a SCI should stimulate cells (endogenous or transplanted) to participate in regeneration, promote oriented axonal growth and mechanically prevent scar ingress. Scaffold's material and architecture are both important to provide regenerative stimuli. Polyurethane urea (PUU) elastomers are tunable materials with high strength and elasticity. Due to these properties we are exploring these materials for use as scaffolds for SC regeneration. We synthetized and characterized by $_1$H NMR and FTIR PUUs based on PCL-diol and including chitosan (PUU-CS) [1]. PUU-CS were processed by electrospinning from solutions employing different solvent systems and polymer concentrations. Randomly oriented and aligned fibrous matrices were obtained and characterized by SEM (figure 1) and their mechanical properties evaluated through tensile tests. Preliminary hydrolytic (in PBS) and enzymatic (10 U/mL lipase) degradation studies and in vitro cytotoxicity tests were performed.

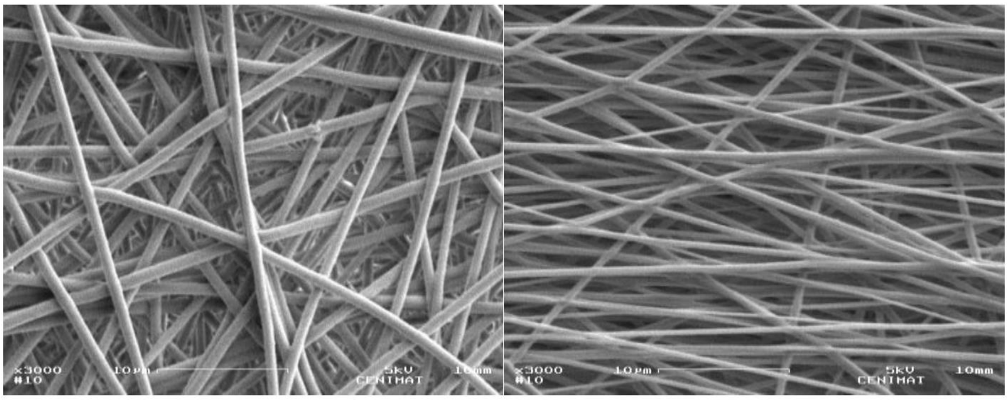

Figure 1 – Randomly oriented (left) and aligned (right) PUU-CS electrospun fibers.

[1] M. Barikani, H. Honarkar, M. Barikani, *Monatsh Chemestry Journal*, **141**, 653- 659 (2010).

P35

STRUCTURAL COLOURS IN CELLULOSE: SCULPTING THE FLOW OF LIGHT

S.N. Fernandes

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Cellulose can be at the origin of structural colors, which is one of the most astonishing characteristics that this polymer can present. One of the main targets in food, cosmetics and paints, as well as in electronic devices are the use of long-term colors, free from chemical or photo decolorizing. Structurally colored cellulose based materials represent potential materials to replace dyes and pigments and serves as an outstanding inspiration to develop new photonic materials. Cellulose liquid crystalline systems are perfect for creating structurally colored materials, as they are easy to prepare, inexpensive and their optical properties can be tuned through synthesis, morphology, and precursor liquid crystalline lyotropic and thermotropic systems.

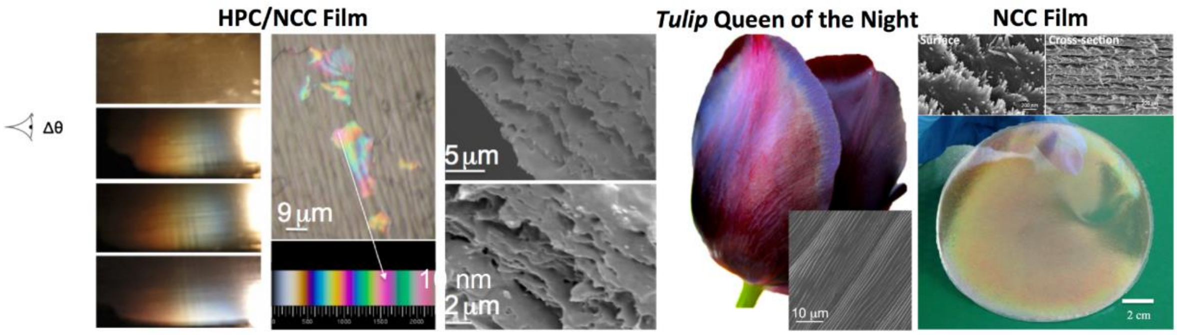

Figure 1 – HPC/NCC film: Iridescence of HPC/NCC films due to periodic structure of the material that mimics the structures found in plants namely in the ***Tulip* Queen of the night** [1]; **NCC Film:** Iridescence in Nanocrystalline Cellulose Film (unpublished work).

[1] S. N. Fernandes, Y. Geng, S. Vignolini, B. J. Glover, A. C. Trindade, J. P. Canejo, P. L. Almeida, P. Brogueira, M. H. Godinho, "Structural Color and Iridescence in Transparent Sheared Cellulosic Films", Macromolecular Chemistry and Physics, 214 (1), 25-32, 2013. DOI: 10.1002/macp.201200351. (Front cover paper)

P36

JANUS PARTICLES

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The main objective is to produce spheroidal and ellipsoidal ferrogel bodies and to study their deformation by applying an external magnetic field, in order to obtain new magnetic stress/strain sensors. These materials are also able to tune their optical properties by the application of an external field and therefore have potential applications for magneto-optical sensors. The materials will be obtained from solutions of polymeric matrices, produced as small spheres and ellipsoids that can be filled with ferro nanoparticles and liquid crystals with ferromagnets. Several networks are tested (as an example polisiloxane membranes and urethane/urea membranes) as well as several kind of magnetic particles and nematic and cholesteric liquid crystals. The morphology of spherical bodies obtained will be affined by controlling the materials used in their synthesis and the processing conditions.

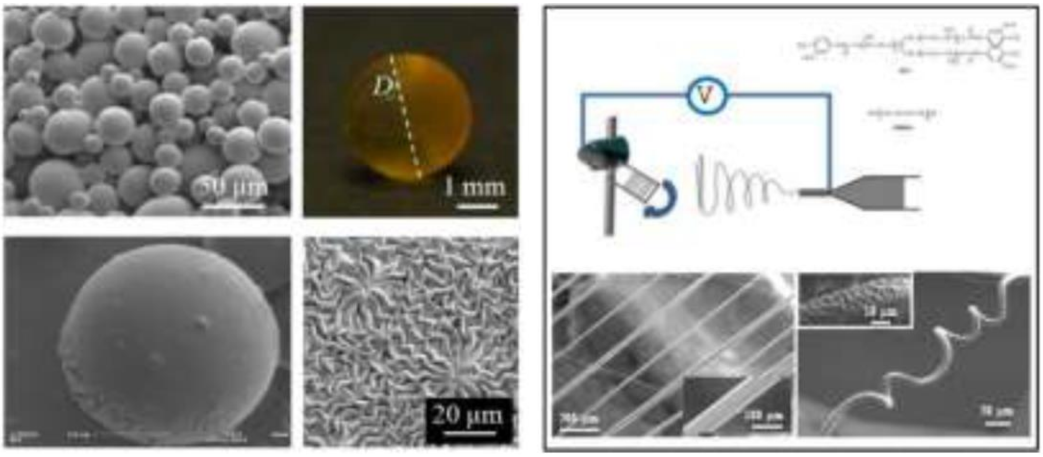

Figure 1 – Janus spherical particle (left) and electrospun janus fibre (right).

[1] A.C. Trindade, J.P. Canejo, L.F.V. Pinto, P. Patrício, P. Brogueira, P.I.C. Teixeira, M. H. Godinho, Wrinkling Labyrinth Patterns on Elastomeric Janus Particles, Macromolecules, **44**, 2220 (2011).
[2] A.C. Trindade, J.P. Canejo , P.I.C. Teixeira, Pedro Patrício, M.H. Godinho, First Curl, Then Wrinkle, Macrom. Rapid Com., **34**(20), 1589 (2013).

P37

LASER WELDING OF SHAPE MEMORY ALLOYS

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Laser welding of shape memory alloys is attracting considerable attention due to the possibility to overcome the problems of machining and obtain complex forms of these materials [1].

Similar welds of NiTi shape memory alloys were performed and their functional properties (shape memory effect and superelasticity) are observed after welding. 600 mechanical cycles up to 10% strain were performed in all samples (Figure 1a). The shape memory effect was evaluated for all samples, even after the 600 mechanical cycles, and full recovery of the initial shape was always observed. Structural characterization using synchrotron X-ray diffraction was performed on NiTi welds and a microstructural gradient is observed in the heat affected and fusion zones as a consequence of the welding procedure (Figure 1b). This microstructural gradient is a consequence of precipitation phenomena in the heat affected zone and preferential evaporation of Ni in the fusion zone. As a result of the presence of martensite at room temperature, when the as-received material is fully austenitic, a unique mechanical behavior of the welds is observed.

Laser welding of these materials is a suitable joining technique and may open doors for new applications based on the microstructural alterations observed.

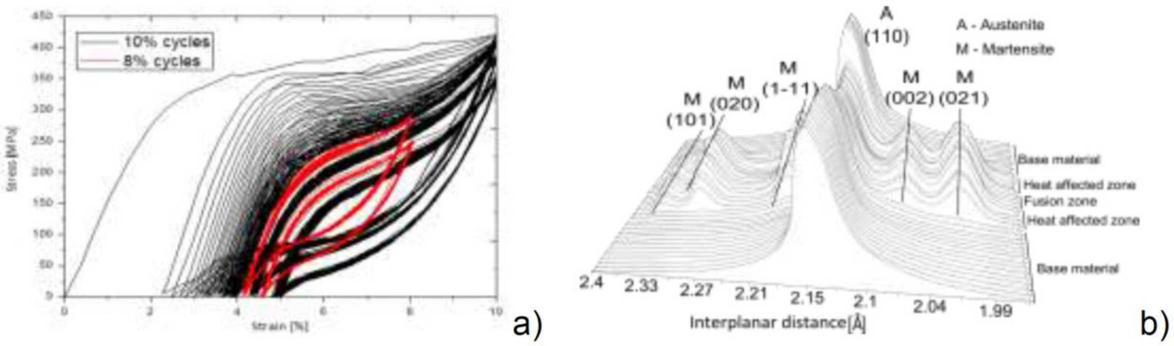

Figure 1 – Welded NiTi: a) superelastic behavior; b) structural characterization by X-ray diffraction.

[1] J.P. Oliveira *et. al*, Laser Welded NiTi, LAP – Lambert Academic Publishing, 2013

P38

MICROPATTERN STRUCTURES FOR GASEOUS DETECTORS – LARGE RADIATION DETECTION AT MICRO-SCALE RESOLUTION

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X-Rays are a very powerful tool in many analytic techniques, with a very wide use in fields ranging from medicine, history of arts, geology, astronomy, etc. Some of these techniques are still limited by the lack of detection technologies that can make full use of the information obtained from the X-Rays. Whenever large areas of detection which require position and energy resolution, Micropattern Gaseous Detectors (MPGD) become very interesting solutions. These detectors are widely used in instrumentation in major Physics experiments with a solid history of success, and have been introduced to other fields of science in the past few years as X- and gamma Ray detectors [1,2,3] and as VUV [4], visible and IR light detectors, when used coupled to photosensitive materials. In this work we present some of the MPGDs based systems [2,4,5] developed at DRIM (Radiation Detection and Medical Imaging) lab for different applications.

[1] "Energy weighting technique in Quantum Computed Tomography using a MPGD," L. F. N. D. Carramate, C, et al., JINST, vol. 6, 2011.
[2] "Multi-slice quantum Computed Tomography system using a MHSP", L F N D Carramate, at al., JINST, vol. 7, 2012.
[3] "Performance of a gaseous detector based energy dispersive X-ray fluorescence imaging system: Analysis of human teeth treated with dental amalgam," A. L. M. Silva, et al., Spectrochimica Acta B, vol. 86, pp. 115-122, 2013.
[4] "Position sensitive VUV gaseous photomultiplier based on Thick-multipliers", T. Lopes, et al., JINST, vol. 8, 2013
[5] "X-ray imaging detector based on a position sensitive THCOBRA with resistive line," A. L. M. Silva, et al., JINST, vol. 8, 2013.

P39

PHOTOLUMINESCENCE STUDIES ON SODIUM NIOBIUM TELLURITE GLASS-CERAMICS FOR OPTICAL SENSOR APPLICATIONS

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The present work deals with preparation of sodium niobium tellurite (SNT) glasses using melt quenching method, in which small quantities of boron and silicon in the form of oxides are added to improve their mechanical properties. Controlled heat treatment is performed to ceramize the prepared glasses based on the thermal data given by DTA. XRD and SEM profiles of the glass-ceramics confirmed the formation of crystalline monoclinic Sodium Tellurium Niobium Oxide ($Na_{1.4}Nb_3Te_{4.9}O_{18}$) phase (JCPDS card No. 04-011-7556). Down conversion and upconversion along with decay measurements in the NIR and visible regions respectively were made for the prepared Er^{3+}-Yb^{3+} co-doped glasses and glass-ceramics laser excitation varying the laser power and concentration of Er^{3+} ions. Results showed that the glasses ceramics exhibit enhanced performance over glasses. Temperature dependent visible upconversion was performed to test the ability of efficient SNT glass-ceramic at low temperatures and variation of upconversion intensities was studied for their use as low temperature sensors.

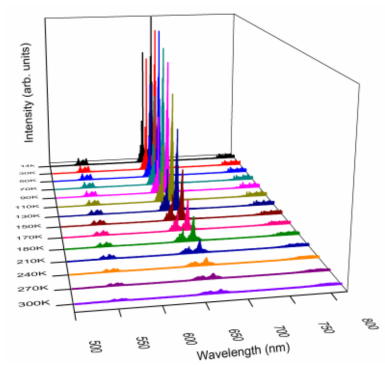

Figure 1 - Temperature dependent upconversion of SNT:ErYb glass-ceramics.

P40

EARLY METALLURGICAL STEPS IN THE PREHISTORIC PORTUGUESE ESTREMADURA

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[2]Centro de Ciências e Tecnologias Nucleares (C2TN), Instituto Superior Técnico, Universidade de Lisboa, Estrada Nacional 10 (km 139,7), 2695-066 Bobadela LRS, Portugal

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The Castro de Vila Nova de São Pedro (VNSP) is an emblematic settlement located at Azambuja (Portugal), occupied during the third and second millennia BC, predominantly during the Chalcolithic period.

The present study focused on the chemical and microstructural characterization of selected metallurgical remains from the VNSP collection aims to contribute to a better comprehension of the copper-based metallurgy on the Portuguese Estremadura. A set of metallurgical production remains (8 crucible and 6 slag fragments and 7 metallic prills) belonging to VNSP were characterized by using different analytical techniques: EDXRF spectrometry, micro-EDXRF spectrometry, optical microscopy and SEM-EDS. Preliminary results on the elemental composition of the metallurgical production remains are consistent with copper and arsenical copper artefact production. These results are also in accordance with the artefact collection from VNSP previously studied mainly composed of copper or arsenical copper (38% of the artefacts copper alloyed with arsenic - As>2%) with low iron contents. Analyses of the metallic prills and slags residues have provided indications of melting and smelting operations.

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FROM ORES TO METAL: INVESTIGATING ANCIENT BRONZE PRODUCTION

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The Northwest of the Iberian Peninsula is particularly rich in raw materials as Sn ores, besides Cu ores. These could have played an active role in the inception and fabrication of the first intentionally man-made metal alloy, bronze (Cu-Sn), during Pre and Proto-historic times (2nd and 1st millennium BC). The present Post-doc research will investigate the possible use of local ores for bronze fabrication by conducting various experimental smelting experiments trying to re-produce probable ancient technologies, and detailed analysis to ores, metal and associated metallurgical products will be made. Results will allow a better understanding of ancient metallurgical technologies based on NW Iberian raw resources and provide a database for future interpretation of archaeological metallurgical vestiges.

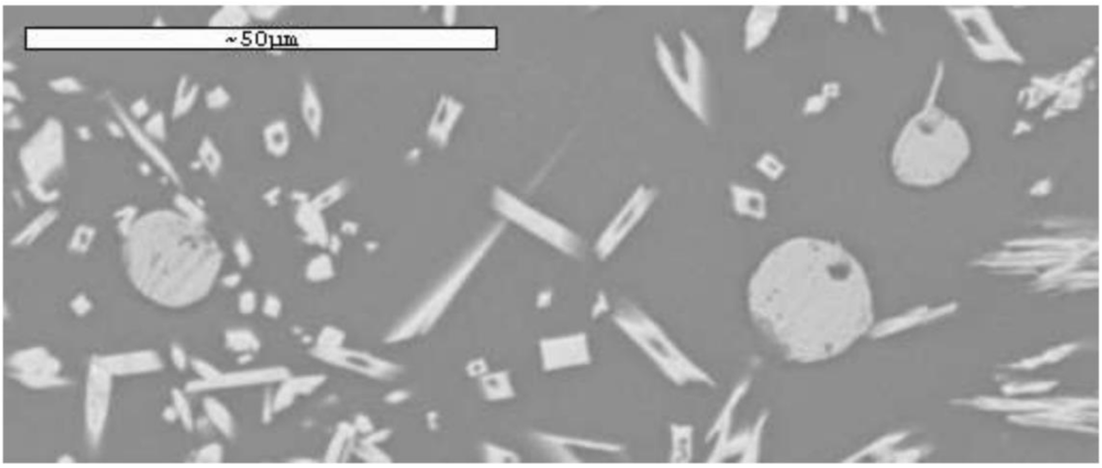

Figure 1 – SEM-EDS (BSE) image of a slag with Sn-O and Cu-O formations in a vitreous matrix.

P42

RAMAN SPECTROSCOPY OF MBE-GROWN INGAAS/ALP ULTRA-SHORT PERIOD SUPERLATTICES

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Ultrashort-period superlattices (USPSL) of ZB materials sharing no-common atom are predicted to present a strong anisotropic unit cell and consequently anisotropic optical properties [1]. They are good candidates for cubic semiconductor-based frequency conversion devices due to their interesting potential for phase matching over long distances. As example, we will study the $In_{0.5}Ga_{0.5}As/AlP$ USPSL structures grown on GaAs substrate by molecular beam epitaxy. High resolution X-ray diffraction scan shows a dominant GaAs substrate peak, and the presence of several superlattice satellite peaks confirming the periodicity of the structures. The knowledge of the optical and vibrational properties of these structures is very important for future applications, however, no information on the optical phonons exists so far. In this work, we report optical phonon spectra measured for the $In_{0.5}Ga_{0.5}As/AlP$ USPSL by micro-Raman spectroscopy for different temperatures. We find that the $In_{0.5}Ga_{0.5}As/AlP$ USPSL still obeys to first order Raman selection rules, and does not contain a high level of structural disorder. We identify the different optical phonons: disorder-activated, GaAs-, InP-, GaP-, and AlP-like LO phonons.

[1] J.-M. Jancu, A. Vasanelli, R. Magri and P. Voisin, Phys. Rev. B, **69**, 241303(R) (2004).

P43

ASSESSMENT OF A FREE CO2 IRON MAKING METHOD

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Although steel production by molten oxide electrolysis offers potential economic and environmental advantages over classic extractive metallurgy, its feasibility is far from being convincingly demonstrated, mainly due to inherent experimental difficulties exerted by harsh conditions and lack of knowledge regarding relevant mechanisms and physico-chemical processes in the melts. The present work was intended to demonstrate the concept of pyroelectrolysis at very high temperature near minimum liquidus point of magnesium aluminosilicate glass, to provide a new insight into electrochemistry behind this process. The results suggest the need for further optimization of the molten electrolyte composition to promote ionic conductivity and to suppress electronic transport contribution, possibly, by tuning Al/Si ratio and altering the network-forming/modifying behaviour of the iron cations.

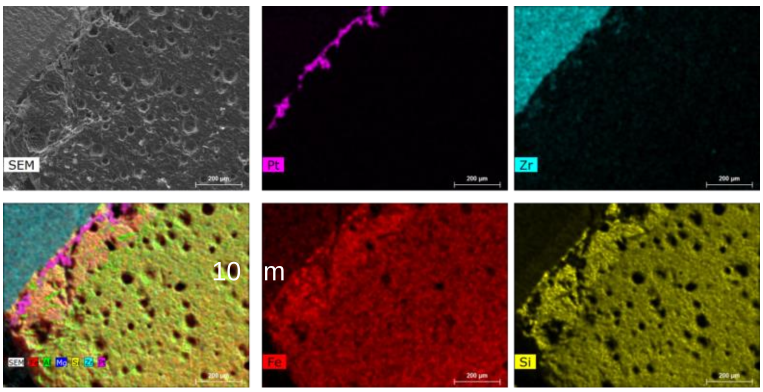

Figure 1 – Post-mortem analysis of the cell after pyroelectrolysis.

[1] N.M. Ferreira et. al. Journal of Alloys and Compounds **611**, 57-64 (2014), http://dx.doi.org/10.1016/j.jallcom.2014.05.118.

[2] N.M. Ferreira et. al., Journal of the European Ceramic Society **34**, 2339–2350 (2014), http://dx.doi.org/10.1016/j.jeurceramsoc.2014.02.016.

[3] N.M. Ferreira et. al., Applied Surface Science **278**, 203–206 (2013), http://dx.doi.org/10.1016/j.apsusc.2013.01.108.

P44

ELECTRONIC DOPING AND MAGNETIC ANISOTROPY IN NANOCRYSTAL QUANTUM DOT SYSTEMS

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Semiconductor nanocrystals (NCs) are crystallites a few nanometers in scale with unusual size-specific optical, electronic, and magnetic properties, unseen in bulk materials. These properties may be useful for various technologies, such as wavelength-tunable lasers, bioimaging, solar cells, and high-density recording media. Our work focuses on two prominent phenomena in NCs: electronic doping [1] and magnetic anisotropy. Doping is expected to enable the control of key NC properties, but many questions remain unanswered, such as the role of interdopant interactions on electronic properties of doped NCs. We investigate the exchange-coupling between donors incorporated in a NC via probing the deviation of the triplet-state magnetic resonance of donor pairs from Curie paramagnetism. With regard to magnetic NCs, magnetic anisotropy is a key issue. We observed unexpected magnetic anisotropic in ensembles of NCs randomly stacked in an isotropic shape. We showed that this can be explained if we consider the magnetic dipole-dipole interactions between dipoles located at the surface of each NC in the ensemble.

[1] R. N. Pereira, A. J. Almeida, A. R. Stegner, M. S. Brandt, H. Wiggers, Phys. Rev. Lett. **108**, 126806 (2012)

P45

NONLINEAR OPTICAL PHENOMENA IN MICROSTRUCTURED OPTICAL FIBERS

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Microstructured optical fibers (MOFs) or photonic crystal fibers (PCFs) are a new class of optical fibers that have a microstructured cross section, enabling a plethora of new effects. They are usually divided in two groups: the solid-core MOFs (SC-MOFs) and the hollow-core MOFs (HC-MOFs). In this work we have determined the propagation modes of MOFs, and their dispersive and nonlinear characteristics. We have also studied the nonlinear dynamics of pulse propagation on such fibers and effects such as supercontinuum generation and deep-UV light generation. We have particular interest on the layered spiral SC-MOF and on the gas-filled kagomé HC-MOF.

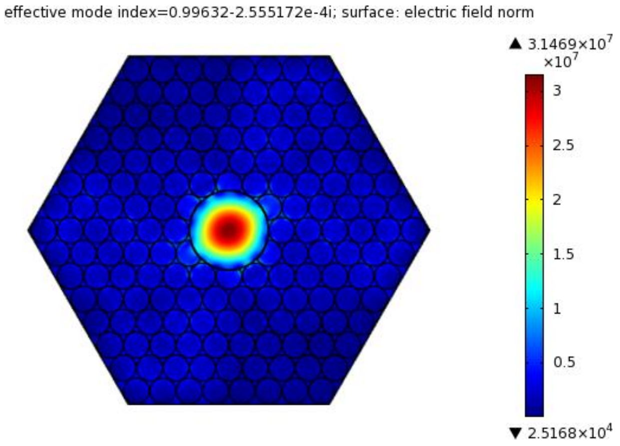

Figure 1 – Fundamental propagation mode of an HC-MOF having a core filled with air.

[1] S.M. Rodrigues, M.M. Facão, S.C. Latas and M.F. Ferreira, “Highly nonlinear layered spiral microstructured optical fiber”, Photonics and Nanostructures - Fundamentals and Applications, vol. 11, issue 3, pp. 226-233 (2013);

P46

NANOSTRUCTURED METAL OXIDES FOR APPLICATION IN ELECTROCHEMICAL DEVICES

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The motivation of using metal oxides is the improved charge storage capabilities, and electrocatalytic, electrochromic and photoelectrochemical properties. Furthermore, comparing with bulk, nanostructured materials present several advantages related with the spatial confinement, large fraction of surface atoms, high surface energy, strong surface adsorption and increased surface to volume ratio. Examples of some applications are evidentiated in Figure 1. Tungsten oxide (WO_3) is a well-studied semiconductor and is used for several applications as chromogenic material, sensor and catalyst. The major important features is its low cost and availability, improved stability, easy morphologic and structural control of the nanostructures, reversible change of conductivity, high sensitivity, selectivity and biocompatibility. The galliumindium-tin oxide (GIZO) nanoparticles applied in electrolyte-gated transistors (EGTs), allowed a good interface and promotes a more efficient step coverage of the channel layer, reducing the operating voltage when compared with conventional dielectrics gating. Both materials were synthesized by a solvothermal process.

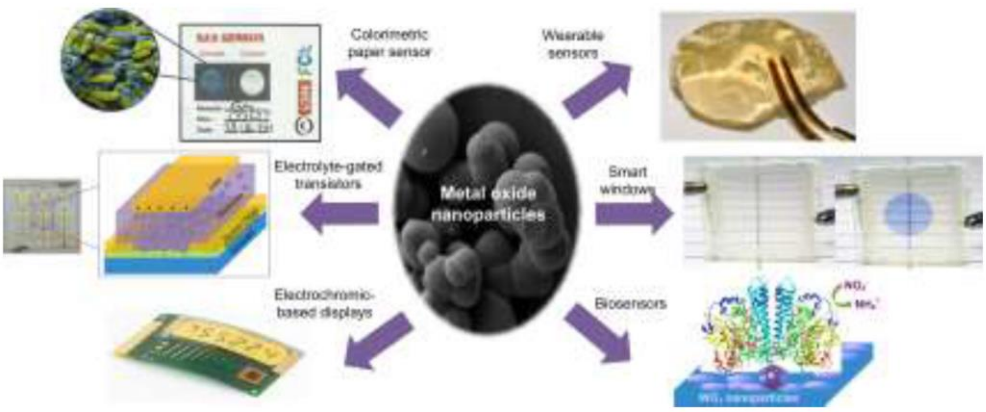

Figure 1 – Examples of metal oxide nanoparticles applications.

P47

LAB-ON-PAPER PLATFORMS FOR ASSEMBLING INEXPENSIVE DIAGNOSTIC ASSAYS

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There is a strong interest in the use of biopolymers in the electronic and biomedical industries, mainly towards low-cost applications. The possibility of developing entirely new kinds of products based on cellulose is of current interest, in order to enhance and to add new functionalities to conventional paper-based products. Focusing on the use of paper as a substrate for microfluidic applications, through an eco-friendly wax-printing technology, we present four main and distinct colorimetric approaches: (i) enzymatic reactions (glucose detection); (ii) immunoassays (antibodies anti-*Leishmania* detection); (iii) nucleic acid sequence identification (*Mycobacterium tuberculosis* complex detection;[1], [2] (iv) electrochromic reactions (electrochemically active bacteria detection)[3].

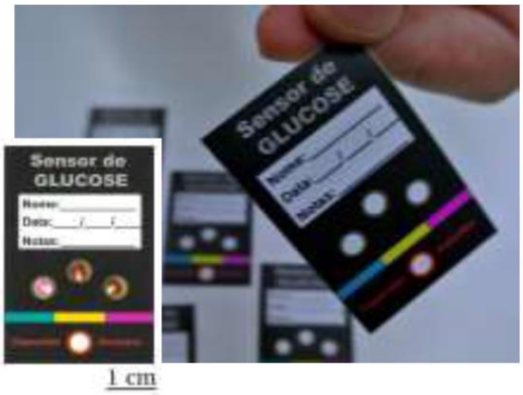

Figure 1 – Paper-based colorimetric glucose sensor

This results are thus promising towards the future development of simple and cost-effective paperbased diagnostic devices.

[1] M. N. Costa, *et al*., A low cost, safe, disposable, rapid and self-sustainable paper-based platform for diagnostic testing: lab-on-paper, Nanotechnology, **25**, 9, 094006, (2014).
[2] B. Veigas, *et al*., Gold on paper-paper platform for Au-nanoprobe TB detection, Lab Chip, **12**, 22, 4802–8, (2012)
[3] A. C. Marques, et al., Office Paper Platform for Bioelectrochromic Detection of Electrochemically Active Bacteria using Tungsten Oxide Nanoprobes, Scientific Reports, Unpublished Manuscript

P48

TRANSPARENT ELECTRONICS: IMPLEMENTATION OF PROCESS/PHYSICAL DEVICE SIMULATION TOOLS AND ANALOG CIRCUIT FABRICATION WITH OXIDE TFTS

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Amorphous transparent oxide semiconductors allow large area uniform fabrication of good performance TFTs [1] even for low process temperatures, as suitable for flexible substrates. However, before fully-oxide TFT-based devices are feasible at a commercial level some aspects are yet to be enhanced as enhancement of p-type oxide TFTs, for CMOS technology, achieving low-temperature, non-vacuum, fabrication methods and finding less expensive oxides. As a way of addressing these needs TCAD tools for device and fabrication processes simulation at a physical level (Figure 1) can be implemented [2]. Supported by physical parameters from the oxide devices being fabricated at CENIMAT, accurate models will be implemented and the viability of these models and of the optimized materials/processes will be shown by designing and fabricating a fully transparent and flexible circuit with oxide CMOS architecture.

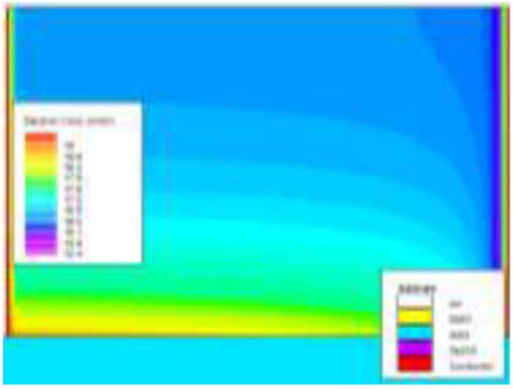

Figure 1 – Simulation in Silvaco's Atlas™ of the electron concentration on the channel of a IGZO TFT.

[1] P. Barquinha, L. Pereira, G. Goncalves, R. Martins, E. Fortunato, Toward High-Performance Amorphous GIZO TFTs, J. Electrochem. Soc., 156, H161-H168 (2009).
[2] H. Hsieh, T. Kamiya, K. Nomura, H. Hosono, C. Wu, Modeling of amorphous InGaZnO thin film transistors and their subgap density of states, Appl. Phys. Lett., 92, 133503 (2008).

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LEAD-FREE MULTIFUNCTIONAL MAGNETOELECTRIC MATERIALS FOR DEVICE APPLICATIONS

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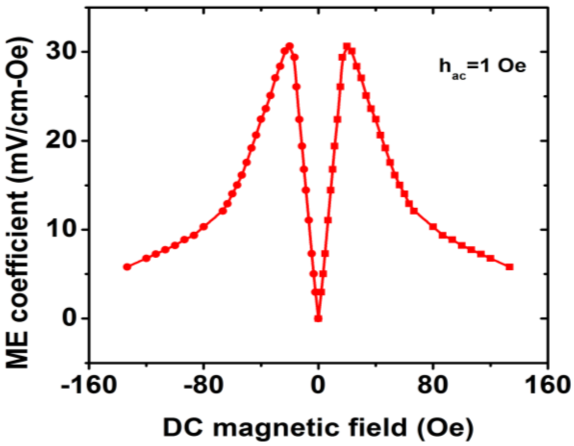
Recently, in view of large demand in energy for electronic devices, and structural health monitoring systems there has been a considerable scientific interest in materials for energy harvesting technologies. Unused power can be tapped from environment in the form of structural vibrations and magnetic field available from industrial machines, transportation vehicles, human activity, and buildings. The emerging technology for large power density is the magnetoelectric (ME) energy harvesters, derived from composite structures possessing large piezoelectric and magnetostrictive strength, in several configurations. Such ME materials also find applications in magnetic random access memory (MRAM) as well as thermally controllable magnetic memories. Apart from device applications, physics involved in single phase multiferroics, dilute magnetic oxides, is interesting. Here, we present significant results obtained in our research on multiferroic ME oxide materials in single phase and composite formats (in bulk as well as thin films).

Fig



[1] M. Liu and N. X. Sun, Phil. Trans. R. Soc. A, **372**, 20120439 (2014).

P50

HYDROGEN PASSIVATION OF TITANIUM IMPURITIES IN SILICON: EFFECT OF DOPING CONDITIONS

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[2]Department of Chemistry, University of Surrey, Guildford GU2 7XH,United Kingdom
[3]School of Electrical, Electronic and Computer Engineering, Newcastle University, Newcastle Upon Tyne, NE1 7RU, United Kingdom

In this work we revisit the problem of the hydrogen passivation of interstitial Titanium in silicon by means of density functional calculations in the light of recent deep-level transient spectroscopy (DLTS) measurements [1] of Ti implanted Silicon samples. To do so we determine the thermodynamic stability of several Ti_iH_n complexes for variable doping conditions. We also calculate the electrical transition levels of these complexes and propose an assignment of these levels to the DLTS data. We assign the levels T_iH (-/0), T_iH_3 (0/+), T_iH_2 (0/+) and T_iH (0/+) to the DLTS electron traps E40', E170', E270 and E170 respectively.

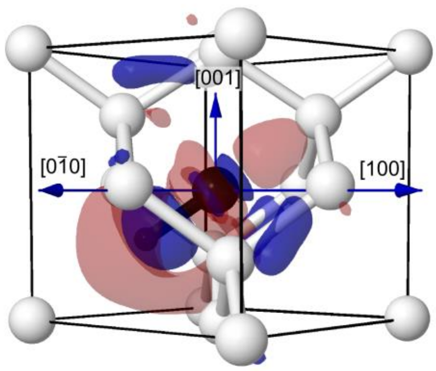

Figure 1 – Isosurfaces of the electron density transfer upon formation of a Ti-H_{ab} bond

[1] S. Leonard, V. P. Markevich, A. R. Peaker, and B. Hamilton, Appl. Phys. Lett. 103, 132103 (2013)

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WEAK PERCOLATION ON MULTIPLEX NETWORKS

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Bootstrap percolation is a simple model of activation networks. It has applications in many areas of science and has been explored on random networks for several decades. In single layer (simplex) networks, We propose an extension of bootstrap percolation to multiplex networs [1]. Which are networks with multiple kinds of edges. There is a diirect mapping betwen multi-layer interdependent networks and multiplex networks [2]. (see fig.1). In sinle layer (simplex) networks, it has been recently observed that bootstrap percolation , each is defined as an incremental proces, can be seen as the opposite of prunning percolation for multiplex networks. We collectively refer to these two models with the concept of "weak" percolation, to distinguish them from the somewhat classical concept of ordinary ("strong") percolation. While the two models coincide in simplex networks, we show that they decouple when considering multiplexes, giving rise to a wealth of critical phenomena. Our bootstrap model constitutes the simplest example of a contagion process on a multiplex network and has potential applications in critical infrastructure recovery and information security.

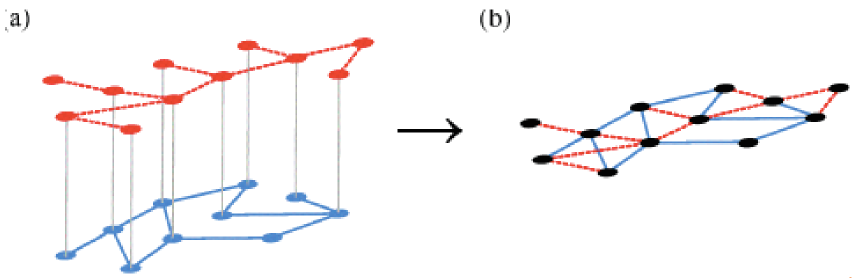

Figure 1 - 'Mapping between interdependent (a) and multiplex (b) networks.

[1] Weak percolation on multiplex networks , Gareth J. Baxter, Sergey N. Dorogovtsev, José F. F. Mendes, Davide Cellai, Phys. Rev. E 89, 042801 (2014)
[2] Heterogeneous-k-core versus Bootstrap Percolation on Complex Networks, G. J. Baxter, S. N. Dorogovtsev, A. V. Goltsev, J. F. F. Mendes , Physical Review E 83, 051134 (2011)

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STUDY AND DEVELOPMENT OF MULTIFUNCTIONAL ZNO:1D NANOSTRUCTURES TO BE USED IN ELECTRONIC DEVICES

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We aim to exploit and develop a new class of electronic devices, based on 1D ZnO nanostructures, either using rigid or flexible substrates, like paper and tetrapak. The ZnO is produced by solvothermal method assisted by microwave radiation and the emphasis will be put on developing nanoparticles to be used in sensor, like UV sensors and biosensors, and in single crystal transistors, transducers or piezoelectric devices, exploiting the properties of ZnO nanoparticles and boosting to its maximum their electronic performances for the next generation of nanodevices and nanosystems away from traditional covalent semiconductors [1]

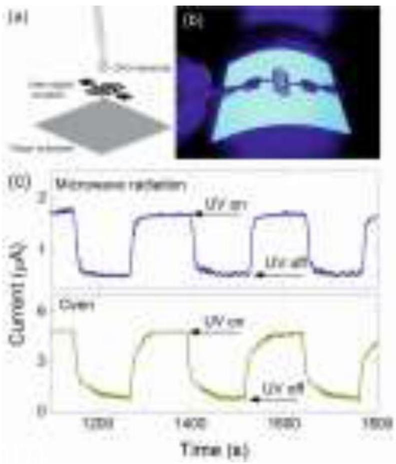

Figure 1 – (a) Scheme of the Inter-digital contacts used to test the ZnO nanorods as UV sensor; (b) paper under the UV light and (c) cycling behaviour of ZnO nanorods based UV sensors.

[1] A. Pimentel, D. Nunes, P. Duarte, J. Rodrigues, F.M. Costa, T. Moneiro, R. Martins, E. Fortunato, Synthesis of Long ZnO Nanorods under Microwave Irradiation or Conventional Heating, The Journal of Physical Chemistry C, **118**, 14629 (2014).

P53

DEVELOPMENT OF NANOMORPHOUS SILICON SOLAR CELLS ON CERAMIC SUBSTRATES WITH BIOMEDICAL APPLICATION

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The present work aims at the development and fabrication of nanomorphous silicon solar cells deposited in ceramic substrates for biomedical and industrial applications, namely long-term field hospitals.

The effects of climate change will continue to exacerbate the natural and humaninduced disasters with which the world has to cope. Solar cells can be of significant importance to field hospitals; since they are completely self-sufficient hospitals, an efficient energy supply is critical when fossil fuels may not be available or their acquisition costs are too high for long term deployments.

As an alternative to the traditional micromorphous solar cells, this work presents a novel and innovative solution to the low efficiency solar cells, by using new deposition conditions [1] to produce a nanostructured n-i-p silicon solar cell. These materials deposited in conditions near to the formation of nanocrystalline silicon, are more compact and have a higher order at short distance, which will present a higher stability and lead to solar cells with 5% efficiencies [2].

[1] H. Águas, et al. Silicon thin film solar cells on commercial tiles, Energy & Environmental Science, **4**, 4620-4632 (2011).

[2] S. Filonovich, et al. Hydrogen plasma treatment of very thin p-type nanocrystalline Si films grown by RF-PECVD in the presence of B(CH3)3, Science and Technology of Advanced Materials, **13**, 4620-4632 (2012).

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OPTICAL FIBER SENSORS IN NON-INVASIVE CARDIOVASCULAR MONITORING

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The assessment of central arterial pulse pressure has been an important tool in hypertension and cardiovascular risk evaluation. In this work, the arterial pulse wave is acquired with two optical fiber probes, one based on fiber Bragg gratings (FBG) [1] and a low cost solution using a plastic optical fiber (POF) intensity sensor [2]. The devices were fully characterized and human tests performed. The results showed a fair compromise between easiness of applicability, technician training, and pressure wave acquisition performance.

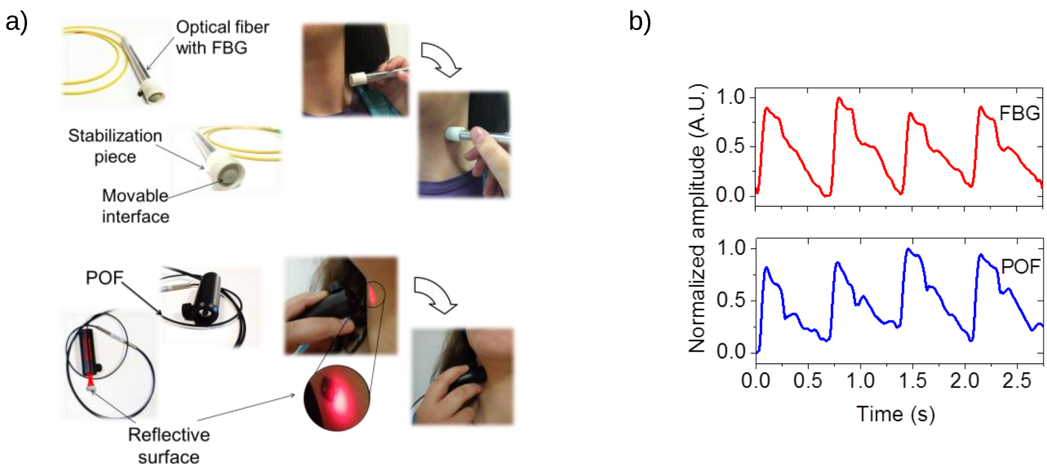

Figure 1 – a) FBG (Top) and POF (Bottom) probes; b) pulse waves acquired with both sensors.

[1] Leitão, C., Antunes, P., Bastos, J., Pinto, J., André, P., "Plastic Optical Fiber Sensor for Noninvasive Arterial Pulse Waveform Monitoring," IEEE Sensors Journal 15(1), 14-8 (2015).

[2] Leitão, C., Antunes, P., André, P., Pinto, J., Bastos, J., "Central arterial pulse waveform acquisition with a portable pen-like optical fiber sensor," Blood Pressure Monitoring Journal 20(1), 43-6 (2015)

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MODELIZATION AND DEVELOPMENT OF MICROWAVE SINTERING CAVITIES

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A bench microwave oven to processes utilitarian porcelain was simulated and designed. The standing waves microwave results in an inhomogeneous electromagnetic field which cause nonuniform heating of the material, giving rise to thermal runaway. A perceptive of how the electromagnetic field propagates and how is absorbed is essential. So, using the COMSOL Multiphysic software, we carried out a 3D electromagnetic field simulation in a microwave oven loaded with a ceramic sample and after analyzing the results we build the cavity and the automated power control system that produces a homogeneous heating of the ceramic material. With lower thermal gradients in the material, it is possible to increase the heating rate and avoid hot spots that may originate the thermal runaway phenomenon. The study was conducted in a multimode cavity microwave oven with 6 magnetrons, working at the frequency of 2.45 GHz.

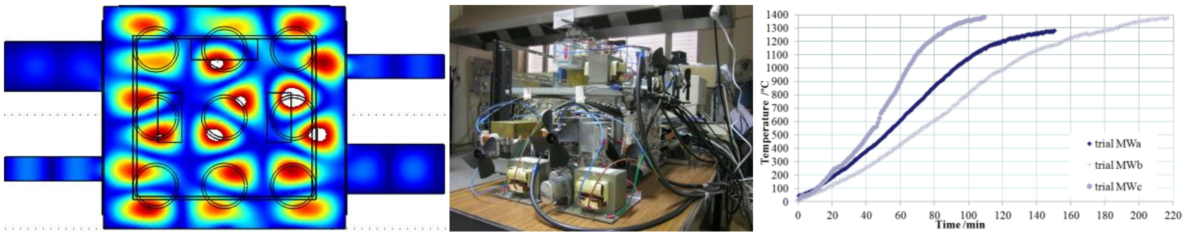

Figure 1 – Microwave furnace, electromagnetic field simulation and temperature sintering curves.

[1] T. Santos, L. C. Costa, L. Hennetier, M. A. Valente, J. Monteiro, and J. Sousa, Microwave processing of porcelain tableware using a multiple generator configuration, Appl. Therm. Eng., **50**, 677-682 (2012).

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DEVELOPMENT OF NEW MATERIALS FOR ENERGY STORAGE BASED ON ALKALI FERRITES

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This project aims to present material(s) that can efficiently storage energy (electric/magnetic). A family of materials with high potential for this purpose is the ferrites because of characteristics like high permeability, low magnetic losses, high electrical resistivity, low eddy current losses, good thermal and chemical stability.
In this work, alkali ferrites nanopowders were prepared by different methods (sol-gel, solid state, combustion, microwave assisted reaction). The synthesis process is crucial because it can allow modification and tuning of fundamental characteristics. XRD, FTIR and Raman spectroscopy were used to analyse their structure.
In a second step the nanopowders were incorporated in a polymer matrix, and this composite was analysed by TGA, DSC, SEM-EDS and TEM.
Electrical and dielectric characterization was made in the frequency range $10^2 – 10^9$ Hz and in the temperature range of 200 - 400 K. VSM was used to measure the magnetic properties.

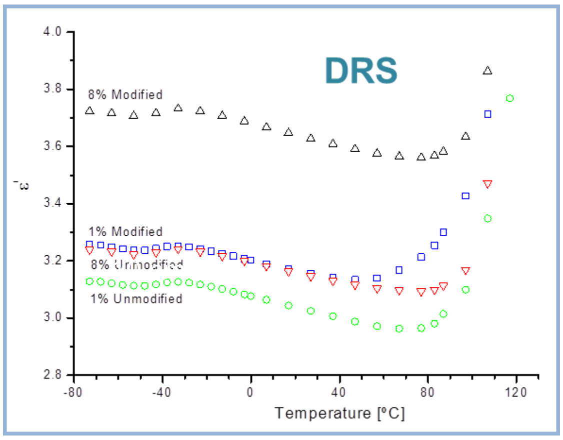

Figure 1 – Dielectric characterization of composites composites with different percentage in weight of lithium ferrite particles (1 and 8%).

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LIGHT TRAPPING IN THIN FILM SOLAR CELLS WITH SELFORGANIZED PLASMONIC NANOSPHERES

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The intense light scattered from metal nanoparticles (NPs) sustaining surface plasmons makes them attractive for light trapping in photovoltaic applications. However, a strong resonant response can only be obtained if the NPs have monodisperse properties. The synthesis of colloidal NPs is the method that produces the highest monodispersion in geometry and material; being also low-temperature, low-cost and scalable [1]. Novel plasmonic back reflector structures were developed using spherical gold colloids with appropriate dimensions for pronounced far-field scattering. The plasmonic back reflectors are incorporated in the rear contact of thin film *n-i-p* nanocrystalline silicon solar cells to boost their photocurrent generation via optical path length enhancement inside the silicon layer. The quantum efficiency spectra of the devices revealed a record broadband enhancement [2].

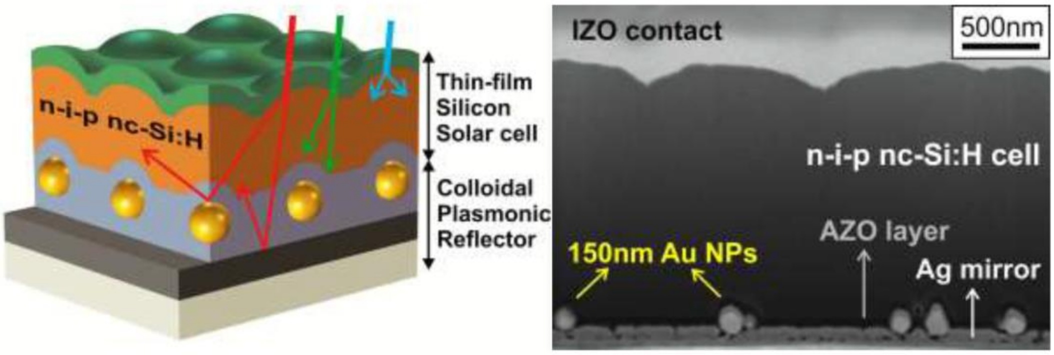

Figure 1 – Sketch and SEM-FIB cross section of colloidal plasmonic back reflectors in a nc-Si:H cell

[1] M. J. Mendes et al., Nanoscale, **6**, p. 4796-4805 (2014).
[2] M. J. Mendes et al., Nanotechnology, **26**, 135202 (2015).