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MONCLOA

1st Workshop
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CIE Moncloa
Campus

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INDEX

Editorial.....	5
i-Health Cluster.....	7
Introduction.....	9
Oscillations and connectivity patterns measured with magnetoencephalography in mild cognitive impairment	11
A telehealth system for chronic disease management at home focused on Parkinson's disease patients	13
Evaluation of new potential chemotherapeutic agents for the treatment of Chagas disease	15
<i>Trichomonas vaginalis</i> : Molecular characterization and rational design of new molecules (screening <i>in silico</i> and biological activity)	17
Cancer stem cell differentiation as therapeutic strategy in breast cancer; structural approach in the search of specific inhibitors of HIF-2 α	19
A fast pathway for fear in human amygdale	22
Modeling and optimization of a positron emission tomography scanner for small animal molecular imaging using Geant4 based tools	23
Role of cannabinoids and autophagy in the pathogenesis and therapeutics of spinocerebellar ataxias.....	25
Spatio-temporal morphology for Microscopy Image Analysis	27
Crowdsourcing malaria image analysis.....	28
Cell therapy in combination with a xenogeneic bone substitute in the treatment of critical-size supra-alveolar periodontal defects in dogs	29
Reprogrammable, modular bio-sensors using Boolean logic	31
Agri-Food and Health Cluster	33
Introduction.....	35
Development of molecular and technology tools for the early detection of food spoilage by sorbate resistant yeast and its altering product, the pentadiene.....	37
Influence of net energy content of barley based diets on productive performance of gilts, boars, and immunocastrated males slaughtered at heavy body weights.....	40
Infotaxis algorithm for the detection and localization of disease-borne volatiles in crop fields....	42
Integrated approach to the analysis of human and animal tuberculosis.....	44
African horse sickness in Spain: New tools for its surveillance and control.....	48
Use of pulsed light to increase the safety of ready-to-eat food products.....	50
Development of a vision system to detect allergen (peanut traces) in powdered foods.....	52
Materials for the Future Cluster	55
Introduction.....	57
Quantum transport in graphene and other materials	59
Magnetism in magnetic/non magnetic/magnetic nanostructures	61
Silica additions in cement pastes obtained from different mixing conditions: Influence on the hydration process	62
Renormalized properties of graphene induced by surface acoustic waves.....	64
Magnetically triggered multi-drug release by hybrid mesoporous silica nanoparticles	66
Smart nanosystems for antitumor therapy	68
Electrostatic doping of strongly correlated oxides.....	70

Hysteretic transport in oxide/graphene hybrid planar nanostructures.....	72
Design and synthesis of two-dimensional magnetic and electric properties in perovskite materials	74
Fabrication, characterization and testing of nanostructured W for nuclear power plants applications.....	76
Phase transitions in colloidal monolayers absorbed at flat interfaces.....	78
Surface acoustic waves in graphene	80
Development of a Molecularly Imprinted Polymer (MIP) for the determination of Enrofloxacin in food samples	82
Heritage Cluster.....	85
Introduction.....	87
Decay assessment, diagnosis and monitoring through wireless sensor networks and non destructive techniques for architectural heritage conservation	89
Comprehensive strategy of assessment of cultural landscapes related to Spanish energy, industry: Stage of identification and catalog.....	91
Public action in social housing estates in Madrid, Paris, and Berlin. Identification, protection and intervention between 1979 and 2010	93
Effects of conservation and restoration treatments on porous inorganic materials in archaeological sites. Case study: Mérida.....	96
Participatory processes for valuing cultural landscapes in rural areas	98
Global Change and New Energies Cluster.....	101
Introduction.....	103
Development of new efficient materials for carbon capture technology	105
New generation nano-structured membranes for solar-driven micro/ultra filtration systems.....	107
Intermediate band materials for a new generation of solar cells.....	110
Plasmonic nanoparticles for the protection of the final optics in inertial-confinement fusion facilities.....	112
Simulation of thermal performance of glazing in architecture using scale models	115
Proactive and reactive thermal optimization techniques to improve energy efficiency in data centers.....	117
Design and characterization of cryogenic low noise amplifiers at the CDT-Observatorio de Yebes	119
Development of high precision FPGA-based noise reduction techniques for infrared interferometers fusion diagnostics	121
Software developments and astronomical researchs for integral field instruments at LICA (Laboratorio de Instrumentación Científica Avanzada).....	123
Soil bacteria adaptive stress-response to the presence of Nanoscale Zero Valent Iron	126
Stridulation variability in dung beetles: An examination of the species <i>Geotrupes mutator</i> (Marsham, 1802) (Coleoptera, Scarabaeidae).....	128
Alpine lizards in Mediterranean mountains: Distribution patterns and prospective evolution under conditions of global change	130
Impact of climate variability on Iberian Peninsula summer cropping systems.....	132
Contributions of active faults in El Salvador to the seismic hazard.....	135
Next-generation materials and devices for energy-efficient systems.....	137
Iceberg discharges of the last glacial period driven by oceanic circulation changes.....	139

The Moncloa Campus, Campus of International Excellence (CIE Moncloa Campus), a joint initiative between the UCM and UPM, is a strategic commitment to excellence between two universities that complement each other in their goals and bring together what is most likely the greatest collection of talent in our country. In its creation and development the CEI Moncloa Campus has set goals that go beyond its planned timeframe, which extends to the end of 2015. These objectives are based on maintaining and enhancing the collaboration between the two institutions with the idea of creating a true international reference in the university community. We are fully confident that this can be achieved and, therefore, it should be achieved.

Clearly, any bid for the future must provide training for those who will oversee that future: our young talent. At a time when the government and the private sector are cutting back on R&D spending, which we consider suicide and which is taking a heavy toll on the development of human resources for research, the CIE Moncloa Campus has earmarked more than four million euros of its budget (over 30%) for the PICATA Program (International Program for Talent Recruitment). This program includes grants and pre- and post-doctoral contracts with very strict standards that are comparable to those of similar international programs such as the European Union's People program, and it requires that the research projects be co-directed by professors from the UPM and UCM. As a result, apart from ensuring that our young talent receives the highest level of scientific training by establishing certain concepts from the very beginning, it reinforces our fundamental goal: the closest possible collaboration between the two universities.

During the course of this conference, which has provided us with a glimpse of the advances these talented researchers have made, we have confirmed that we are on the right track. The scientific level of the work fully meets our expectations and the level of maturity achieved by our young researchers is inspiring. We would like to offer our thanks to all of the speakers and their directors. Thank you for living up to our expectations and for showing us that the future of CIE Moncloa Campus is in good hands.

Joaquín Plumet

Pro-vice-chancellor of Research

UCM

Roberto Prieto

Pro-vice-chancellor of Research

UPM

M^a Inés Mínguez

Delegate of the UPM Vice-chancellor

CIE Moncloa Campus

The background of the slide is a vibrant teal watercolor splash that spreads across the entire frame, creating a dynamic and artistic feel. The splash is darker in the center and fades towards the edges, with some white space visible at the top and bottom right.

1st Workshop
PICATA

i-Health Cluster

The Workshop of i-Health was coordinated by Prof. Andrés Santos (UPM - ETS Ingenieros Telecomunicación) and Prof. Ignacio Lizasoain (UCM - Facultad de Medicina). This session included presentations by four post-doctoral contracts and seven predoctoral students. As requested, they presented the provisional results of their research projects and all of them were supervised jointly by the UCM and UPM with one Director from each university.

The results presented by the **post-doctoral contracts** were part of their post-doctoral research. In this context, Dr. Moisés García Arencibia showed us the neuroprotective effects of some new cannabinoid drugs acting on CB2 receptors, which can be used for the treatment of spinocerebellar ataxias. He also discussed about the utility of these new drugs in other neurodegenerative diseases such as Parkinson's disease, Huntington's disease and multiple sclerosis. The data presented by Dr. Fabio Vignoletti were also related with new therapies. But in this particular case, he demonstrated that cell therapy in conjunction with the use of a xenogeneic bone substitute is able to promote periodontal regeneration in experimental periodontal defects. Dr. Miguel Ángel Luengo Oroz presented two interesting works that he is currently developing: one related to the analysis of zebrafish embryo microscopy images using spatio-temporal mathematical morphology, the other on the use of crowdsourcing techniques and on-line games for the analysis of malaria microscopy images through the Internet. Dr. Niall Paul Murphy presented his work on the design and simulation of biological sensing devices that use plasmids as detection mechanism, producing modular and reprogrammable systems that detect complex combinations of plasmids and external signals.

On the other hand, most of the **predoctoral students** presented results which are intended to form part of their doctoral thesis. Ms. Alexandra Ibáñez and Ms. Cristina Fonseca presented data regarding the evaluation of new potential agents for the treatment of infectious diseases such as *Trichomonas vaginalis* infection which is the most common non-viral sexually transmitted infection, and for Chagas disease which is also one of the most neglected tropical diseases according to WHO classification. Ms. Nagore I. Marín studied the HIF-2 α specific inhibition as a novel antineoplastic strategy in breast cancer. She showed that the inhibition of HIF-2 α (a transcription factor) which can control cancer stem cell differentiation and could render tumors more susceptible to the chemo and radiotherapy currently used. Mr. Jorge Cancela-González showed his work on telehealth systems for chronic disease management at home, focusing on Parkinson's disease patients. Mr. Constantino Méndez-Bértolo presented his studies on a fast subcortical pathway for threat-related signals to the human amygdala. Ms. María Pilar Garcés-López showed her work on oscillations and connectivity patterns in mild cognitive impairment, using magnetoencephalography signals. Finally, Ms. Sneha Nidhi described her working on the modeling and optimization of a positron emission tomography scanner for small animal molecular imaging that replaces the conventional photomultipliers by solid-state silicon photomultipliers.

All these interesting works will allow the i-Health cluster of the Moncloa Campus of International Excellence to achieve its goals of integrating clinical and preclinical research, together with information and communication technologies, for improving human health and quality of life.

Andrés Santos Lleo

Ignacio Lizasoain Hernández

Coordinators i-Health Cluster

Oscillations and connectivity patterns measured with magnetoencephalography in mild cognitive impairment

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Keywords: Magnetoencephalography, MCI, connectivity, oscillations

1. Introduction and Contents

Mild cognitive impairment (MCI) is a state of cognitive function that lies between normal aging and dementia, particularly Alzheimer Disease (AD). People with MCI have objective cognitive disturbances that do not interfere with daily functioning and are classified as amnesic and non-amnesic MCI, depending on the presence of memory impairment. Both subtypes can further be classified as single or multidomain, based on the number of cognitive domains affected. The amnesic MCI subgroup presents the higher risk of developing Alzheimer disease compared with their age-matched healthy controls (annual conversion rate 5-10% [1]). Thereby there has been an increasing interest in studying the MCI over the past few years, since the early detection of this prodromal stage as well as those MCI patients at higher risk of converting to AD, would be of huge importance in the development and testing pharmacological or neuropsychological measures.

Electrophysiological signs of Alzheimer disease have been widely studied with electroencephalography (EEG) or magnetoencephalography (MEG). In particular, an increase in power in the lower frequency bands, and a general decrease in connectivity have been shown in many instances. However there is less information about MCI. Some studies show a slight shift of the power towards the low frequency range, and others indicate variations in the connectivity patterns, when compared to healthy controls.

We examined resting state and task MEG registers of MCI patients and controls, looking at differences in power spectrum and connectivity patterns.

2. Methodology

69 controls, 53 amnesic-MCI and 84 multidomain-MCI underwent a MEG register. Subjects sat inside a magnetically shielded room for about 1.5 hours and performed two memory tasks (face delay match to sample and arithmetic task). Resting state registers of eyes open (4min) and eyes closed (3min) were also registered. Magnetic fields outside the brain were measured with an Elekta Neuromag MEG device, consisting in 102 magnetometers and 204 planar gradiometers.

Data was preprocessed the following way: after a temporal signal space separation (MaxFilter, Elekta), data was separated into trials (4 seconds segments for the resting state data), trials with artifacts were discarded from the analysis, notch filtered to remove power line and harmonics and finally bandpass filtered in 1-150Hz (FieldTrip [2]).

For spectrum computation a multi taper method with dpss window and 1Hz smoothing was used, and connectivity between all pair of sensors was assessed with Phase Locking Value (PLV), after filtering the signals into delta (2-4Hz), theta (4-8Hz), alpha (8-12Hz), beta (12-30Hz), low gamma (30-60Hz) and high gamma (60-120Hz). For statistical analysis Wilcoxon and Kruskal-Wallis tests were employed, with permutations to account for the multiple comparison problem.

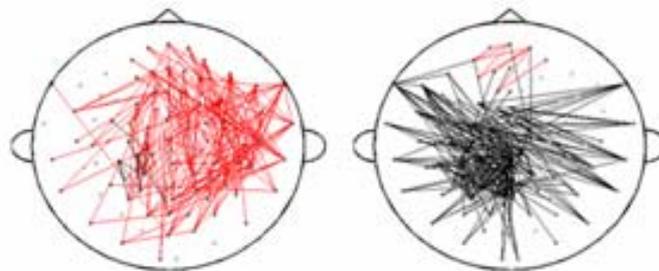
3. Results and Discussion

We looked for differences in connectivity between controls and MCI, both in resting and the arithmetic task. We found that in general MCIs had a higher connectivity in lower frequency bands, although there was a big dependency on the regions. As an example, the links that were significantly altered ($p=0.02$) between controls and multidomain MCI in resting state data are shown for theta and alpha bands.

4. Conclusions and Future research

We showed that MCI has an impact on the electrophysiological signals produced in the brain, and that it can be seen non-invasively through the connectivity patterns of MEG signals. Alterations of connectivity are also different than the ones found in Alzheimer Disease, indicating that the path control-MCI-Alzheimer is probably non-linear. However, to gain more insight into what is really happening in the MCI brain, we need to extract more information out of our MEG signals. For instance, going to the source level (i.e. reconstructing the electrical currents that were produced in the brain and that created the magnetic field that we measured in the MEG sensors) would be extremely useful. However, the reconstruction of the brain areas that were activated and its dynamics is a quite recent topic, and requires the use and testing of some recent algorithms. Right now we are working on that, since functional connectivity at the source space which will characterize better the impaired functional networks in the early stages of Alzheimer Disease.

Figures



Links showing statistical differences in PLV between multidomain MCI and controls in resting state eyes closed data for theta (left) and alpha (right). Red lines show links with higher PLV in MCI, black lines for higher values in controls.

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A telehealth system for chronic disease management at home focused on Parkinson's disease patients

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Abstract. Chronic diseases are prolonged conditions that normally do not improve with the time and are rarely cured completely. Most of them are strongly related with the ageing process and consequently nowadays chronic diseases represent a major health burden worldwide and specially in the developed world. In response to these changes healthcare services should shift their focus from episodic care to a continuous care approach where the patient acquired a main role within the healthcare path. In this shared-care model it is essential to get the patient involved in its own disease through the patient education and empowerment. At this point, the use of the information and communication technologies (ICT) provides tools for both patients and clinicians in order to facilitate the monitoring and empowerment of patients and the communications between them and the clinicians.

Keywords: Parkinson's disease, wearable sensors, telehealth, data mining

1. Introduction and Contents

In developed countries, chronic diseases now accounts for more than 75% of health care expenditure [1]. This work targets the remote monitoring and management of patients with Parkinson's disease (PD). PD is one of the most common neurodegenerative disorders. It occurs in about 1% of the population over the age of 60 and its prevalence increases with age. Telemedicine brings healthcare delivery to the home environment by connecting the patient with medical professionals. It is not intended to replace health professional care, but rather to enhance the level of care [2]. The major motor disturbances in PD are bradykinesia (i.e. slowed movement), hypokinesia (small amplitude movements), resting tremor, rigidity, and postural instability. PD is typically characterized by severe, unpredictable and abrupt changes in the patient motor performance whereby OFF periods, characterized by the temporary loss of drugs effectiveness, alternate, sometimes within minutes, with ON periods, during which the medication effectively attenuate motion symptoms. The loss of dopaminergic neurons compromises the speed, the automaticity and fluidity of movements. As the disease evolves, PD patient's motion becomes slower and tremoric and the response to medication fluctuates along the day (ON-OFF periods). Currently, motor assessment in PD is mainly based on historical information, home diaries and neurological examination during visits to the clinic. These methods clearly suffer from many drawbacks: data from these sources can be highly subjective, they rely on the patient's memory and perception of his own symptoms and they depend on the physician's experience on the field. Moreover, most of the patients may not be aware of mild symptoms, they may not necessarily understand medical terminology, or they may unconsciously exaggerate or attenuate symptoms severity. Finally, PD can affect short-term memory. In an attempt to solve these problems and to find more objective assessments, several rating scales have been designed and used. Among them, the Unified Parkinson's disease Rating Scale (UPDRS) [3] is the most widely used. This rating scale tries to quantify selected symptoms and parkinsonian signs in a 5-points scoring system (from 0 for no sign, to 4 for a marked severity of the sign). Unfortunately, the UPDRS, like any other semi-objective rating scale, has several limitations. In fact intra and inter-observer inconsistencies and bias by subjectivity issues related to the historical information have been demonstrated. The system platform is composed by a set of wearable sensors devices for the recording of the motion signals and a set of software algorithms for the signal processing (Support Vector Machine algorithms). The hardware was formed by a set of four tri-axial accelerometers positioned at each patient limb used to record signals from legs and arms; a belt sensor, composed by an accelerometer and a gyroscope, used to record body movement accelerations and angular rate;

and a data logger used to receive and store all recorded signals in a SD card. All sensors transmit data using Zigbee protocol to the logger device, with 62.5 Hz sampling rate before a synchronization phase. All accelerometers transmit data at the same time and no retransmission of lost packets has been implemented in order to save battery. Apart from the wearable sensor network, each patient was provided with touch-screen PC at his/her home.

2. Materials and Methods

The current status of the project is a fully operative prototype which has been tested in three different hospitals across Europe: University of Navarra Medical School Hospital (Spain), the University of Ioannina Hospital (Greece) and the Nuovo Ospedale Civile S.Agostino-Estense of Modena (Italy). A iterative design process was followed. Three different phases were designed involving 92 PD patients and 20 health subjects. On each phase of the design raw signals were collected using the wearable sensor network. In order to assess the status of the patient the patient's computer was equipped with ad-hoc software for the detection and quantification of the PD symptoms. The technology used is based on machine learning algorithms; specifically in classifiers (knowledge about a given problem is learnt from examples also called the training data). As general approach the raw signal is preprocessed with a linear interpolation algorithm in order to fix the dataloss holes. Then, the signal is split out in "epochs" using a slide window (between 1 and 5 seconds length). For each "epoch" different features are calculated (e.g. rms, entropy or range). These features will feed the classifiers which were previously trained using the UPDRS as reference.

3. Results and Discussion

About the technical performance of the system it shows an maximum level of accuracy of 86% of bradykinesia severity [4], [5]. Also, a special module for the assessment of the gait has been developed showing an accuracy of 98,12% in the characterization of the step frequency and arm swing frequency [6]. Entropy analysis was also used in the assessment of the gait degradation has been proved to be an excellent discriminator of the On/Off status) [6].

4. Conclusions and Future research

The nature unsupervised environments creates a number of challenging problems with regards to signals interpretation and signals quality validation, nevertheless the future of the eHealth system require the monitoring and assessment of the patients at their own homes. Future research will involve a global survey involving all the past and ongoing projects of telehealth systems related to PD patients in order to extract the trends and bottlenecks of this field.

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Evaluation of new potential chemotherapeutic agents for the treatment of Chagas disease

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Abstract. The lack of a suitable therapy for the treatment of Chagas disease is today a reality. The only two drugs commercialized for the specific treatment of the parasitic illness caused by *Trypanosoma cruzi*, show important limitations in terms of efficacy and safety. In this context, our research group works in the rational synthesis and evaluation of new trypanocidal prototypes based on *virtual* and classical screening methods, as well as in the development of new pharmaceutical formulations of the reference drug benznidazole, contributing in this way to the search of therapeutic alternatives for the treatment of the disease.

Keywords: Chagas disease, trypanocidal agents, benznidazole, solid dispersions

1. Introduction and Contents

The WHO classifies Chagas disease as one of the most neglected tropical diseases according to the chronic nature of a parasitosis that affects more than 8 million people in Latin America, where is naturally transmitted by hematophagous vectors [1]. However, alternative routes of transmission (i.e. contaminated blood transfusions or congenitally) and international migrations have spread this illness to non-endemic areas, acquiring an emerging character in countries like Spain and becoming a worldwide public health problem [2]. Concerning the chemotherapy, neither satisfactory drug nor a vaccine has been developed since the commercialization of the only two drugs available for its specific treatment. In spite of the fact that nifurtimox and benznidazole report parasitological cures during the acute phase, both turn into ineffective in the chronic disease [3]. Moreover, their toxicity [4] together with the existence of resistant *T. cruzi* strains [5] hinders this situation supporting the priority in the search of antichagasic drugs.

According to this, our research team has great experience in the synthesis and evaluation of antichagasic prototypes by applying *virtual* [6] and classical [7] screening. Furthermore, the new formulations of benznidazole suppose an alternative to the synthesis, enhancing its effectiveness by improving the physicochemical properties of this poor water soluble drug [8].

2. Methodology

2.1 Chemistry - The designed 1,2-disubstituted 5-nitroindazolinones are generally prepared by sequential alkylation at positions N-1 and N-2 of 5-nitroindazolinones, with the corresponding alkyl halide. Other indazole derivatives are also obtained from these synthetic procedures [7].

2.2 Solid dispersions (SDs) - Drug (benznidazole) and carrier (sodium deoxycholate) were co-dissolved in a common solvent later removed by a freeze-drying process. Scanning electron microscopy, powder X-ray diffraction, differential scanning calorimetry and *in vitro* dissolution studies were performed for their characterization.

2.3 Biological assays - *In vitro* evaluation consists in a sequential screening against *T. cruzi* (epimastigotes and amastigotes) and mammalian cells (unspecific cytotoxicity). Only those compounds with excellent results are also tested in a murine model of acute Chagas disease.

2.4 *In silico* identification of trypanocidal compounds - A data set of 1308 compounds, 759 active and 549 inactive against *T. cruzi*, has been elaborated to find classification models that allow the discrimination of trypanocidal drugs from molecular descriptors calculated with the software TOMOCOMM-CARDD and linear discriminant analysis performed with STATISTICA.

3. Results and Discussion

3.1 Several 5-nitroindazole derivatives show activities on epimastigotes better than nifurtimox ($IC_{50}=3.61$) and benznidazole ($IC_{50}=27.12$), holding also complete growth inhibition of amastigotes at concentrations lower than 8 μ M. Two of them were assayed in mice, reaching both compounds reductions in parasitemia up to 52% and 77% at the end of the treatment.

3.2 SDs: An enhance in benznidazole:sodium deoxycholate ratio supposes an increase in trypanocidal activities, but also in the cytotoxicity. According to this, the ratio 1:3 was selected as the most promising SD and thus, tested *in vivo* reaching significant reductions in parasitaemia.

3.3 *In silico* procedures: The first linear discriminant analysis-based QSAR models obtained provide accuracies higher than 86% and 82% in the training and test sets, respectively.

4. Conclusions and Future research

4.1 The 5-nitroindazole derivatives are promising trypanocidal agents. Nevertheless, additional studies are needed to assess their potential use as antichagasic drugs. At the moment, our research team is working in the synthesis and evaluation of new structures and fluorescent derivatives to study the intracellular distribution by using confocal microscopy.

4.2 Solid dispersions in sodium deoxycholate improve benznidazole effectiveness. Likewise, new SDs in a cellulosic carrier (L-HPC) and other pharmaceutical systems will be designed and applied to benznidazole. These formulations will be also useful for our synthetic derivatives.

4.3 Serological tests (ELISA) will be introduced in the sequential screening in order to evaluate the evolution of the chronic disease in mice treated during the acute phase.

4.4 Our data set of experimental compounds, together with the first *in silico* models, will permit us to classify chemicals in the chemotherapy of Chagas disease. However, a validation of these models is needed to ensure their quality and predictive power. In fact, new classification models will be calculated, to develop useful tools for the discovery of trypanocidal compounds.

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***Trichomonas vaginalis*: Molecular characterization and rational design of new molecules (screening *in silico* and biological activity)**

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Abstract. Trichomoniasis is the most common nonviral sexually transmitted infection (STI) in the world. This STI is associated with a wide range of clinical patterns, however, very little is known about the pathogenic features of this parasite. In the current research, diverse aspects of trichomoniasis have been studied. On the one hand, different *Trichomonas vaginalis* strains have been genotyped using the ITS1/5.8S/ITS2 region, with the aim of searching a robust molecular marker to correlate phenotypic features and genotypic diversity; on the other hand, a high-throughput *in vitro* procedure has been optimized providing a sensitive and rapid method to evaluate potential trichomonocidal compounds. Further studies searching other genomic regions and the development of virtual screening models are currently being investigated.

Keywords: *Trichomonas vaginalis*, Internal transcribed spacer (ITS), Inter simple sequence repeats (ISSR), experimental screening, virtual screening

1. Introduction and Contents

Trichomonas vaginalis is the causative agent of trichomoniasis, a sexually transmitted infection (STI) responsible of almost half of all curable infections, with more than 180 million cases per year [1]. This parasitic disease presents a wide range of clinical manifestations ranging from asymptomatic cases to severe inflammatory sequelae. Trichomoniasis is also a risk factor for cervical and prostate cancer and plays an important role in HIV acquisition and transmission [2]. Despite its importance, little is known about the pathogenic features and the genetic relatedness. One of the objectives of the current investigation has been the study of the ITS1/5.8S/ITS2 region of *T. vaginalis* strains with different features to determine possible correlations between mutations and phenotypic differences.

5-Nitroimidazoles are the unique drugs approved by the FDA to treat trichomoniasis. However, no alternative treatments are available for hypersensitivity cases and clinical drug resistance is becoming widespread [3]. So, alternative curative therapies are needed. The microscopic-based counting of viable trophozoites has been the traditional procedure to evaluate *in vitro* activity of new scaffolds; however this method is time-consuming and highly dependent on the observer. One of the aims during this period has been the development of a sensitive, fast and reliable *in vitro* assay for the screening of trichomonocidal drugs using the redox dye resazurin.

2. Methodology

2.1. Parasites: *T. vaginalis* isolates are cultivated at 37 °C and 5% CO₂ in TYM modified medium. Six isolates with different pathogenic behavior, metronidazole sensitivity and geographic origin, have been characterized.

2.2. Molecular characterization: The DNA extraction has been performed by the use of the Speedtools DNA Extraction kit. PCR amplification and sequencing has been carried out according to the procedures of Felleisen [4].

2.3. Resazurin *in vitro* assay optimization: A fluorimetric microassay using a redox dye has been validated. Experimental conditions have been adjusted as described Ibáñez et al. [5].

3. Results and Discussion

3.1. Molecular characterization of the ITS regions: The ITS1-5.8S rRNA-ITS2 sequences of the isolates examined proved to be genetically identical. The low polymorphism was supported with other sequences obtained from the GenBank. The alignment report revealed 5 different sequence patterns among the different trichomonadid sequences with only one mutation.

3.2. In vitro screening assay: The results have demonstrated the reductive character of the TYM medium producing the spontaneous reduction of the resazurin. Finally, 200 µl of the trophozoites cultivated with the drugs were seeded into microplates. TYM medium was replaced by PBS and 10% of 3 mM resazurin solution. To confirm the applicability of the new *in vitro* assay, different therapeutic drugs were assayed by microscopic and fluorimetric method in parallel. No statistical difference in IC₅₀ activities were obtained by both procedures (Table 1).

4. Conclusions and Future research

4.1. Molecular characterization of the ITS regions: The ITS regions have provided to be useful markers for intraspecific differentiation in other parasites [6]. Although *T. vaginalis* genome is highly repetitive with ~250 rDNA copies [2], only one stable mutation in the position 66 of the ITS1 region was observed in the 24% (6/25) of the sequences analyzed with a possible correlation with a geographical origin. Hence, the low polymorphism found, suggests the suitability of the ITS regions as molecular markers for the determination of closely related species and clinical diagnosis in trichomonads.

Currently, inter-microsatellites regions (ISSR-PCR) are being explored for intraspecific characterization. Diverse *T. vaginalis* strains are being amplified with 20 different primers based on dinucleotide and trinucleotide repetitions.

4.2. In vitro screening assay: The activity results obtained by both methods were quite similar, proposing the resazurin assay as a sensible, one-step, reliable and easily automated method for high-throughput screening against *T. vaginalis*.

Moreover, new LDA (linear discriminant analysis)-based QSAR models are being developed for virtual screening of potential trichomonacidal compounds. A large dataset composed by 782 compounds (370 active and 412 inactive) assayed against the parasite by different research groups has been performed. The compounds have been clustered into training and test sets. Different molecular descriptors are being calculated with TOMOCOMD-CARDD® software.

Tables

Table 1: Trichomonacidal activity of therapeutic drugs determined by resazurin and microscopic methods.

Therapeutic drugs	IC ₅₀ activity (µg/mL)*	
	Resazurin	Microscopic
Metronidazole	0,579±0,07	0,563±0,05
Secnidazole	0,389±0,04	0,234±0,08
Clotrimazole	3,459±0,43	2,786±0,89

*Data are expressed as mean ± standard deviation obtained from at least three independent experiments. Statistical comparisons were performed by Wilcoxon T test with SPSS software (v.20, IBM).

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Cancer stem cell differentiation as therapeutic strategy in breast cancer: structural approach in the search of specific inhibitors of HIF-2 α

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Abstract. The main objective of this work is to explore the HIF-2 α specific inhibition as a novel antineoplastic strategy in breast cancer. By controlling cancer stem cell differentiation, HIF-2 α inhibition could render tumors more susceptible to the chemo and radiotherapy currently used.

Keywords: HIF, hypoxia, cancer stem cells, cell differentiation, breast cancer

1. Introduction

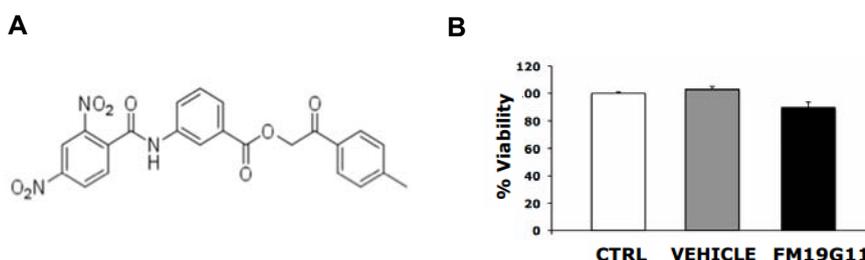
During the last years, the strategy to re-orientate antineoplastic therapies towards cell differentiation has been reinforced in Oncology. In this context, the cancer stem cell (CSC) subpopulation has arisen as a novel target for pharmacological action, as they seem to have an especial resistance to chemo and radiotherapeutic treatments. Solid tumors with areas of hypoxia are generally associated with bad prognosis. The hypoxia inducible factor (HIF) has shown to have a key role in oncogenesis by promoting the generation and expansion of the CSCs [1]. To be transcriptionally active, HIF must be a heterodimer formed by a constitutively expressed β subunit and a hypoxia inducible subunit, known as α . There are different α isoforms, being HIF-2 α [2] the one that specifically regulates genes involved in stemness and pluripotency, such as Oct4, Sox2 and Nanog.

2. Methodology

Cellular experiments were carried out in human breast cancer cell lines (MCF-7, BT474, SKBR3 and MDA-MB-436), in cells derived from mice breast xenograft models and in cells from human breast tumors obtained by surgery at University Hospital of Getafe. Standard biochemical and molecular biology techniques were used, including cell culture, MTT proliferation assay, reporter assays, flow cytometry, DNA cloning, protein expression and purification and xenografts for in vivo cancer models. For structural biology studies, protein NMR and crystallization techniques have also been used.

3. Results and Discussion

3.1. The HIF- α inhibitor FM19G11 [3] decreases the number and size of mammospheres, without inducing general cytotoxicity



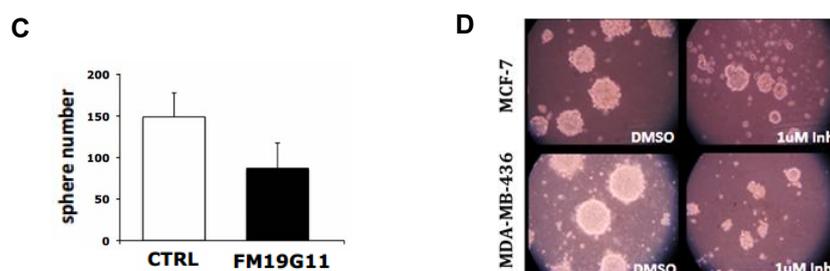


Fig. 3.1. (A) Structure of FM19G11. Addition of FM19G11 (1µM) to MCF-7 cells does not affect their viability (B), but it decreases the number and size of mammospheres derived from MCF-7 (C, D) and MDA-MB-436 (D) cell lines.

3.2. HIF- α inhibition reduces expression of breast CSC markers

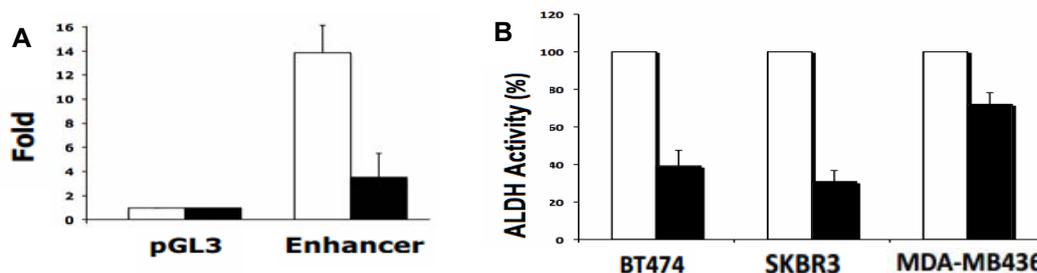


Fig. 3.2. (A) Treatment with FM19G11 (1µM, black bars) decreases mammosphere-induced Sox2 expression, as assessed by a luciferase reporter assay with MCF-7 cells transiently transfected with an empty vector (pGL3) or a vector encoding the Sox2 enhancer R1 region. (B) Treatment of different cell lines (BT474, SKBR3 and MDA-MB-436) with FM19G11 (1µM, black bars) reduces the aldehyde dehydrogenase (ALDH) activity, traditionally considered a stemness marker. In all cases, white bars represent vehicle-treated cells. Data are expressed as the average \pm SEM of at least three independent experiments carried out in triplicates.

3.3. HIF- α inhibition significantly reduces tumor formation and growth in mice breast xenografts

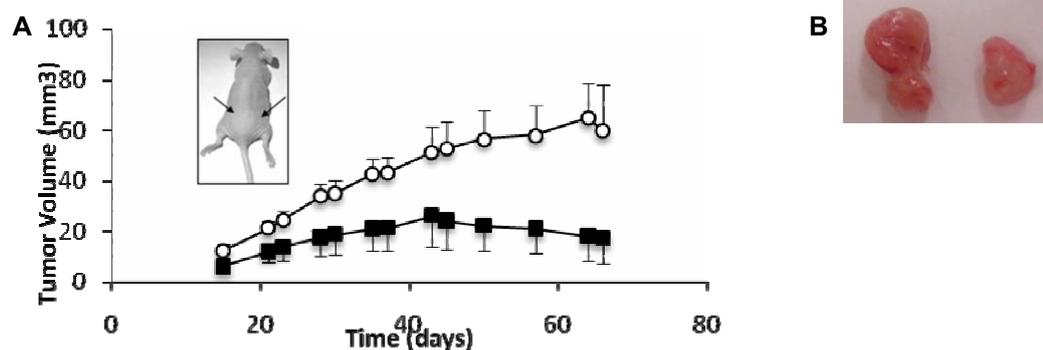


Fig. 3.3. (A) FM19G11 (1µM, black squares) inhibits the growth of BT474 xenografts compared with vehicle control (white circles). 100.000 cells pretreated with FM19G11 or vehicle were injected in each flank of the mouse. Points represent tumor volume for each experiment group and bars indicate the SEM. (B) Representative tumors from xenografts formed from cells previously treated with FM19G11 (right) or vehicle (left).

3.4. Identification of new HIF-2 α inhibitors

In order to be functionally active, HIF α and β isoforms must interact through their PAS-B domains. These protein domains of both the α and β subunits were cloned, expressed, purified and used for carrying out a Saturation Transfer Difference (STD) screening of several commercially available libraries. These experiments, which are ongoing in our laboratory, may allow us to identify new HIF-2 α inhibitors and that will be subsequently used in the hit-to-lead process.

4. Conclusions and Future research

- FM19G11 shows no significant cytotoxicity when used at concentrations required for its antineoplastic effects.
- The decrease in mammosphere formation, as well as in the levels of expression of stem cell markers (ALDH, Sox2) consolidate the role of HIF- α in the stability of breast CSCs.
- The fact that cell viability is not affected by FM19G11 means that the observed reduction in the percentage of CSCs subpopulation (mammospheres) is not a consequence of its toxicity, but of a differentiation process from CSCs to tumor cells.
- Results observed *in vitro* turned out to be reproducible *in vivo* when we studied the effects of FM19G11 administration in mice xenograft models of breast cancer, getting a significant reduction in tumor formation and progression with the addition of the inhibitor.
- Finally, the expression and purification of PAS-B protein domains will allow us to carry out a structure-based design and subsequent rational design and synthesis of HIF-2 α specific inhibitors. These compounds could become an effective therapy, especially in the most aggressive tumors (metastasis and tumor relapse-prone, and chemo- and radiotherapy resistant). It is in those tumors, resistant to current antineoplastic treatments, where the differentiation of the CSCs to cancer cells would suppose a new way of tumor eradication with better possibilities of success.

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A fast pathway for fear in human amygdala

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Abstract. A fast, subcortical pathway to the amygdala is thought to have evolved to enable rapid detection of threat [1]. Its existence is fundamental for understanding non-conscious emotional responses, but has been challenged due to lack of evidence for short latency fear-related responses in primate amygdala, including for humans. By recording electrophysiological responses directly from human amygdala, we show that a fast amygdala response is observed to fearful, but not neutral or happy, facial expressions. Critically, this response, beginning 80 ms after stimulus onset, is limited to the low spatial frequency components of fearful faces, as predicted by a fast magnocellular route to the amygdala [2]. Furthermore, such an early latency effect is not evoked by more complex photographs of arousing scenes, indicating a selective early response for socially-relevant visual information conveyed by fearful faces. These data therefore support the existence of a phylogenetically old subcortical pathway providing fast, but coarse, threat-related signals to the human amygdala [3,4].

Keywords: fear, amygdala, intracranial EEG, spatial frequency

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Modeling and optimization of a positron emission tomography scanner for small animal molecular imaging using Geant4 based tools

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Keywords: positron emission tomography, PET, small animal molecular imaging, PET detectors, positron emission imagin

1. Introduction and Contents

The aim is to simulate ring-type PET system under design [1] and optimize it. The current system will use photo multiplier tubes (PMT) [2] based detectors and it is intended to replace them in the near future with SiPMs (Silicon Photomultipliers).

Positron Emission Tomography (PET) is a molecular imaging technique that uses short-lived positron emitting radionuclide (tracer, introduced into the subject's body) which binds with an active molecule and emits two 511 KeV gamma rays (produced when a positron interacts with an electron) in opposite directions. By detecting the linear gamma rays in photomultiplier tube based scanners a three dimensional image (tracer concentrations of tissue metabolic activity) of the functional processes in the body is constructed.

The use of advanced SiPM detectors is advantageous over PMTs as they provide higher gain with low voltage inputs. They have a faster response time and are very compact in nature. Being less sensitive to external magnetic field [3] they have attractive prospects to be used in the development of next generation PET scanners.

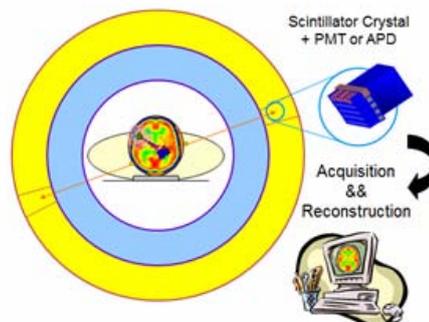


Figure 1: Block Diagram of PET scanner

2. Methodology, Materials and Methods

The PET system is modeled and simulated with GAMOS [4] (Geant4-based Architecture for Medical Oriented Simulations) and GATE [5] (Geant4 Application for Emission Tomography). Both tools are based on GEANT4 [6] high energy physics package for Monte Carlo simulation for interactions between particles and matter. These tools have facilities for geometric design (design and analysis of physical layout of the detector), setting up physics processes for the experiment, tracking (simulation of passage of particles through matter involving decays and interactions processes), detector response (when particle crosses a detector volume), run management and visualization.

A PET system using PMTs was designed in GATE as this tool is very extensive in simulating system functionality close to the real system as compared to GAMOS. Features such as noise addition, extensive digitizer and readout parameters (crystal blurring, energy blurring, transfer efficiency, light yield for each layer, intrinsic resolution for each layer, quantum efficiency of

photo-detector, coincidence sorter, etc.) simulate the system to produce data close to a real system output.

Currently, the design and simulation of the SuperArgus PET (Sedecal, Algete, Spain) system using PMTs under the project AMIT has been completed. The binary data obtained from simulation is being analyzed to reconstruct the three dimensional functional image in Matlab.

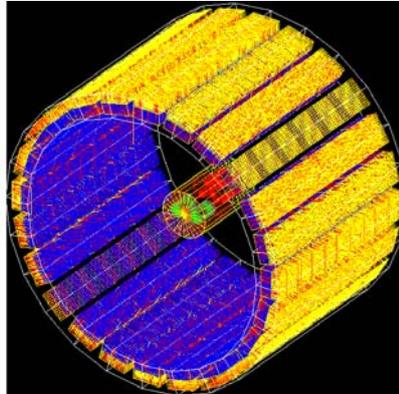


Figure 2: 3D view of SuperArgus PET Scanner

3. Results and Discussion

The geometric design and simulation of the PMT based PET system has been completed in GATE. The binary output is being used to reconstruct the three dimensional image.

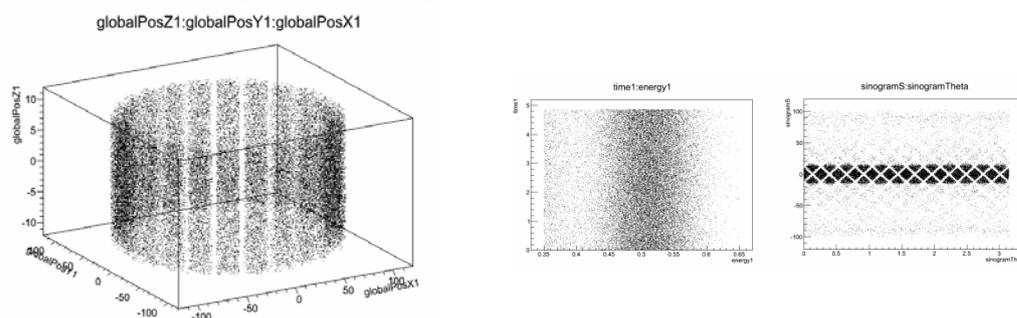


Figure 3: Global Crystal Position, Energy v/s Time, Sinogram Graph

4. Conclusions and Future research

GATE is a very convenient tool for simulation of such advanced PET systems. In future the aim is to replace the PMTs with advanced SiPM detectors and reassess the reconstructed image for higher resolution and quality. Also to compare the simulated data with real data collected from SuperArgus PET system under construction.

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Role of cannabinoids and autophagy in the pathogenesis and therapeutics of spinocerebellar ataxias

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Keywords: ataxia, cannabinoid, autophagy, drug development

1. Introduction

Spinocerebellar ataxias (SCAs) result from variable degeneration of neurons in the cerebellar cortex, brain stem, spinocerebellar tracts and their afferent/efferent connections. To date, over 30 dominantly inherited SCA subtypes have been described. Polyglutamine expansion SCAs are more frequent than are other forms of SCAs. They all show as common features, the progressive neurodegeneration of neuronal subsets in distinct brain areas and the formation of polyQ containing protein aggregates forming characteristic nuclear or cytoplasmic inclusions. There are currently no known effective treatments to modify disease progression in any of the SCAs.

Cannabinoids have been reported to serve as neuroprotective agents in several chronic neurodegenerative pathologies where processes such as glutamate-induced excitotoxicity, intracellular calcium increase, energy failure and mitochondrial dysfunction, inflammation or oxidative stress are cooperative events in the pathogenesis. Even, the early malfunctioning of the cannabinoid signaling system has been associated with the initiation and the progression of these disorders. These pathologies include mainly Alzheimer's disease, Parkinson's disease, Huntington's disease, amyotrophic lateral sclerosis and multiple sclerosis. However SCAs remain to be studied in relation with a possible therapy with cannabinoids.

Finally, cannabinoids can be neuroprotective in polyglutaminopathies by enhancing autophagy, an important cellular process in clearing protein aggregates in proteinopathies. Interestingly, certain cannabinoid agonists have demonstrated to stimulate cell autophagy in human glioma cells. and to act on mTOR, a master regulator of autophagy. To date, no one has showed a neuroprotective effect of cannabinoids via autophagy which may have therapeutic value in polyglutamine disorders such as SCAs.

The aim of this project is to explore the potential neuroprotective effects of cannabinoids in SCAs and the underlying mechanisms, and to check whether autophagy is involved in such effects. At the same time, we aim to develop new cannabinoid drugs with improved neuroprotective profiles, such as bivalent activity, improved solubility, etc.

2. Materials and Methods

The new cannabinoid compounds will be evaluated *in vitro* for their ability to displace [³H]CP55940 from human cannabinoid CB1 and CB2 receptors in transfected cells. They are first subjected to a preliminary screen at a concentration of 40 μM. A complete dose-response curve is generated for compounds that displaced the radioligand by > 50 % in the preliminary screen. The functionality of the compounds will be analyzed by evaluating their effect on PGE2 release by BV-2 microglial cell line and/or their effect on cAMP levels.

The neuroprotective properties of the different cannabinoid compounds will be evaluated *in vitro* in a rat mesencephalic cell line stably transfected with expanded ataxin 3, and *in vivo* in a

transgenic mouse model for SCA3, which shows a progressive motor coordination impairment starting before 16 weeks of age. The potential efficacy of the different cannabinoids as neuroprotective agents will be examined by analyzing the progression of functional (e.g. rotarod), neurochemical (e.g. GABA and glutamate analysis) and neuropathological (e.g. Nissl, FluoroJade B or TUNEL staining, and immunohistochemistry for several neuronal and glial markers) abnormalities in the animal model of SCA and the cell survival in the *in vitro* experiments. We will also explore the cellular substrates and molecular mechanisms that could explain the possible beneficial effects. At the CTB-UPM, we will evaluate the effect of the different cannabinoids on the dendritic trees and the dendritic spines of the cerebellar neurons of SCA3 mice.

The analysis of the different endocannabinoid elements (receptors and enzymes) in the cerebellum of patients (in samples obtained from brain banks) and our animal model of SCAs will be done by qRT - PCR, autoradiography, in situ hybridization or immunostaining. The levels of endocannabinoids will be carried out in collaboration with the group of Vincenzo Di Marzo in Naples, Italy.

To further confirm the involvement of different endocannabinoid targets in the neuroprotective effects of cannabinoids in SCAs we will examine whether mice genetically deficient in these targets (e.g. CB1 - / - , CB2 - / - or FAAH - / - mice) are more vulnerable to the lesion caused by the different damaging stimuli (e.g. excitotoxins, mitochondrial toxins, LPS) in the cerebellum or in nuclei afferent to cerebellar structures.

3. Results and Discussion

We have set up a platform for the testing of new cannabinoid drugs, optimizing the cost and the time of the assays so we can analyze several compounds. So far, we have analyzed more than 50 new cannabinoid drugs, and we have selected 15 of them for the functionality analysis. After analyzing their CB2 receptor-mediated activity, we have one CB2 agonist which can be a good candidate to use as neuroprotectant.

We have seen an overexpression of the cannabinoid receptors and enzymes in the cerebellum of SCA patients. The study of this changes will be helpful in selecting the cannabinoids with a better neuroprotective profile.

We are now characterizing the animal and cellular models of SCA3, in order to use them to test the new drugs under development.

4. Conclusions and Future research

Once we finish the characterization of the animal and cellular models of SCA3, we will start testing the new cannabinoid drugs.

These new drugs can also be useful in other neurodegenerative diseases, so we will test them in other animal and cellular models available in our laboratory, such as models for Parkinson's disease, Huntington's disease and multiple sclerosis.

Spatio-temporal morphology for microscopy image analysis

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Abstract. We propose to directly process 3D+t image sequences from in-vivo microscopy imaging of zebrafish development with spatio-temporal structuring elements.

Keywords: image processing, mathematical morphology, 3D+T imaging, zebrafish

1. Introduction

Developmental biology is under revolution with the inclusion of new microscopy technologies and automated processing methods [1]. The zebrafish is a vertebrate model in developmental biology and in the study of cancer and stem cells. The goal of image processing tools when analyzing zebrafish imaging is to be able to digitalize each cell in time and space, leading to the cell lineage tree sequencing. Because of the inherent 3D + t nature of the data which is not fully exploited when analyzing separately 3D images and the requirement of fast and efficient algorithms to analyze massive data produced by the new microscopy technologies, this work proposes a general 3D+t mathematical morphology approach for analysis [2].

2. Methodology

We propose to directly process 3D+t image sequences with mathematical morphology operators, using a new classification of the 3D+t structuring elements (spatio-temporal shapes). Several methods (filtering, tracking, segmentation) dedicated to the analysis of 3D+t datasets of zebrafish embryogenesis are introduced and validated through a synthetic dataset. Then we illustrate this methodology with the analysis of datasets of zebrafish early development acquired with various microscopy techniques.

3. Results and Discussion

The following methods have been proposed: 1) Denoising cell membrane images with the twister segment filtering, a multidimensional extension of the morphological filtering based on openings by line segments. 2) Cell tracking based on the morphological reconstruction by dilation, starting from a nuclei marker and identifying the cell trajectory as a single 4-D object. 3) Generation of virtual cell fate maps with standard and viscous 3D + t watershed from seeds in one 3D frame. 4) Skeletonization of spatio-temporal topologies to simplify and quantify gene expression domains.

4. Conclusions and Future research

The proposed methodology is a conceptual extension that sets up a common flexible framework to apply morphological operators and exploits both temporal and spatial features of 3D + t images. The main advantage of analyzing directly 3D + t images comes from the inherent redundancy of the temporal dimension. Future research lines aim to provide mathematical models of the developmental processes that have been digitized using these image analysis techniques.

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Crowdsourcing malaria image analysis

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Abstract. This research proposes an online gaming approach for crowdsourced counting of malaria parasites in images of digitized thick blood films.

Keywords: crowdsourcing, malaria, image analysis, telepathology

1. Introduction

There are 600,000 new malaria cases daily worldwide [1]. The gold standard for estimating the parasite burden and the corresponding severity of the disease consists in manually counting the number of parasites in blood smears through a microscope, a process that can take more than 20 minutes of an expert microscopist's time. This research tests the feasibility of a crowdsourced approach to malaria image analysis [2]. In particular, we investigated whether anonymous volunteers with no prior experience would be able to count malaria parasites in digitized images of thick blood smears by playing a Web-based game.

2. Methodology

The experimental system consisted of a Web-based game where online volunteers were tasked with detecting parasites in digitized blood sample images coupled with a decision algorithm that combined the analyses from several players to produce an improved collective detection outcome. Data were collected through the MalariaSpot website. Random images of thick blood films containing *Plasmodium falciparum* at medium to low parasitemias, acquired by conventional optical microscopy, were presented to players. In the game, players had to find and tag as many parasites as possible in 1 minute. In the event that players found all the parasites present in the image, they were presented with a new image. In order to combine the choices of different players into a single crowd decision, we implemented an image processing pipeline and a quorum algorithm that judged a parasite tagged when a group of players agreed on its position.

3. Results and Discussion

Over 1 month, anonymous players from 95 countries played more than 12,000 games and generated a database of more than 270,000 clicks on the test images. Results revealed that combining 22 games from nonexpert players achieved a parasite counting accuracy higher than 99%. This performance could be obtained also by combining 13 games from players trained for 1 minute. In addition, we propose a mathematical equation that accurately models the collective parasite counting performance.

4. Conclusions and Future research

The findings support the conclusion that nonexperts are able to rapidly learn how to identify the typical features of malaria parasites in digitized thick blood samples and that combining the analyses of several users provides similar parasite counting accuracy rates as those of expert microscopists. This experiment illustrates the potential of the crowdsourced gaming approach for performing malaria parasite quantification, and more generally for solving biomedical image analysis problems, with future potential for telediagnosis related to global health challenges.

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Cell therapy in combination with a xenogeneic bone substitute in the treatment of critical-size supra-alveolar periodontal defects in dogs

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Abstract

Introduction. The objective of this in-vivo experimental study was to test the regenerative potential of periodontal ligament derived stem mesenchymal cells seeded in a xenogeneic bone substitute.

Materials and Method. In 9 beagle dogs, PI, PII and MI were extracted and critical-size 6 mm supra-alveolar periodontal defects were created around the PIII and PIV. Defects were chronified by placing ligatures around the teeth and allowing dental plaque accumulation for two months. Defects were then surgically accessed, notches were created as reference at the crestal level and were then randomly treated with either a BioSS-Collagen® seeded with with 2×10^5 canine periodontal ligament-derived line cells or BioSS-Collagen® seeded with saline serum. The histomorphometric analysis at 3 months assessed the total length of the root surface; the amount of new cementum formation (NC); the linear extension of the root surface covered by NC adjacent to newly formed bone, with functionally-oriented collagen fibres and the extension of the root surface covered by epithelium and connective tissue.

Results. The histological analysis of the furcation areas showed that the cell group presented a length of new cementum of 4.79 ± 1.9 mm versus 4.82 ± 1.01 mm in the control group ($p=0.96$). The root surface covered by epithelium and connective tissue was less in cell group when compared with the control group (2.71 ± 1.47 mm vs. 3.93 ± 1.16 mm ($p=0.09$)). The calculated amount off periodontal regeneration was superior in the cell group when compared with the control group, 2.57 ± 2.25 mm and 2.07 ± 1.51 mm, respectively ($p=0.39$).

Conclusion. The present study suggests that cell therapy in conjunction with the use of a xenogeneic bone substitute (BioSS-Collagen®) promoted periodontal regeneration in experimental critical-size supra-alveolar periodontal defects without the use of a barrier membrane.

Keywords: periodontal regeneration, mesenchymal stem cells, critical size defects

1. Introduction

The periodontium is comprised of four mesenchymal tissue components, cementum, bone (hard tissue components), gingiva and periodontal ligament (soft tissue components). Although each tissue component presents its own structural and functional characteristics, they behave as one functional system responsible of the tooth attachment apparatus.

In a previous investigation from our research group (Nuñez et al 2010) we have reported the method for isolating cementum derived cells (CDC) and undifferentiated mesenchymal stem cells extracted from human PDL (PDL-MSC) and tested their regenerative potential in a three-wall self-contain intrabony periodontal defect model in beagle dogs (Nuñez et al 2011) demonstrating promising results. It is, therefore, the objective of this investigation to assess the regenerative potential of undifferentiated mesenchymal stem cells extracted from canine PDL (PDL-MSC) when combined with xenogenic compound graft (Bio-Oss collagen®; Geistlich) in the treatment of critical size supra-alveolar defects in a dog model.

2. Materials and Method

In vitro study: Cell Culture Dog CDC and PDL-MSC cell lines obtained from extracted premolars were obtained and characterized as previously reported (Nuñez et al. 2010). Prior to the surgical implantation of the scaffold in the defects, the tested carrier (Bioss-Collagen®) were tested for its ability to attach and release the CDS and MSC-PDL cells. In vivo study: Experimental Surgeries. Mucoperiosteal flaps were raised in both posterior lower jaws to create critical-size 6 mm supra-alveolar periodontal defects around PIII and PIV (Wikesjö et al. 1991). Defects were chronified and after two months were then surgically accessed. Each quadrant was treated with either test or control treatments according to randomization by tossing a coin (n=9) (Fig. 1, 2).

Histological Study. Three months post-surgery, animals were sacrificed and both experimental premolars were hemisected in a mesio-distal direction and tissue blocks were processed for histomorphometrical analysis.

All specimens were analyzed with a 10X-100X objectives in a 10 X eye-piece under a light microscope (Eclipse E800, Nikon Inc., Tokyo, Japan) (Fig. 3).

3. Results and Discussion

Results from histometric measurements are presented in table 1 and represented in fig. 4 and 5. In detail, the histological analysis of the furcation areas showed that the cell group presented a length of new cementum of 4.79 ± 1.9 mm versus 4.82 ± 1.01 mm in the control group ($p=0.96$) whereas the calculated amount of periodontal regeneration was superior in the cell group when compared with the control group, 2.57 ± 2.25 mm and 2.07 ± 1.51 mm, respectively ($p=0.39$). Data from the present investigation are not as promising as data recently reported in a similar investigation (Suaid et al. 2012.). Nevertheless, this is the first experiment that used a critical size supracrestal chronic defect that reproduces the microbiological and inflammatory condition of the chronic furcation defect, and thus may be in part responsible for the observed difference.

4. Conclusions and Future research

The present study suggests that cell therapy in conjunction with the use of a xenogeneic bone substitute (Bioss-Collagen®) promoted periodontal regeneration in experimental critical-size supra-alveolar periodontal defects without the use of a barrier membrane warranting a promising field of future research.

Table 1. Histometric results at 3 months post-surgery.

Group	TDL	TFDL	NC	PR	E/CTE
Control	10.53 (1.35)	4.55 (1.92)	4.82 (1.01)	2.07 (1.51)	3.93 (1.16)
Test	10.58 (1,20)	5.18 (2,25)	4.79 (1.90)	2.57 (2.25)	2.71 (1.47)

Table represents data from the extension (mean (SD), mm) of the linear histometric measurements of the Total Defect Length (TDL); Tissue Free Defect Length (TFDL); New Cementum (NC); Periodontal Regeneration (PR) and Epithelium/Connective Tissue Extension (E/CTE).

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Reprogrammable, modular bio-sensors using Boolean logic

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Abstract. Plasmids are a mobile genetic element and a major carrier of virulence genes and antibiotic resistance in bacterial populations. Our long term aim is to develop technology to avoid using antibiotics that kill bacteria indiscriminately and instead detect and react to the presence in a cell of undesirable plasmids or combinations of plasmids. In this work we have designed and simulated a biological sensing device that uses plasmids as a detection mechanism. That is, we use cells as computational devices that detect and respond appropriately to plasmids and environmental signals. The system is modular so that we can assemble arbitrary detectors and detect complex combinations of plasmids and external signals.

Keywords: plasmids, conjugation, bio-sensors

1. Introduction

Plasmids are DNA molecules encoding genes for accessory functions that often increase bacterial fitness in a given environment. They often encode genes for a type 4 secretion system that allows for autonomous transfer between adjacent bacteria, even those of different bacterial species. This process is known as “conjugation” and is one of the methods of horizontal transfer of genes which allows bacteria to rapidly adopt new behaviours. For example virulence and anti-biotic resistance genes are often carried and spread via plasmids. In this work we have developed a method to detect and react to plasmids using synthetic plasmids as autonomous programmable biological sensors.

Existing bio-sensors implemented in bacteria often use carefully engineered genetic circuits. These systems require extensive fine tuning and development of new sensors is slow. These systems suffer from noise, high error rates, and lack of modularity. Recently, distributed circuits have been developed [2,4] which improves modularity. However the cells use pheromones or quorum sensing signals to communicate with other cells in the sensor and so have a limited number of channels of communication and there is a danger of cross talk if other micro-organisms use the same pheromone.

We have designed a modular, conjugation based bio-sensor that distributes simple computations across a population of cells. The ambition of our design is to change the behaviour of certain bacteria in a population depending on the presence of specific combinations of inputs such as environmental signals (toxins, quorum sensing signals etc.) and plasmids (bearing traits such as anti-biotic resistance, virulence etc.). The resulting behaviour can be a visible signal to a human observer or some autonomous action such as expression of a toxin.

2. Methodology

A Boolean circuit is a directed acyclic graph with input gates (nodes with no incoming edges), and logic gates (nodes labelled by one of AND, OR, or NOT). The gates are connected by directed arcs called “wires”. Each input gate is assigned a value 0 or 1. The value of each logic gate is defined recursively as the application of the Boolean function of its label to the value of the gates on incoming wires (note that a NOT gate can have only 1 incoming wire). Outputs of the circuit are read from designated output gates. We implement AND and OR logic gates using conjugative plasmids that lack genes for their own relaxase and/or other proteins crucial for conjugation. The missing genes are on other plasmids that act as inputs for this gate. For example an AND gate plasmid is immobilisable if any one of its input plasmids is not in this cell (input 0). Once all the input plasmids are present in the cell (input 1) the AND gate plasmid becomes mobilizable and spreads through the population. In turn it becomes an input for other logic gate plasmids. In this way, gates are chained together to make a Boolean circuit.

Traditionally, differential equations have been used to model the spread of plasmids in a well mixed bacterial populations. However, our experimental data comes from 2D and 3D cell

cultures growing on a solid surface. Here the vertical spread of the plasmids via cell division and the spatial structure of the population are crucial in predicting the effectiveness of the bio-sensor. To capture the spatio-temporal structure of the colony we have developed individual based models of bacterial conjugation using simple agent systems.

3. Results and Discussion

We have developed a new technique to promote and control the spread of synthetic plasmids in a population. We have developed an individual based model of bacterial conjugation which we have verified using experimental data from our laboratory partners [1]. Using this model (at its conjugation rates) we have simulated various circuit designs. For example, simulations using show that a 3 input circuit with 3 gates (5% input cells, 50% cells with computing plasmids and 45% plasmid free cells) results in 0.1% of the cells having completed the circuit computation within 5 generations.

While our models match the global behaviour of a single plasmid transfer, we do not have the experimental data to validate the accuracy of our model for multiple plasmids. Moreover, there is still uncertainty of the molecular mechanism of conjugation. We are currently working with our laboratory partners to design wet and computational experiments that will allow us to predict and confirm which model of conjugation is closer to nature.

4. Conclusions and Future research

Using conjugative plasmids in our distributed circuit design avoids or mitigates many of the problems associated with previous bio-sensor designs. The resulting bio-sensor may be re-programmed to detect combinations of inputs expressed as a Boolean functions. Our bio-sensor design also increases its own sensitivity (by the conjugative spread of the logic plasmids) once the target signal is detected.

Our current model is limited to simulations of approximately 10,000 cells which gives us less than 5 generations. To properly study large circuits (> 5 plasmids) we are currently developing a conjugation system for CellModeller [3].

This project has been expanded into a proposal for a FP7 FET emerging technology project. We will further develop and perfect our models with microscopic images of conjugation and implement more ambitious designs of bio-sensing circuits. Learning how to control and program the distribution of plasmids will be a huge advance in medicine, biotechnology, synthetic biology.

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1st Workshop
PICATA

Agri-Food and
Health Cluster

AGRI-FOOD AND HEALTH (A&H) is one of the six thematic CIE Moncloa Campus clusters and it is focused on Sustainable Production of safety and health in the food production. The activities of the groups working in the specialized areas of agricultural and livestock production, and the processing of safe, healthy and high-quality food products for human and animal consumption.

The proposal of the A&H cluster includes the activities that the Complutense University of Madrid (UCM), and the Polytechnic University of Madrid (UPM) and associated organism are carrying out in the field of generation of agricultural and livestock products, their processing to production of safe, healthy and quality food for human and animal consumption, obtained through sustainable techniques and system and respecting the welfare standards through the development and application of new technologies.

On February 12, 2013 took place a workshop at the Seminar Room of the School of Forestry Engineering of the UPM. This workshop was intended to know the people recently incorporated thank to PICATA Programme of Moncloa Campus and who are researching and assessing this cluster.

The participants explained the description of the research carried out and the work plan developed within the Moncloa Campus and their results and their scope perspective.

Within the A&H cluster priority lines, the subjects studied was classified as follow:

PRE-DOCTORAL GRANTS PICATA

- Rivas Fernández, Eva M^a
- Cámara García, Lourdes
- Duque Rodríguez, Juan Ramón
- Navarro García, Yurena
- Sánchez Matamoros, Almudena

POSTDOCTORAL CONTRACTS PICATA

- Gañán Martínez-Ballesta, Mónica

1. **Animal Production and Health: nutrition, public health and welfare in livestock and aquaculture.**

- Integrated approach to the analysis of human and animal tuberculosis (Navarro García, Yurena).
- African horse sickness in Spain: New tools for its surveillance and control (Sánchez Matamoros, Almudena).
- Influence of net energy content of barley based diets on productive performance of gilts, boars, and immunocastrated males slaughtered at heavy body weights (Cámara García, Lourdes).

2. **Vegetable production systems: production and sustainable management, including risk in agro-food sources.**

- Infotaxis algorithm for the detection and localization of disease-borne volatiles in crop fields (Duque Rodríguez, Juan Ramón).

3. **Agri-Food technology: advanced technologies for quality, safety and traceability.**

- Development of molecular and technology tools for the early detection of food spoilage by sorbate resistant yeast and its altering product, the pentadiene (Rivas Fernández, Eva M^a).

4. **Food-safety and Hygiene: safety and Health in the food production.**

- Development of a vision system to detect allergen (peanut traces) in powdered foods (Lunadei, Loredana).
- Use of pulsed light to increase the safety of ready-to-eat food products (Gañán Martínez-Ballesta, Mónica).

Lucas Domínguez Rodríguez

Margarita Ruiz-Altisent

Coordinators Agri-Food and Health Cluster

Development of molecular and technology tools for the early detection of food spoilage by sorbate resistant yeast and its altering product, the pentadiene

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Keywords: sorbates, colony, yeast, food spoilage

1. Introduction

Yeasts are relevant agents in food spoilage. Their main manifestations are surface growth, gas production, off-flavours and bad odors (Deák, 2008). Weak acids as sorbic acid and derived salts (sorbates) are common preservatives added to foods. There are resistant microorganisms that can metabolize such preservatives, transforming them into non-toxic molecules with spoiling properties. Our group was the first to describe the production of 1-3 pentadiene from sorbate by yeasts (Casas *et al.* 1999, 2004). This metabolite has an unpleasant petroleum odour and has been detected in marzipan and nuggat. Therefore, a predictive model of risk spoilage that would link yeast contamination and 1-3 pentadiene production would be of great use. Up to date, predictive growth models have been made mainly in liquid media whereas most of food shows some degree of structure. In solid food yeasts can grow as surface colonies, whose behaviour can not be predicted accurately by the available models (Theys *et al.* 2010). To solve this problem a collaboration has been established between the LPF_TAGRALIA (UPM) and HOLEIAL (UCM). LPF_TAGRALIA is credited by works on data modeling derived from instrumented quality such as gas sensors, electronic noses and sensor networks. HOLEIAL is a recognized expert on yeast and filamentous fungi. Together we propose to develop complementary approaches to produce predictive models of risk spoilage. The specific objectives of this study are:

- Screening and selection of strains 1-3 pentadiene producers. Physiological studies of 1-3 pentadiene production (UCM)
- Development of methods to measure growth of yeast, including image analysis algorithms to automate measurements of growth in the different structures, with classical invasive and non-destructive, noninvasive, techniques. Development of predictive kinetic models of growth and physiological models linking growth and spoilage metabolite production in different structures. Validation in artificially contaminated food. (UCM-UPM)
- Development of an economic sensor for detecting and quantifying 1-3 pentadiene. (UPM)

2. Materials and Methods

2.1 Screening of strains 1-3 pentadiene producers. The sensorial detection, using strains of *Z. rouxii*, *W. anomalus*, *D. hansenii* has been made in YMA and ME4 media (10 and 300g/l glucose, respectively) with 0.75 g/l of sorbate, as described previously (Casas *et al.* 1999).

2.2 1-3 pentadiene detection in foods using MWIR technology. In collaboration with New Infrared Technologies (NIT), the capacity of MWIR detectors, with specific filters, has been evaluated in samples of flavored water with sorbate as preservative, which presented a strong petroleum odor.

2.3 Analysis of growth in broth and on solid medium. Modelling the yeast growth kinetics on solid media. Colony growth has been studied in model food systems, especially agar plates (Wilson *et al.* 2002). Colonies originated from 1 to 10⁶ cells from 4 different species of yeast (two of them 1-3pentadiene producers) were analyzed with respect to their number of total and viable cells and also their area, for more than 500h of incubation at 28°C. Viable cells was determined by

plate count; total cells, by DO_{620} nm and Thoma Chamber counting; area and radius by an image analysis algorithm, developed in MATLAB (UPM). We have also carried out a comparative monitoring with the area of the two strains 1-3 pentadiene producers in YMA with 0.75 g/l of sorbate.

2.4 Yeast growth detection by hyperspectral images: Images of YMA plates, inoculated with *Z. rouxii* Bch were taken with a hyperspectral vision system. Extracted spectra were analyzed by means of principal component analysis.

3. Results and Discussion

It has been shown that sorbates decarboxylation capacity depends on the strain and is independent of the glucose concentration of the medium. The use of MWIR detector has enabled a first detection and quantification of 1-3 pentadiene in water. Pentadiene 1-3 presents an absorption band at 3.4 microns when the spectrum is normalized to 4.6 microns (Figure 1).

Hyperspectral images of colony growth of *Z. rouxii* Bch showed that the first component can discriminate between agar and colonies and the second one distinguishes different agar conditions due possibly to differences in the degree of hydration (2 congresses).

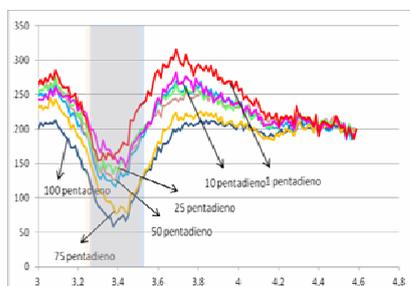


Figure 1. Absorption spectrum of samples of bottled and flavored water with 1-3 pentadiene diluted to final concentrations between 1 and 100 ppm.

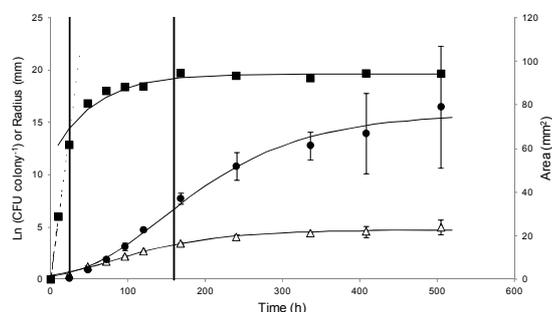


Figure 2. Triphasic general model of the growth of yeast colonies. Dashed line represents the expected growth similar of liquid culture. Continuous lines are the Gompertz fitting of viable cells, area and radius growth.

In contrast with the biphasic model for liquid cultures, we have established a triphasic model to describe the growth of yeast colonies (Figure 2). The model is based on data regarding colony area and viable cells. Thanks to the image analysis algorithm developed and validated in this work we have been able to measure automatically the area growth. Furthermore we have observed that the area of the colonies is proportional to the number of total cells. The sigmoid Gompertz model can be used to describe the kinetics growth of viable cells and the area of the colonies (Fig. 2). The parameters of this model are being used to analyze the effect of others environmental conditions. So far results have been disseminated in 3 congresses, 1 research paper has been submitted (Microbiology paper no. mic/2013/066704).

4. Conclusions and future research

The development of image analysis routines has triplicated the capacity of microbiological experimentation. The model developed allows describing the yeast growth on solid medium but its validation in selected foods artificially contaminated is required.

Current methodologies for detection of microorganisms in solid foods are destructive and hyperspectral analysis is proposed as a new non-destructive and highly complementary method for the detection of changes that occur in food due to contamination and growth of yeasts. Although more tests are required, 1-3 pentadiene detection by MWIR detector is a first step in the development of IR low cost sensors for detecting and quantifying 1-3-pentadiene in batches of foods with sorbates. The kinetic model will be an excellent tool to analyze and identify the limiting factors that affect growth on solid food and to establish the relationship between colony growth and food spoilage. Our future experiments will also include the characterization of food microstructure parameters, and specific experiments are to be designed within that purpose.

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Influence of net energy content of barley based diets on productive performance of gilts, boars, and immunocastrated males slaughtered at heavy body weights

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Keywords: gender, growth performance, immunocastrated male, net energy

1. Introduction

An increase in energy concentration of the diet results usually in improved feed efficiency (Smith et al. 1999) and increased backfat depth and intramuscular fat content of the meat (Liu et al. 2007). However, the effects of net energy (NE) concentration of the diet on average daily gain (ADG) are inconsistent (Quiniou and Noblet., 2011; Coca et al., 2012). Factors such as genetic background and sex of the pigs, energy system used for feed evaluation and the use of balanced or unbalanced diets, might affect the response of pigs to increases in energy concentration of the diet. Pigs destined to the dry cured industry are slaughtered at heavier body weight (BW) than pigs destined to fresh pork production (Latorre et al., 2004;). However, excessive BW at slaughter hinders feed efficiency and increases the incidence of boar taint in the carcass (Font i Furnols et al., 2003). Active immunization against GnRF is a recommended option to surgical castration to avoid boar taint in pork meat (Dunshea et al., 2001). The objectives of this research were to study the effect of NE concentration of the diet on productive performance of gilts, boars, and immunocastrated male (IMC) pigs slaughtered at heavy BW.

2. Materials and Methods

Five hundred and forty pigs with an initial body weight (BW) of 28.5 ± 4.1 kg were used to study the effects of NE concentration of the diet (2.29, 2.33, 2.37, 2.41 and 2.45 Mcal NE/kg) and gender (gilts, boars and IMC) on productive performance of pigs slaughtered at 117 kg BW. The IMC pigs were immunized against GnRF with Improvac at 90 (18 days of experiment) and 143 (71 days of experiment) days of age. Each of the 15 treatments was replicated 3 times (12 pigs per pen). Individual BW and feed consumption per pen were recorded at 72, 90, 126, 143, 168 and 188 d of age (0, 18, 54, 71, 96, and 116 d of experiment). Excess of feed was removed from the feeders at the end of each period, weighed, and discounted from the total feed supplied. From this data average daily feed intake (ADFI), ADG, Gain:Feed ratio, NE intake (g feed intake per day x Mcal NE/kg diet), and NE efficiency (g ADG/Mcal NE intake) were calculated per replicate. All pigs were slaughtered at the same age (117 days of experiment and 189 days of age as an average).

3. Results and Discussion

For the entire experimental period (Table 1), ADFI was not affected by NE concentration of the diet and consequently, energy intake increased as the NE content of the diet increased. In contrast Smith et al. (1999) did not observe any difference in energy intake in pigs from 29 to 107 kg BW fed diets varying in ME from 3.31 to 3.57 Mcal/kg. ADG increased as the energy concentration of the diet increased, consistent with the higher energy intake of the pigs, and in agreement with data of De la Llata et al. (2001). In contrast, Coca et al. (2012) observed that an increase in NE concentration of the diet did not have any effect on ADG. For the entire experimental period, G:F ratio was improved as the NE concentration of the diet increased, but NE efficiency was not affected. No interactions between energy content of the diet and gender were detected, suggesting that the 3 genders responded similarly to increases in NE content of the diet. Immunocastrated males had higher ADFI and ADG than gilts and boars, in agreement with data of Fábrega et al. (2010) in pigs slaughtered at 120 kg BW. However, boars had better gain:feed ratio than gilts and IMC.

Table 1. Effect of net energy (NE) concentration of the diet and gender on productive performance from 72 to 188 d of age (28.5 to 117 kg BW)

Item	NE, Mcal/kg					Gender (G)			Rsd ²	Probability	
	2.29	2.33	2.37	2.41	2.45	Gilt	Boar	IMC ¹		NE	G
										L ³	
Final BW, kg	116.1	115.9	117.4	118.3	118.7	115.8 ^b	116.3 ^{ab}	119.8 ^a	3.618	+	**
ADFI, kg/d	2.02	1.99	2.00	1.96	1.98	1.97 ^b	1.93 ^b	2.08 ^a	0.0975	NS	**
ADG, kg/d	0.756	0.758	0.773	0.776	0.779	0.741 ^b	0.766 ^b	0.798 ^a	0.0288	*	***
G:F	0.375	0.382	0.388	0.395	0.394	0.377 ^b	0.397 ^a	0.386 ^b	0.0119	***	***
NE intake, Mcal/d	4.621	4.636	4.736	4.739	4.850	4.657 ^b	4.579 ^b	4.910 ^a	0.230	**	***
NE efficiency ⁴	0.164	0.164	0.163	0.164	0.160	0.159 ^b	0.167 ^a	0.163 ^{ab}	0.0051	NS	***

¹ Immunocastrated males. Pigs received the Improvac injections at 90 and 143 d of age. ² Residual standard deviation. Nine replicates of 12 pigs each for NE concentration of the diet and 15 replicates of 12 pigs each per gender. ³ L = linear effect of NE content of the diet. ⁴ kg ADG/ Mcal NE intake. ^{a-b} Within a row, means without a common superscript differ ($P < 0.05$). The interactions between NE concentration of the diet and gender were not significant ($P > 0.10$).

4. Conclusions and Future research

It is concluded that increasing the NE concentration of the diet improves feed conversion ratio and average daily gain. Also, IMC have better BW gain but similar feed conversion ratio and energy efficiency than gilts and boars. The use of high energy diets might be recommended for the production of pigs destined to the dry cured industry. However, the economical benefits of this practice will depend on the relative cost of feed ingredients.

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Infotaxis algorithm for the detection and localization of disease-borne volatiles in crop fields

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Keywords: disease-control, odor sensing, search algorithms, robotics, crop production

1. Introduction

The goal of this project is to identify the presence of an infected plant inside an open crop field and locate the infectious focus using automated non-destructive methods. This is a major task to be solved in order to ensure safe and sustainable agriculture.

In this work we present a theoretical information based strategy known as *infotaxis* as an effective navigation system of a robotic platform to locate the source of a disease in a crop field using the information obtained from the chemical detection of volatile compounds.

Chemical methods offer real-time and large distance detection capabilities, and are based on the application of the Volatile Organic Compounds (VOCs) as possible biomarkers of the presence of a disease.

Infotaxis was recently proposed as a strategy for searching an odor source in a noisy and turbulent environment such as air or water. Its implementation in mobile robotic platforms equipped with gas sensors promises to be useful in the localization task of plant diseases. Based on Bayesian inference, infotaxis strategy decodes the information contained on the molecules transported by the air and detected along the search process to build a subjective probabilistic map that represents the belief or degree of knowledge of the agent about the source position. As the agent gathers and accumulates information, the probability map (or belief function) becomes sharper and its associated Shannon entropy, which measures the uncertainty of the location of the source, decreases.

Infotaxis strategy consists of moving in a way that maximizes the expected gain in information about the location of the target, and consequently, the decrease in entropy of the belief function. The algorithm ensures an optimal balance between

- ✧ *exploration* of the environment, where the agent collects information encoded in the trace of detections (or lack thereof) of volatiles emitted by the source) and
- ✧ *exploitation*, where the agent directs its motion towards the most probable location of the source.

In this study we analyze numerically the robustness of the infotaxis strategy with respect to inaccurate modeling of the medium and under other non ideal conditions such as the existence of obstacles due to land topology or weeds and the systematic errors of the odor sensors. A comparison with other well established olfactory search strategies such as systematic or random ones is also carried out in terms of efficiency and success measures.

2. Material and Methods

The infotaxis strategy assumes that the information comprises molecules that are emitted by the source at a rate γ , and are transported by a turbulent flow defined by a mean wind velocity V and a diffusion coefficient D . The non uniform and fluctuating concentration profile of volatiles formed under the mechanism of turbulent and molecular diffusion can be modeled in a simple way as the solution of an advection-diffusion equation, and the mean rate of encounters experienced by the agent in its movement through the medium using Smoluckowski's arguments. Moreover, in order to simulate the time varying process and the intermittence of the odor detection, we suppose that detections are distributed according to a Poisson distribution of mean proportional to the mean rate of encounters.

In all the simulations we have considered that the strategy takes place on a regular lattice, and that the robot sensors are capable of measuring a finite number of detections. The search algorithm consists mainly of two steps: an update of the belief function and a decision to move according to the maximal information gain. Searches begin with a uniform belief function, and end either when this probability map converges to a delta function or the source is found (successful search), or when a predefined maximum number of steps or the boundary domain are reached (unsuccessful search).

3. Results and Discussion

The optimal trade-off between exploration and exploitation makes this algorithm the most efficient one among the different simulated strategies. Systematic searches overexplore the space looking for detections that guide the agent towards the source, while random motions lack directionality and spend too much time in regions far from the source.

Infotaxis also appears as a robust strategy with respect to the searcher's model of the turbulent medium and to its fluctuations and inhomogeneities. This result also extends when the parameters employed internally to guide the search differ from the instantaneous characteristics of the environment, emphasizing the capacity of infotaxis to cope with unpredictable real environments, as it will be the case in crop fields or greenhouses.

With obstacles, the efficiency of infotaxis reduces drastically but success rates remain high thanks to the Bayesian formalism used. Even in the case of immobile agents, localization is possible due to the convergence of the probability map to a delta function centered in the real position of the source. In order to improve efficiency, a fleet of cooperative agents able to change and share information can be used.

Another significant point is that searches in a triangular percolated lattice are more robust than in square ones, which can be explained by a greater freedom of motion. This is particularly relevant since crop production using triangular geometries has shown to be more effective in the production of biomass than the traditional furrow geometry.

4. Conclusions and Future research

We have evaluated numerically the robustness of infotaxis with respect to spatial and temporal constraints and have established a comparison with other olfactory search techniques in terms of efficiency and success rates. Our results show that infotaxis is a promising, robust and successful strategy for the location of infectious foci in open crops. It offers a good response as a method for early stage control of plant diseases.

Our next step consists on the implementation of the algorithm in a simple and cost effective robotic platform and testing the performance of infotaxis under controlled laboratory conditions. Signal analysis to improve the decoding and discrimination problem of volatiles in complex mixtures of odors will be also studied in order to improve the specificity of electronic noises.

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Integrated approach to the analysis of human and animal tuberculosis

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Keywords: *Mycobacterium tuberculosis*, *Mycobacterium bovis*, genotyping, clonal variants

1. Introduction

Tuberculosis is a respiratory disease caused by *Mycobacterium tuberculosis* complex. Among the species of this complex, *Mycobacterium tuberculosis* (MTB) causes human disease and *Mycobacterium bovis* (MB) affects animals, but zoonosis produced by both pathogens has been described [1,2]. Coordination between human health and veterinary research is needed to better analyze the human-animal interphase in the infection by these pathogens. The aim of our collaboration in the CEI is to define a collaborative scheme aiming to fill this gap. For this first year of coordinated work we defined a research strategy supported in three axis of activity:

- a) Integration of the genotyping and epidemiological data of MB causing infection in humans and animals in a population-based sample to get a global snapshot of its transmission
- b) To develop specific methodology to adapt our standard protocols to versions more suitable for a high-throughput analysis of MB in forthcoming collaborative studies
- c) To define scientific points of common interest in human health and veterinary within the topic of clonal complexity in the infection by MT and MB

2. Materials and Methods

Microbiological methods

Specimens were processed by standard methods and inoculated on Lowenstein-Jensen (MTB) or Coletsos (MB) slants. The MTB cultures were boiled in 200µl of water for 7 minutes, and they were frozen until genotyping analysis. MTB strains to inoculate were grown at 37°C in Middlebrook 7H9 broth supplemented with Middlebrook ADC Enrichment (Difco) with daily agitation. Once the culture reached an OD of 0.9-1, stocks of 200µl were prepared and stored at -70°C until used.

Genotyping Methods

Spoligotyping

Spoligotyping was performed using the spoligotyping kit (Isogen, Ijsselstein, The Netherlands and VISAVET Health Surveillance Centre) and following the manufacturer's instructions.

Mycobacterial interspersed repetitive units-variable-number tandem repeat (MIRU-VNTR) typing

MB: We selected the nine MIRU-VNTR loci published by Rodríguez-Campos [3]. Simplex PCR format was made following conditions published elsewhere [4].

MTB: Multiplex PCR format was made as reported in other publications [4].

Infectivity characterization

Intracellular growth in THP-1 cells: The human monocytic cell line Thp-1 was cultivated and differentiated to macrophages as the published paper by Alonso et al. [5]

Infectivity models: we have made two kinds of infections: a) individual infections with each strain and b) co-infections with all strains simultaneously infecting. These infections were made on two kinds of macrophages models 1) differentiated macrophages and 2) activated macrophages con IFN following conditions published elsewhere [5].

3. Results and Discussion

a) Population-based study of human-animal tuberculosis caused by *Mycobacterium bovis*

Seventeen patients were detected with tuberculosis infection caused by MB between 2006 and 2010 in Asturias (Hospital Universitario Central de Asturias). These cases were genotyped by spoligotyping and MIRUtyping and only 2 patients were clustered. In 9/17 cases we identified a farm infected by a MB which shared identical genotype with that involved in the human case (Table1). An epidemiological survey supported the existence of links between the human cases and the farms sharing genotype.

b) Methodological development: MIRUtyping by multiplex PCR

We have optimized a new method to high throughput genotype MB supported in three new multiplex PCRs: Mix1 (MIRU4, MIRU26, MIRU31) Mix2 (Qub11b, VNTR48, 1955) and Mix3 (Qub11a, Qub3232 and ETRA). Thermocycling conditions and sizing of PCR products by capillary electrophoresis have been optimized and the protocol is being evaluated with a prospective selection of 45 MB isolates.

c) Analysis of clonally complex infections

- **Mixed infections by MB:** We applied MIRU-VNTRtyping to all the MB strains isolated from 15 farms apparently infected by a single strain according to the spoligotyping analysis. The MIRU data confirmed a homogeneous infection in five farms. However, the remaining 10 farms revealed the simultaneous infections by 2 to 7 different strains with a variable degree of heterogeneity (differences from 1 to 7 different loci).

- **Compartmentalized infections by MB and MTB:** We spoligotyped isolates from independent lymphnodes of 84 single infected cows. In eight animals we identified a compartmentalized infection, as indicated the presence of different strains in different nodes (Fig1).

- **Microevolution in MB:** We selected 6 farms with persistent infection by a MB strain (isolation of MB along 2 to 13 years) to search for microevolution phenomena in MB along its persistence period (Table 2). MIRU typing is being applied to identify subtle changes in the pattern of these strains.

- **Infectivity characterization:** We selected human cases with microevolution events and among those we selected a case involving the four clonal variants infecting different sites and a case involving five clonal variants infecting respiratory site. Our aim was to evaluate whether these clonal variants could have different infectivity. We evaluated the infectivity of these clonal variants in four different ex vivo infection models. Infectivity differences were found in the two patients among their coinfecting variants (in one case when these were evaluated in the simultaneous coinfection assay and in the other when these were infected on activated macrophages (Fig2 and 3).

4. Conclusions and Future research

The integration of the genotyping datasets available for MB isolated from human cases and animals together with the epidemiological information has allowed us to obtain a complete snapshot of the transmission by MB in a population-based sample. The optimization of a multiplex MIRU version for genotyping *M. bovis* will allow us the highthroughput analysis of this pathogen. The different clonal complexity features that are being explored in the infection by MTB are also found to have a major role in the analysis of the infection by MB.

Figures and tables

Year	Patient	Spoligotype	MIRUtype	Coincidental human-animal MIRUtype
2008	8	SB0130	3 6 3 1 5 4 8 8 3	NO
2008	7	SB0130	3 5 3 1 5 4 9 8 4	NO
2009	10	SB0130	3 6 3 2 5 4 8 8 4	NO
2010	14	SB0130	3 6 3 2 5 4 9 8 4	YES
2010	16	SB0130	3 6 3 2 5 4 9 8 4	YES
2006	2	SB0134	3 5 3 4 2 5 8 5 5	NO
2008	9	SB0134	3 5 4 3 2 5 9 5 6	YES
2009	11	SB0121	3 5 3 2 3 4 10 7 6	NO
2009	13	SB0121	3 5 3 2 4 5 10 8 5	YES
2010	15	SB0121	3 5 3 3 4 5 10 2 5	NO
2007	5	SB1019	3 6 3 2 5 4 9 8 4	YES
2009	12	SB0265	3 5 3 2 4 4 8 8 5	NO
2006	1	SB1305	3 2 3 2 4 5 10 7 6	YES
2008	6	SB1312	3 6 3 1 5 4 9 8 4	NO
2007	3	SB1569	3 6 3 2 5 4 9 8 5	NO
2007	4	SB1641	2 5 3 3 6 4 9 8 5	NO

Table 1. Genotypes of patients with tuberculosis caused by *M.bovis* and matches with animal MIRUtypes

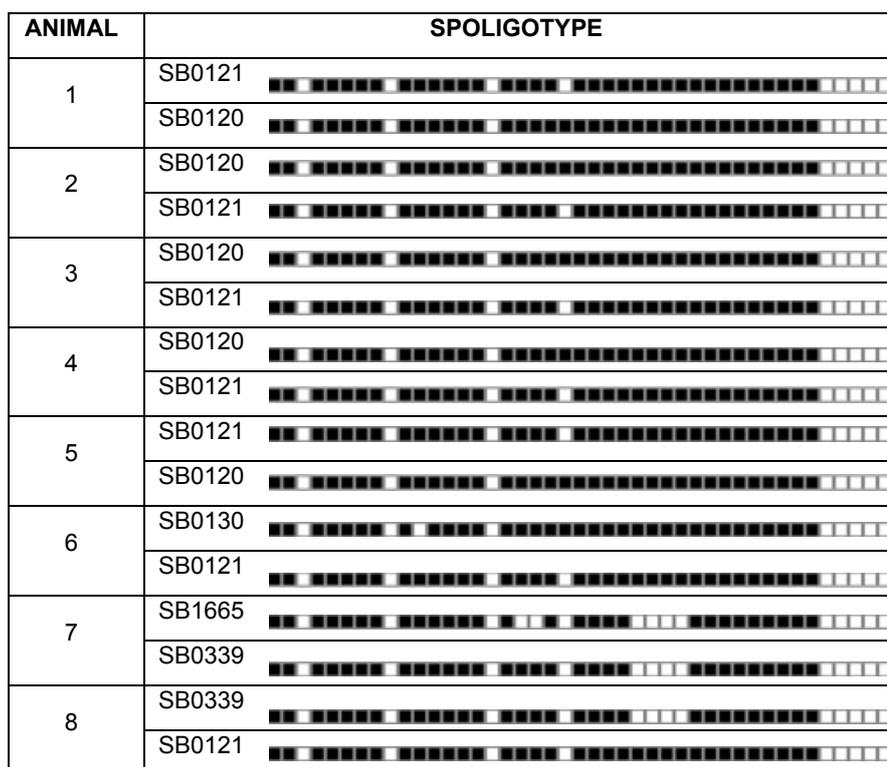


Fig. 1. Spoligotypes of different lymphnodes from compartmentalized animals

Spoligotype	Length (month)	%1	%2	%3	%4	%5	%6	%7	years
SB0867	49	3% (3/93)	10% (8/78)	Q	3% (1/64)				2006-11
SB0265	41	1,5% (2/127)	Q	2,5% (2/79)	6% (4/69)	2% (1/42)			2007-11
SB0339	17	0,2% (3/1439)	2% (19/989)	0,7% (7/933)	0,1% (1/917)	0,2% (2/920)	0,1% (1/901)	0,1% (1/968)	2007-09
SB1142	156	1	0,3% (1/311)	3	3	0,6% (2/300)	0,7% (2/278)	2	1998-11
SB1142	22	0,5% (1/181)	0,5% (1/153)						2009-11
SB0339	21	1% (1/108)	2,5% (2/78)	1,5% (1/59)					2009-12

Table 2. Selected farms with prevalent infection. Q:qualified time farms

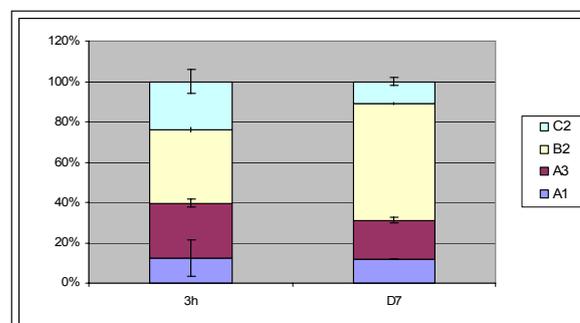


Fig. 2. Co-infection assay of the clonal variants (A1, A3, B2 and C2) from the compartmentalized patient on macrophages non-activated. Increase of B2 clonal variant and reduction of C2 clonal variant at seventh day (D7) of co-infection assay

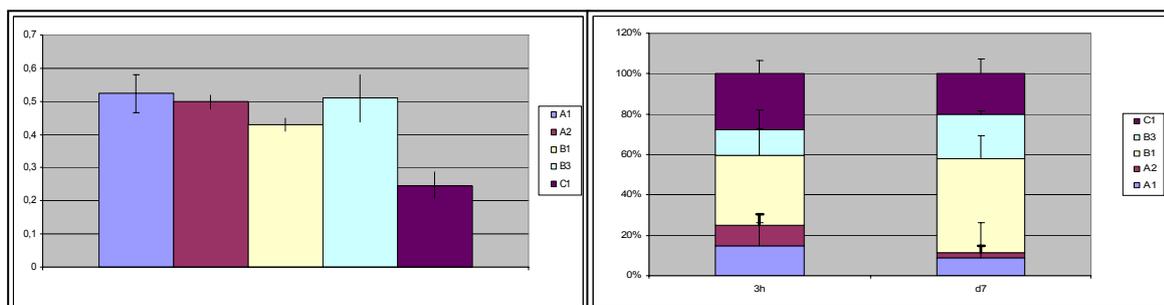


Fig. 3. Infection and co-infection assays of the clonal variants (A1, A2, B1, B3, C1) from respiratory patient on activated macrophages a) reduction of growth rate of C1 clonal variant; b) reduction of proportion of C1 and A2 clonal variants at seventh day (D7) of co-infection assay

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African horse sickness in Spain: New tools for its surveillance and control

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Keywords: african horse sickness (AHS), surveillance and control methods, risk assessment, risk mapping, immune response

1. Introduction

African Horse Sickness (AHS) is one of the most severe viral diseases affecting equidae, which is transmitted by species *Culicoides* genus [1]. This disease is included on the OIE list due to its severity, rapid spread and the important socio-economic impact in the affected regions. Its causal agent is AHS virus (AHSV), which belongs to *Orbivirus* genus, such as Bluetongue virus (BTV). Nowadays, nine different AHSV serotypes have been serologically identified. Its endemic distribution is limited to Sub-Saharan Africa and Yemen, but has periodically caused outbreaks in other areas where the vector-borne is adapted, such as Spain [1, 2]. Therefore, global warming, recent experience with BTV and Schmallenberg, and also the presence of new *Culicoides* species in Europe indicate that, at the moment, AHS can be considered a re-emergent disease of special concern in Europe [3].

Spain is one of the European countries with high risk for the re-introduction and spread of the disease in relation with the main risk factors of AHSV. It is the second largest country in Europe in terms of equidae census with animals of high economic and genetic value. In addition, Spain had reported twice the disease, [2] having a capable culicoide population to spread the disease. These circumstances require the application of new epidemiological tools for qualitative assessment and spatial analysis of AHSV in Spain, which are essential to improve the surveillance and control measures against the disease. These measures are based on early detection with effective diagnosis assay and adequate control methods, especially vaccination [2]. The knowledge of the immunology of the animals against this disease is crucial to develop new control methods. Therefore, the study of immune response against AHS is essential to reveal more information about host defense and allow the development of new tools to enhance the control measures in dealing with equidae production needs.

The present study provides new tools for surveillance and control of AHS integrating the epidemiological and immunological aspects of the disease. We analysed the serotypes at highest risk to be re-introduced and the high suitable areas for AHS outbreaks in equine population in Spain. Therefore, we evaluated the innate and adaptive immune response against AHS infection.

2. Methodology

Three different methodologies were used to achieve the aim of this study. The qualitative assessment of the serotypes at highest risk to be re-introduced into Spain was performed considering AHSV worldwide distribution, the imported equidae and the entry of infected *Culicoides* through air drafts. This information was mapped using ArcMap 9.2 (ESRI® 2006). Results were used to know the serotypes which have higher risk of potential re-emergence.

The analysis of main risk factors of the disease was performed altogether using the multicriteria decision framework based on geographical information systems (GIS), which allows the identification of high suitable areas for AHS outbreaks in Spain.

The host immune response against AHS was analyzed by means of three experimental infections with different serotypes. In each horse, clinical form of the disease, viraemia, serological response and cytokine expression [15] were measured to understand the immune response.

3. Results and Discussion

The result of qualitative assessment in Spain shows that the serotypes at highest risk to be re-introduced are AHSV2, AHSV4 and AHSV9. This result is associated with the recent outbreaks of the disease outside the endemic area and historical outbreaks in Spain. This funding could help to assess effective strategies to control the disease, such as the establishment of vaccine stock against these serotypes and the development of new generation vaccines and diagnosis techniques. These tools could be used in the high suitable areas for AHS to limit the spread of the disease and to avoid severe economic losses. The model revealed that South-Western and Northern-Center Spain are the most suitable areas for the development of AHS. On one hand, the South-Western region corresponds to the ones that historically were more affected by AHS outbreaks, which are related with *C.immicola* distribution [5]. On the other hand, Northern-Center suitable regions overlapped mainly with *C.obsoletus* distribution [5]. The official veterinary services could use this information for equine disease control and prevention programs and to reduce the consequences associated to AHS.

The evaluation of AHSV infection allowed us to identify that only horses with an efficient immune response survived to the virus. Several cytokines (IL-1, IL-10, IL-12 and/or TNF α) were involved in the innate immune response, which depended on the clinical form of the disease that the horse showed. This innate response is related to the control of the early stage of the disease until the development of a specific adaptive immunity, which allows the improvement of an antigen-specific defense that is fundamental to host survival. The adaptive immune response was represented by the expression of TNF α probably associated with cytotoxic T lymphocytes (LTc, CD8+), altogether antibody production for the effective resolution of the disease. This new knowledge of the immune response will enable the improvement of treatments and vaccinations as methods of control and prevention.

4. Conclusions and Future research

These AHS epidemiological results may be useful to support risk-based surveillance and control strategies which, ultimately, are intended to more cost-effectively prevent and control potential incursions and the spread of AHS in Spain. The acquired knowledge has allowed to identify and to map AHS risks in Spain. Further research will also be oriented to assess its economic value as an effective means to reduce vulnerability and mitigate social and economic consequences associated to introduction and spread of AHS. A simulation and scenario-based approach will be developed to evaluate the potential economic impact. Furthermore, new information about general immunology knowledge of AHS has been acquired. This knowledge will allow developing new vaccine against the serotypes at highest risk to be re-introduced into Spain, as well as to develop new effective diagnosis methods for a better control of AHS disease in equidae production. Future work will address the design and implementation of effective strategies to risk-based surveillance and control of the disease.

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Use of pulsed light to increase the safety of ready-to-eat food products

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Abstract. Pulsed light (PL) is an emerging food decontamination technology with a great potential for the superficial decontamination of ready-to-eat (RTE) foods. The efficacy of PL on the microbiological safety and shelf-life of different RTE food matrices (raw, dry-cured, smoked and cooked) was studied. Even though PL presented different degrees of surface decontamination depending on the characteristics of the food matrix, in all the cases it showed to be effective in reducing pathogenic bacteria and in increasing the shelf-life of the products, minimally affecting their sensory properties. PL could be thus considered a useful alternative for increasing the safety of RTE products.

Keywords: pulsed light, RTE foods, microbiological safety

1. Introduction

The production of ready-to-eat (RTE) foods is a highly dynamic sector in Western countries. However, these products may pose a safety risk for consumers since they have been linked to a number of food-borne outbreaks (Rocourt *et al.*, 2003). Pathogenic bacteria reach their surface mainly during post processing handling (cutting, slicing, and packaging) and remain in the product along the storage. Different non-thermal technologies are being studied for the control of pathogens in RTE, in order to ensure food safety while minimizing nutritional and sensory damage caused by traditional thermal processing methods. These technologies include high pressure processing (Porto-Fett *et al.*, 2010), irradiation (Cabeza *et al.*, 2009) and pulsed light (PL) (Hierro *et al.*, 2011). PL consists on the application of short duration flashes of an intense broad-spectrum, rich in UV light. Its bactericidal effect is exerted at a surface level and is mainly attributed to photochemical damage in DNA, induced by the UV-C component (Wang *et al.*, 2005). In comparison to continuous UV systems, PL allows a greater energy input and reduces the exposure time. The evaluation of the effect of PL on the target matrices is critical, since properties such as their topography or transparency may influence the effectiveness of the technique.

The purpose of this study was to evaluate the efficacy of PL for the inactivation of food-borne pathogens in different matrices of RTE foods, and to analyze their effects on different aspects related to safety and acceptability, such as oxidation, color, shelf-life, and sensory characteristics, in view of a future industrial application of this technology.

2. Materials and Methods

Pulsed light treatment. A desktop SteriBeam SBSXeMatic-2L-A device (SteriBeam Systems, Kehl am Rhein, Germany) was used for the PL treatment (Hierro *et al.*, 2011). Samples were flashed with different fluences (0-11.9 J/cm²).

Microbiological analysis. Samples were plated on selective media according to the microbial group to be detected.

Lipid oxidation. Measurement of the TBARs index was performed.

Protein oxidation. The methodology described by Oliver *et al.* (1987) was followed.

Color measurement. A tristimulus colorimeter (ChromaMeter CR-400, Konica Minolta, Osaka, Japan) was used for the determination of the CIELAB profile.

Sensory analysis. A rank order test was performed.

3. Results and Discussion

In our studies, we observed that pulsed light might be useful to increase the microbiological safety of different RTE products. For instance, on smoked salmon we found that PL was effective in reducing *Listeria monocytogenes* loads, with a dose-rate effect (Fig 1). Significant inactivation rates ($p < 0.05$) were obtained for fluences of 4.2 J/cm^2 or higher. Bacterial counts remained lower ($p < 0.05$) in these samples along 28 days of storage at 4°C . Regarding quality parameters, no differences in lipid oxidation were detected after applying the treatment. Furthermore, PL treatment seems not to affect the CIELAB profile or the sensory attributes right after the treatment or during the storage. Similar studies were performed in order to analyze the effect of PL on other food matrices (raw, dry-cured and cooked products). The technique showed different degrees of efficacy on surface decontamination and a range of effects on the product's quality. Both depended on the fluence tested and the composition, texture and opacity of the matrix. In general, the negative effects of PL on the quality parameters of RTE foods were neglectable compared to the decontamination levels offered by the technique.

4. Conclusions and Future research

Pulsed light is effective in reducing pathogenic bacteria on the surface of RTE products, alone or as part of a hurdle technology, minimally affecting the sensory properties of foods. As it can be easily integrated at the processing lines, this technology could be considered a simple and cost-effective alternative to increase the safety of food products. Further research is needed for the industrial implementation of this technology.

Figures

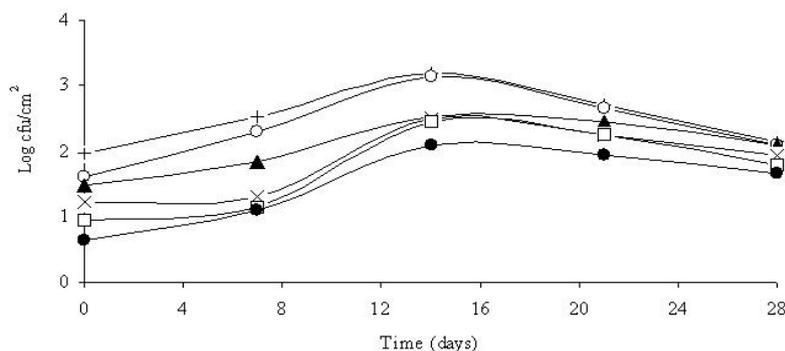


Figure 1. *L. monocytogenes* counts (log cfu/cm²) in vacuum-packaged smoked salmon slices during 28 days storage at 4°C after applying several PL fluences (+ 0 J/cm^2 , ○ 0.7 J/cm^2 , ▲ 2.1 J/cm^2 , X 4.2 J/cm^2 , □ 8.4 J/cm^2 , ● 11.9 J/cm^2).

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Development of a vision system to detect allergen (peanut traces) in powdered foods

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Abstract. Cross-contamination occurs when a safe food comes in contact with bacteria, germs or food allergens. Regarding food allergens, the intake of even the slightest trace can cause serious consequences in sensitized individuals. Thus, food industries must test their products for the presence of allergenic components due to cross-contamination and must provide suitable information on food label. Among allergenic ingredients, peanuts are one of the most prevalent. In order to provide the food manufacturers with a sensitive, non-destructive and rapid technique to detect peanut traces in foods, this research was focused on the development of a method based on a Red-Green-Blue (RGB) vision system. This technique was tested on mixtures of different powdered foods (cocoa, milk and wheat flour) with increasing concentrations of crushed peanuts. Interesting results were obtained: after analyzing RGB images through various Image Texture Analysis (ITA) techniques (texture filters, co-occurrence matrix, Multivariate Image Analysis, MIA), it was observed that methods based on MIA in all cases allowed the separation of non-contaminated mixtures from those with even the lowest contamination levels.

Keywords: allergen detection, Red-Green-Blue (RGB) vision system, Texture Image Analysis (TIA), Multivariate Image Analysis (MIA)

1. Introduction

ITA is defined as a function of the spatial variation in pixel intensities of a given zone of an image [2]. Texture classification is one of the major issues of ITA. The approaches for analyzing texture are very diverse, and differ from each other mainly by the method used for extracting textural features. The principal methods for ITA are: *i) statistical methods*, based on extracting textural features from a gray level co-occurrence matrix (GLCM); *ii) filtering methods*, which provide information about the local variability of the intensity values of pixels in an image; *iii) MIA methods*, which involve unfolding the RGB image cube into a data matrix that can be analyzed by PCA[1]. Through PCA the original number of variables could be reduced to a much smaller number of variables (PCs), which accounted for most of the variability in the data [3]. Through MIA it is thus possible to view pairs of score vectors (columns of T, i.e. t_a) as point clusters of scatter plots (score space), to investigate individual point clusters in the score space by manual masking and to calculate the Hotelling's T^2 and the Residual Sum of Square (RSS) images [4].

2. Materials and Methods

Digital images of wheat flour, powdered milk and cocoa with different peanut contamination levels (0%, 0.1%, 1% and 5%) were acquired through a RGB vision system. RGB images were analyzed by applying the most popular texture analysis techniques (texture filters, GLCM, and MIA based methods): *i) four of the most commonly used descriptors (Contrast, Correlation, Energy, and Homogeneity)* were used to extract textural features from the GLCMs of the RGB images and PCA was then applied to these textural features; *ii) performance of three texture filters* was tested (one based on the entropy of the of the 9-by-9 neighborhood around the pixel i of the input image I , one based on the local standard deviation of I , and one based on the range value, minimum and maximum values, of the 3-by-3 neighborhood around the pixel i in the input image I); *iii) The total number of pixels falling under the t_1 - t_2 and t_2 - t_3 score space masks* obtained through MIA was employed as a measure of image texture, since it was related to the count of pixels belonging to peanut traces in each image, and this feature was employed to classify flour samples. ANOVA was applied to the number of pixels falling under the t_1 - t_2 and the t_2 - t_3 score space masks. Milk and cocoa samples were classified on the basis of geometric characteristics of the t_1 - t_2 score space density regions and by analyzing T^2 and RSS images.

3. Results and Discussion

The results obtained through the mentioned ITA techniques were: *i)* after applying PCA to the textural features derived from GLCMs, it resulted that samples with a low contamination level were usually separable from those highly contaminated; *ii)* the best results were obtained with the filter based on entropy applied to the flour samples, which in all cases was able to identify regions with dark specks (trace of peanuts or other type of contaminants) in contaminated and no contaminated samples; *iii)* after applying ANOVA to the number of pixels falling under the t_1 - t_2 and the t_2 - t_3 score space masks and after analyzing T^2 and RSS images, all mixtures were correctly classified according to their contamination levels (Fig. 1).

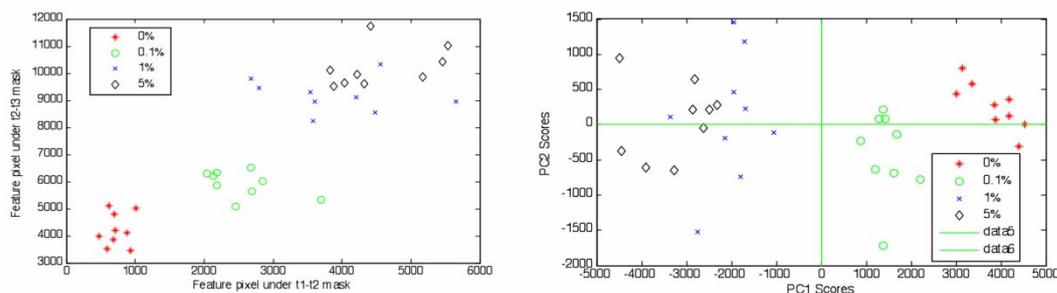


Fig. 1 – Image classification of flour mixtures obtained through MIA.

4. Conclusions and Future research

Different approaches to image texture analysis were overviewed and were used to classify a set of RGB images of powdered samples with different contamination levels. The proposed MIA-based image texture analysis method produced better classification results than those obtained employing different types of texture filters and the GLCM features. The approach based on MIA methods could be successfully used to classify images on the base of textural information; it let to identify no contaminated samples and it let to separate samples with a low contamination level from samples with the highest contamination level. This approach could be successfully used as a cheap and fast screening test in the food industry. It would be interesting to implement further ITA, such as transform-based methods (i.e. Fourier and Wavelet transforms) in order to detect lower levels of peanut contamination.

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1st Workshop
PICATA

Materials for
the Future Cluster

The Cluster of Materials for the Future (**Mat4Future**) is coordinated by Prof. José M. González Calbet (UCM – Facultad de Ciencias Químicas) and Prof. José Ygnacio Pastor Caño (UPM – ETS de Ingenieros de Caminos, Canales y Puertos). The activities of the groups working in the specialized areas of materials are quite transversal and include over one hundred high specialized research groups from *ab initio* computation and quantum behavior to structural, functional, biomedical and energy applications of materials. So transversal activities involved a close contact with real human and social problems, and, so that, two of the priorities of this Cluster is the social divulgation of the results and the collaboration with the industry.

On February 13, 2013 took place a workshop at the Seminar Room of the School of Forestry Engineering of the UPM. This workshop was intended to meet the people recently incorporated thank to PICATA Programme of Moncloa Campus and who are researching and assessing this Cluster. During the 2013 sessions it was presented the work performed by 33 predoctoral students and 22 postdoctoral contracts. The participants explained shallowly the ongoing results of the collaborative research projects, between the UCM and UPM, in which they are involved, their scope perspective. All the research projects were directed jointly by the UCM and UPM with one Director from each institution.

The subjects presented within the Mat4Future Cluster can be classified in the following priority lines:

Materials for Functional Applications

- Quantum transport in graphene and other materials, C. Gaul
- Magnetism in magnetic/non magnetic/magnetic nanostructures, M. Abuin
- Renormalized properties of graphene induced by surface acoustic waves. D. González González
- Electrostatic doping of strongly correlated oxides, A. Pérez
- Hysteretic transport in oxide/graphene hybrid planar nanostructures, M. Rocci
- Design and synthesis of two-dimensional magnetic and electric properties, in perovskite materials, R. Cortés-Gil
- Surface acoustic waves in graphene, J. Pedrós

Materials for Biomedical Applications

- Magnetically triggered multi-drug release by hybrid mesoporous silica nanoparticles, A. Baeza
- Smart nanosystems for antitumor therapy, M. Martínez-Carmona

Materials for Energy Applications

- Fabrication, characterization and testing of nanostructured W for nuclear power plants applications, N. Gordillo

Materials Processing

- Silica additions in cement pastes obtained from different mixing conditions: Influence on the hydration process, D. Alonso-Domínguez
- Phase transitions in colloidal monolayers absorbed at flat interfaces, F. Martínez-Pedrero
- Development of a Molecularly Imprinted Polymer (MIP) for the determination of Enrofloxacin in food samples, J. L. Urraca

The presentations saw transversal studies, which make clear the transversality of our Cluster, where the interdisciplinary and multidisciplinary approaches to the different problems presented where a constant of the most of the works performed by the PICATA young researches. As well, a good combination between basic knowledge with applied objectives has been a common characteristic of the work developed in the PICATA projects in this Cluster.

We fell that the work performed by this young talent PICATA people is an inspiring and motivating promised of a future, where a strong and tough collaboration between the two Universities involved in the CIE Moncloa Campus, can guide us to successful results thanks to the synergies created by the complementarity of the research groups.

José M. González Calbet

José Ygnacio Pastor

Coordinators Materials for the Future Cluster

Quantum transport in graphene and other materials

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Abstract. This work is dedicated to quantum transport in complex environments and sheds light on several fundamental questions. The four main parts are: (a) disordered Bose gases, (b) Bloch oscillations with interactions, (c) electron-electron scattering in graphene, and (d) spin filtering in graphene. Here, I focus on the last two points. Main results are the prediction of scattering resonances due to interactions and the design of a graphene-based spin filter.

Keywords: graphene, Bloch oscillation, spin filtering, Bose-Einstein condensation, disorder

1. Introduction

The microscopical understanding of quantum transport is not only of fundamental theoretical interest, but it also paves the way for novel technological developments. There are great hopes to build more efficient computers and other devices with the help of:

- ✦ Ultracold atoms and trapped ions which are promising systems for the realization of novel concepts of computation and simulation, namely quantum computing and quantum simulation.
- ✦ Graphene, which is a (nearly transparent) two-dimensional carbon allotrope with extraordinary transport properties, high electrical and heat conductance, and good spin coherence.
- ✦ Spin-tronics. Conventional computers only use the charge of electrons, but do not take advantage of the spin degree of freedom. Using the spin as information carrier may allow for more efficient computers with less power consumption.

Before the technical application of these novel concepts, more basic research and knowledge is needed. In the field of ultracold atoms, we have realized several publications that contribute to the understanding of these systems, concretely on (a) disordered Bose-Einstein condensates [1, 2] and (b) Bloch oscillations [3, 4]. Due to the time constraints in this presentation, I restrict myself to the more recent topics (c) and (d), dealing with graphene.

The most particular property of graphene is its electronic band structure (a *band* is the energy of a particle as function of its momentum), which (neglecting electron-electron interactions) consists in two bands that are intertwined and touch at the so-called Dirac points, as represented in Figure 1. In part (c), we address a particular aspect of the interaction, namely the interaction of two electrons energetically well separated from the other electrons, which form the Fermi sea. These background electrons screen the Coulomb interaction of the two electrons of interested, which results in an effective short-range interaction.

In part (d) we address the spin transport in graphene and propose a device to create a current of strongly spin-polarized electrons, a pre-requisite for spin-tronics. This is achieved with a graphene nanoribbon with ferromagnetic strips placed in a regular manner in top of it, resulting in a spin-dependent superlattice.

2. Methodology

Parts (a) and (b) make use of the Bogoliubov approximation, the diagrammatic Green function approach, collective-coordinates techniques, and linear stability analysis.

In part (c), we rely on the T-matrix formalism and on the approximation of a short-range separable interaction potential.

In part (d), we use the quantum transmission boundary method in the numerical part, and a transfer-matrix formalism based on the Dirac equation in the analytic part.

3. Results and Discussion

(c) We have tackled the scattering problem of two electrons in graphene well above the Fermi sea [Figure 1]. In the approximation of a short-range separable potential (justified for low-energy scattering), we have computed the T-matrix analytically. The problem separates into several energetically separated channels, depending on whether the incoming particles are both from the same part of the Dirac cone (the upper part has helicity +1, whereas the lower part has helicity -1). The most interesting results occur in the channel, where both electrons have the same helicity [(++) channel]: at certain energies, narrow resonances of Feshbach type occur, which are related to bound states in the closed (+-) channel.

(d) The transmission through the graphene nanoribbon with the across a spin-dependent super-lattice shows transmission bands that depend strongly on the electron spin [Figure 2]. This allows tuning the device in such a way that it work as a spin filter, which makes it a source of spin-polarized electrons, a pre-condition for spin-tronics. Furthermore, in the resulting current across the sample, regions of negative differential resistance (NDR) occur, i.e., a further increase of voltage leads to a decrease of the current. These regions of NDR occur at different parameters for spin up and spin down.

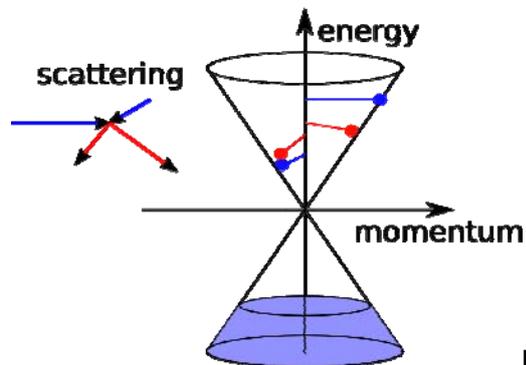


Figure 1: Electron-electron scattering in graphene well above the Fermi sea (blue shaded region). The incoming electrons are represented in blue, the outgoing in red.

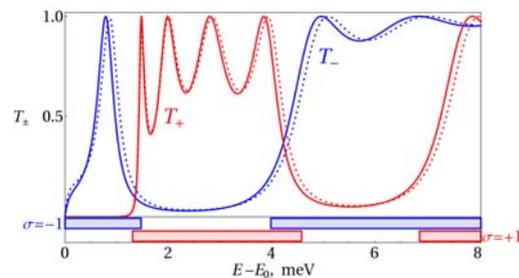


Figure 2: Transmission as function of energy for spin up (red) and spin down (blue). Ref. [5]

4. Conclusions and Future research

In part (c) we have gained quite some insight on the effects interactions can have in the two-particle scattering problem. The next steps are to extend this to the many-body problem and to propose concrete experiments and applications for the predicted effects. Similarly, we seek to study how the device proposed in part (d) can be actually used in real spin-tronics applications.

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Magnetism in magnetic/non magnetic/magnetic nanostructures

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Keywords: thin films, sputtering, AFM, VSM, XRD, micromagnetic calculations

Abstract This project focuses in the fabrication and study of trilayer thin films formed, by magnetic/non-magnetic/magnetic layers, used rectangular patterns (ratio ~1:10). The investigation on the magnetic proper ties of low dimensional materials is considered one of the main research topics worldwide. Furthermore, the possibility of building new materials with at least one dimension in the nanometer scale has revolutionized the research of functional materials, as they opened up new applications in areas as spintronics [1] or biomedicine [2]. One of the leading interests of nanostructured systems resides in the manipulation of their electric and magnetic properties. The patterning of multilayer films has made possible the fabrication of complex structures like Synthetic Antiferromagnets with a very low remanence in the absence of an applied field [3]. In these structures, magnetic layers are separated by non-magnetic spacers and exhibit a magnetostatic coupling between them. This coupling promotes the antiparallel orientation of magnetization, contrary to non-patterned films, where the weak interactions between magnetic layers depends on sample roughness and tends to align magnetization parallel in the two layers [4].

We have selected FeCo for the magnetic layers for its high magnetization and the possibility to tune its coercivity by changing the growth conditions [5]. The nanostructures have been obtained by lithography. Sample fabrication has been carried out by DC and Pulsed-DC magnetron sputtering. The structural quality of the grown trilayer and the surface has been determined by AFM, XRD and SEM (EDAX). Magnetic measurements on films have been made by VSM. In addition, we have initiated a project to correlate the structure and the magnetic properties of Co islands on Ru. In order to do that, we have measured the magnetic pattern of the Co layer by spin-polarized low-energy electron microscopy (SPLEEM) and we have reproduced them by means of micromagnetic calculations. Magnetic thin films often present different properties than bulk materials [6]. These differences arise from the increasing importance of the surface contribution to the magnetic anisotropy when the thickness of a film is reduced.

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Silica additions in cement pastes obtained from different mixing conditions: Influence on the hydration process

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Keywords: cement paste, silica additions, ²⁹Si MAS- NMR, microstructure, ettringite

1. Introduction

The use of nanosilica additions in cement-based materials has actually attracted much attention in the last decade. Nanosilica together with several different oxides is among the most employed additions [1]. The main searched targets in obtaining new materials depend on the type of nanoparticle chosen. Thus, nanosilica and nanoalumina addition mainly aims to improve the characteristic properties of cement paste materials: enhancement of mechanical strength, densification of the aggregates/paste interface, increase of the permeability and therefore optimization of durability, etc [2]. In all cases, one of the main difficulties arises for their application due to operational problems associated with the difficulty in workability. In order to optimize the additive efficiency, a good dispersion inside the material is required, and this implies to ensure a good dispersion of particles in the mixing water and a subsequent successful compaction of the material.

The present work reports on the changes produced in the hydration process of cement pastes additivated with nano and microsilica, obtained under different addition methodologies. The principal aim deals with establishing the most relevant changes occurring in the hydrated compounds, when comparing mixing methods. In the first method the samples prepared by means of the dispersion of particles in the mixing water, in the second method the anhydrous cement is additivated with the silica (nano and micro size).

2. Materials and Methods

The plain cement paste (PCP) used as base and reference material is an Ordinary Type I 52.5R Portland cement. In this study two sets of samples have been studied. The samples of one set (denoted AC) were prepared starting from anhydrous cement in which the additions were already incorporated, whereas in the samples of the second set (denoted as AW) the additions were included during the mixing process. All the phases were prepared at a water–cement ratio $w/c=0.4$ using different concentrations of two types of additions: commercial silica nanoparticles (dry powder), supplied by Cab-O-sil® and microparticles (silica fume), supplied by Ferroatlantica SL. The selected concentrations were, for both sets of samples, 4 and 10% of nanosilica (denoted with N) and 5 and 10% of microsilica (denoted with F). In the notation of water manual mixed samples, i.e. AW ones, a “MA” is included at the end of the name in order to avoid ambiguity. TGA/DTA profiles were registered using a Setaram Labsys Evo TGA-DTA apparatus. A total quantity of 50-100 mg of sample was heated at 10°C/min up to 1200°C. Solid state ²⁹Si MAS-NMR- (Magic Angle Spinning Nuclear Magnetic Resonance) spectroscopy was used to characterize the molecular composition and structure of the hydrated samples. The experiments were carried out on a Bruker Avance 400MHz spectrometer, with a 9.39T widebore superconducting magnet, operating at 79.49 MHz, with spin rate of 12KHz, 90° pulse length of 4.5 μs. Scanning electron microscopy (SEM) was performed using a JEOL JSM6335FEG, with resolution of 12Å. Samples were metallized by covering with Au. Semiquantitative chemical analyses were made from energy dispersive X-ray spectroscopy (EDS).

3. Results and Discussion

From ²⁹Si MAS-NMR data it is observed that, in general, polymerization values are greater for the AC samples than for the manual mixed ones, which indicates that they are more easily hydrated as they present a greater percentage of anhydrous phases (alite and belite), and this is also supported by the thermogravimetric analyses. In the manual mixed samples no

isomorphical Al^{3+} substitution in the silicate chains takes place, whereas for the AC samples $\text{Q}^1(1\text{Al})$ signals prompted to the existence of aluminosilicate chains, in which Al^{3+} cations are located in terminal positions of dimers and/or in the middle of trimers, as, $\text{Q}^2(1\text{Al})$ signals do not appear (see Figure 1-right). New ^{27}Al NMR experiments are now in route in order to get deeper insight about these structural details.

From SEM images, it is observed that the employed nano and microsilica additions from both tested mixing methods lead to a considerable modification of the microstructure, especially concerning the morphology of portlandite and ettringite species. Portlandite crystals size is drastically reduced (ca. 60%) when the cement is nanosilica additivated, even with a concentration as low as 4%. Ettringite is present as needle-type crystals grown inside the pores of the specimens (see Figure 1-left). The deposition type of addition employed in AC samples provokes the apparition of a great quantity of aciculate AFt species efficiently coating the pores surface and therefore leading to promising durability parameters.

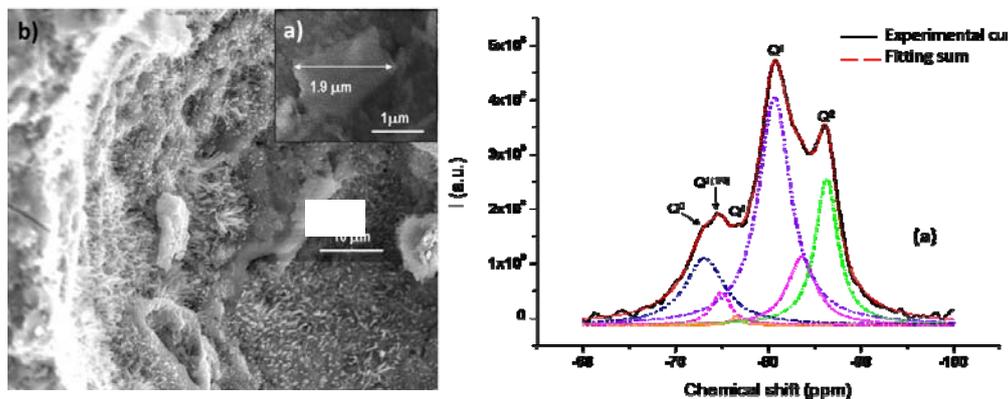


Figure 1. Left side: SEM images for the sample 4N, with 7 days of curing age; Right side: ^{29}Si MAS-NMR experimental spectrum and deconvoluted curves for the 10N specimen, with a curing age of 28 days.

4. Conclusions and Future research

Several cement pastes with different addition content and size, nano and micro silica, have been prepared, following two different ways in incorporating the additives. Paste test specimens of dimensions 1x1x6 cm have been prepared and characterized by TGA, SEM and ^{29}Si NMR. In order to evaluate the rate of samples hydration, measurements were performed in samples with different curing ages: 2, 7 and 28 days. The obtained results show a higher degree of hydration for previously additivated samples compared to manual mixing cements with the same curing age. Moreover, relevant changes concerning the structure of hydrated compounds have also been detected. The behavior of previously additivated samples is consistent with the presence of hydrated calcium silicoaluminates. Finally, regardless of the method employed, the addition of nanoparticles modifies the size of the obtained crystals. SEM images show a significant reduction in the size of portlandite crystals [3].

In the presented work we have reported on the changes produced in the hydration process of cement pastes with additions of nano and microsilica, obtained under two different addition methodologies. With the aim of verifying our previous hypothesis and to get deeper insight about the implied processes, we are now carrying out some complementary ^{29}Si MAS NMR, ^{27}Al MAS NMR, MIP, FTIR, EDS and SEM experiments.

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Renormalized properties of graphene induced by surface acoustic waves

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Keywords: surface acoustic waves, graphene

1. Introduction

Graphene has made frequent headlines in the scientific press during the last few years. The Nobel Prize awarded in 2010 for the discoverers of this “father” of many allotropes of carbon, such as graphite (consisting of many weakly coupled graphene layers), carbon nanotubes and fullerenes, has contributed to give worldwide attention to this single-atom thick material with unique electronic and mechanical properties, which generates a rare combination of both fundamental and applied interest [1].

On the other hand, a new technique has emerged to control electron motion in semiconductor structures which relies on the use of surface acoustic waves (SAWs) as conveyor belts for electrons [2]. The potential of this technique in the context of graphene structures has not yet been investigated and is one of the main thrusts of the current research project.

2. Methodology

In the context of semiconductor structures, some theoretical calculations on the transport of electrons by SAWs have been made which have provided good results and have helped in the applications [2]. However, these calculations have been mostly based on classical descriptions of the electron motion. It is our intention to generalize this type of calculations to include a full quantum-mechanical treatment of the electron dynamics in semiconductors and to investigate in detail the interaction between graphene electrons and SAWs in the underlying dielectric.

Our collaboration with the UPM group led by Fernando Calle, which has a research line on “Electronic devices and microsystems”, is focused on that theme. A fruitful collaboration between theory and experiment is already taking place and interesting basic and applied results will be reported soon.

3. Results and Discussion

My theoretical and experimental colleagues from UCM and UPM, Jürgen Schiefele and Jorge Pedrós, respectively, are already investigating some applications of this technique for the development of plasmonic devices. It should be pointed out that very promising applications are expected from the emergent field of graphene plasmonics [3], which is already yielding exciting new results.

Moreover, we are paying attention to the recent use of surface acoustic waves in double quantum dot semiconductor systems as means of conveying single electrons between neighboring quantum dots. The potential applications of this technique include topological quantum computation [4].

4. Conclusions and Future research

As happens often in research, we do not know yet exactly where graphene plasmonics and SAWs in graphene will lead us, but the range of potential applications is very large indeed. On the short term, we plan to focus on the inclusion of quantum-mechanical effects in the description of the electron-SAW interaction and in general to apply the current knowledge of SAWs in semiconductors to the case of graphene structures.

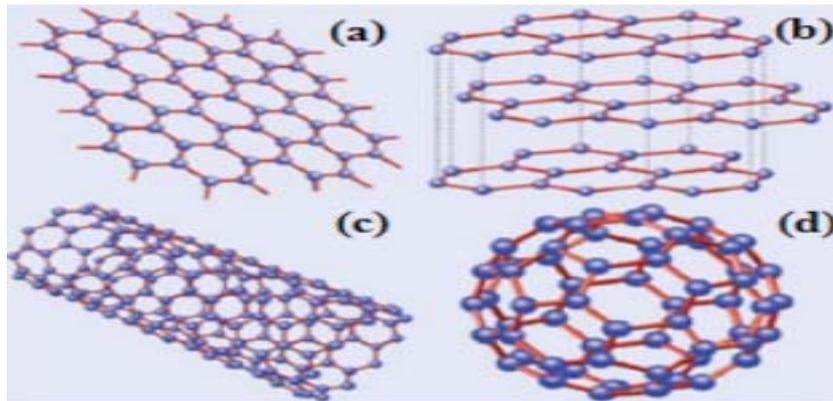


Fig. 1: Carbon allotropes: (a) Graphene, our “king”. (b) Graphite, (c) A carbon nanotube, (d) Fullerene

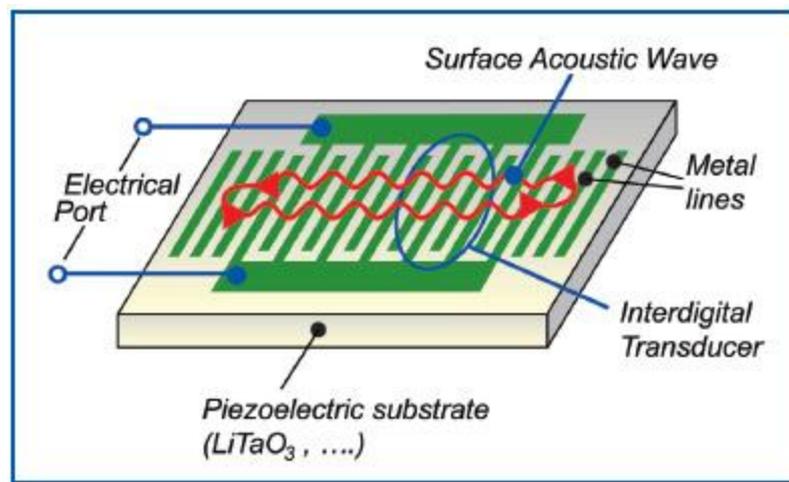


Fig. 2: Sketch of a surface acoustic wave generated by the transducer on top of a piezoelectric.

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Magnetically triggered multi-drug release by hybrid mesoporous silica nanoparticles

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Keywords: controlled drug release, magnetic mesoporous nanoparticles, stimuli-responsive

1. Introduction

The treatment of complex diseases such as cancer pathologies, requires the simultaneously administration of several drugs in order to improve the effectiveness of the therapy. In this work, the objective is the synthesis of a new thermoresponsive hybrid polymer/magnetic mesoporous silica nanocarrier able to release different cargos, proteins and small molecules, housed in the polymer branches and inside the mesoporous matrix respectively, in a controlled manner in response to an external alternating magnetic field. Superparamagnetic iron oxide nanocrystals have been trapped inside the mesoporous silica matrix, in order to provide the heating capability under alternating magnetic fields, which is also suitable for hyperthermia treatment of cancer.^[1] As reversible gating system, thermoresponsive polymer based on the well-known properties of Poly(N-isopropylacrylamide) (PNIPAM) has been attached on the mesoporous surface. This polymer exhibits phase transition at a lower critical solution temperature (LCST) of approximately 32°C in water.^[2] This transition (shrinkage) allows the drugs trapped inside the pores to release if the temperature is above the LCST. Different strategies for producing mesoporous silica-PNIPAM hybrid nanoparticles have been recently published,^[3] ^[4] but all of them are focused on the release of a small molecule encapsulated inside the mesoporous matrix in response to temperature changes. Branched Polyethyleneimine (PEI) chains have been grafted to the end of each PNIPAM chains, and N,N'-methylenebis(acrylamide) (MBA) has been used as crosslinker in order to increase the electrostatic interactions with the housed proteins and to create a more extensively branched polymeric network, respectively, hampering the premature protein release. The nanodevice should combine different interesting properties: the release of two different therapeutic agents and the ability to increase the temperature of the surroundings in response to a nontoxic and highly penetrating in living tissues external stimulus, as magnetic field. Also can improve the therapeutic effect of the released cytotoxic drugs by a synergic effect.^[5] Finally, the nanocarriers can be magnetically targeted to the desired place^[6] or could be used as contrast agents in magnetic resonance imaging (MRI).^[6]

2. Materials and Methods

Synthesis of maghemite, γ -Fe₂O₃. The superparamagnetic maghemite nanocrystals were obtained by coprecipitation of Fe(II) and Fe(III) chloride according to Massart's method^[7].

Synthesis of magnetic mesoporous silica nanoparticles MMSNs. A modification of previously published method by Zink et al. has been employed^[8]. In this approach, tetraethyl orthosilicate (TEOS) was added to an aqueous solution of non-functionalized iron oxide particles, hexadecyltrimethylammonium bromide (CTAB) and NaOH as base, at 80°C.

Synthesis of MMSN-MPS. Dry toluene containing 3-(Trimethoxysilyl)propyl methacrylate (MPS) was added under N₂ to a dried MMSN100, being stirred during 12 h at 110°C, for the nanoparticle acrylate functionalization.

Synthesis of MMSN-NIPAM. The polymer shell was obtained mixing NIPAM, MBA and PEI in a degassed water/ethanol solution with MMSN-MPS with ammonium persulfate (APS) as initiator, and the solution was stirred overnight under N₂ at 30°C.

3. Results and Discussion

Different amounts of iron particles have been added to the synthesis mixture and all of the samples show a narrow average size distribution for drug delivery applications, centered on 50-100 nm measured by dynamic light scattering and showing good magnetic properties by vibrating sample magnetometer. FT-IR and thermogravimetric analysis were employed to verify the successful functionalization with MPS and the polymer attachment. In order to establish the LCST of the polymer grafted onto the nanoparticle surface, MMSN-NIPAM was loaded with fluorescein and heated between 20-50°C, establishing its LCST around 35°C.

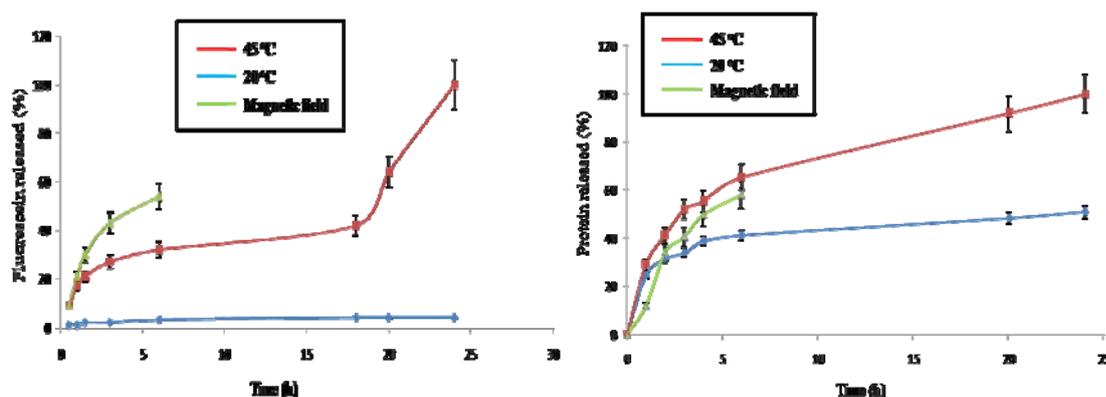


Figure 1. Time dependent fluorescein and protein release at 20°C, 45°C and under alternating magnetic field exposition.

Once the carriers were loaded with fluorescein inside the pores and Soybean Trypsin inhibitor (STI) protein within the polymer branches, the release profile obtained for both cargos call for the ability of this material to release two different molecules (Fig.1).

4. Conclusions and Future research

In this work, a proof of concept of a new smart nanodevice able to release two different cargos, proteins and small molecules, in response non-toxic and highly penetrating in human tissues external stimulus such as magnetic field, has been presented. The results demonstrate that the phase state of the polymer can act as gate-keeper opening or closing the pores of the silica matrix and may also control the release of the macromolecules attached into the polymer branches. This dual release along with the synergistic effect of hyperthermia treatment, could greatly improve the effectiveness of the current antitumoral therapy. Further work is underway to achieve a precise control in the trigger temperature, comprised in the upper limit of hyperthermia range (42-45°C), as well as to extend the application to different therapeutic macromolecules such as DNA, siRNA among others. AC susceptibility measurements depending on frequency and field intensity applied will be useful to appreciate the required amount of material for biological applications.

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Smart nanosystems for antitumor therapy

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Keywords: photolinker, transferrin, mesoporous, bone metastasis

1. Introduction

Mesoporous silica nanoparticles (MSN) constitute one interesting class of inorganic materials for potential applications in nanomedicine because of the advantages of high surface area, tailorable pore size, controllable particle shape and size, versatile surface modification and biocompatibility [1]. Properties that make MSN as well suited drug delivery carriers in the performance of cancer diagnosis and treatment [2].

These nanocontainers equipped with stimuli-responsive gatekeepers can provide unique benefits for precise, controlled release under specific conditions. In recent years, special attention is devoted to these “smart systems” designed to respond to certain concrete stimuli, which may be caused by the disease process itself (pH, redox changes, enzymes, etc)[3] or externally generated (light, heat, ultrasonic, etc)[1][4]. In this field, light is a powerful tool because the release of the cargo can be spatially and temporally controlled by finely selecting the area and the time of exposure to the light stimulus. Here we report a new photosensitive system with an innovative approach, the dual function of transferring, which simultaneously acts as a pore nanocap and as targeting agent towards tumor cells.

Statistics demonstrate that the bone is ranked third in terms of the preferred places of migration (metastasis) by primary tumors of lung, breast, prostate, kidney and thyroid among others, being present in 70% of patients dying of cancer [5]. The approach here presented is the preparation of MSN provided of dual targeting capacity to treat bone metastasis. First MSN will be functionalized with several bisphosphonates with high affinity for hydroxyapatite acting as primary targeting to bone. Short peptides with high affinity for receptor ligands overexpressed in tumor cells will be grafted to the MSN surface, acting as secondary targeting. Antitumor drugs will be confined into the mesoporous channels to be subsequently released once endocytosed by the targeted cancer cells.

2. Methodology

MSN end-capped with Transferrin (TfMSN) via photocleavable linkages.

The synthesis of the MSN was carried out by the sol-gel process as reported elsewhere [6]. Then MSN were functionalized with a previously silylated photolinker. Finally the resulting material was loaded with orange acridine (OA) (as a model molecule) and pores were capped by linking transferrin to the photolinker.

After deeply characterizing TfMSN materials, their gating properties were evaluated. Samples were suspended in phosphate buffer saline (PBS) and exposed to 254 nm irradiation for 30 min under continuous stirring. As a control, dye release was also determined by repeating the same experiment in the absence of light. Photo-triggered molecular gate performance was monitored through the fluorescence band (λ_{em} =525 nm, λ_{ex} =502 nm) of the OA delivered to the PBS.

MSN for dual targeting for treating bone metastasis.

The surface of MSN were functionalized with (3-triethoxysilylpropyl)succinic acid anhydride) TESPASA to obtain –COOH groups for further grafting with the primary and secondary targeting agents. To obtain MSN tuned with TESPASA (TMSN) two different strategies were followed: 1) sol-gel method and postfunctionalization with TESPASA; 2) co-condensation of (tetraethyl orthosilicate) TEOS and TESPASA. By co-condensation several samples were synthesized using increasing amounts of TESPASA (5-20%) to achieve a sample which compromise higher functionalization without loss of the mesostructural order. Several techniques were used to characterize the TMSN such as SEM, XRD and FTIR.

3. Results and Discussion

The data DERIVED FROM OA release experiment by action of light were not significantly different from those obtained for the control. To elucidate what was the element of the system that doesn't work properly, two additional experiments of release (similar to the OA one) were carried out. One to check the photolinker union to the MSNs and it was observed that the fmc released in presence of light was 7 times higher than the control. Then the presence of transferrin in solution was confirmed by the BCA detection method. In view of the results we assume that the proposed methodology conceptually operates but, either the degree of transferrin functionalization is insufficient or transferrin does not block the pores properly.

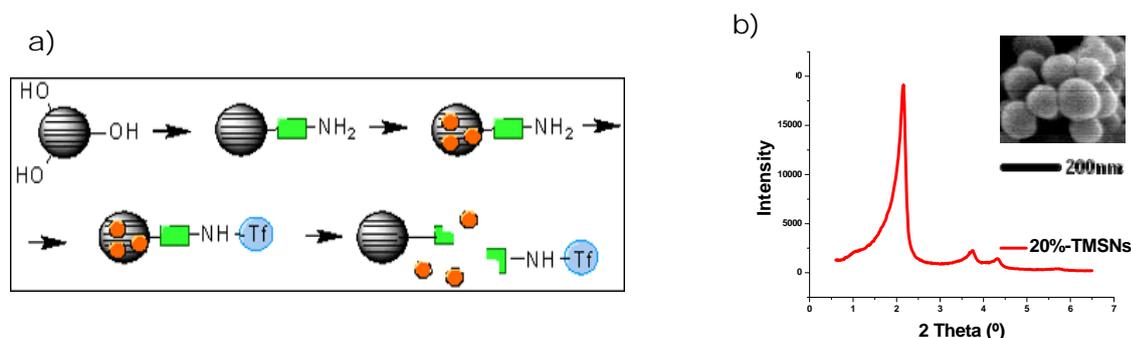


Fig.1. a) Synthesis scheme of TfMSN; **b)** RXD spectra and SEM image of 20%-TMSN.

Characterization of TMSN materials revealed the successful functionalization of samples, by using both, post-synthesis and co-condensation processes. TMSN synthesized by co-condensation show an increase in the functionalization degree when increasing the proportion of TESPSA using during the synthesis process. SEM images and XRD spectra show that all samples preserved both morphology and mesoporous.

4. Conclusions and Future research

Although designed photosensitive system is not fully functional at present, we believe it is of great interest in clinic and has a promising future. We are currently optimizing each step of the synthesis process to ensure smooth operation and to perform cell death experiments in vitro. Also improvements have arisen in the system as the use of photodynamic therapy (not require a zero release) or motors anchoring inside the nanoparticles to favor the exit of the load through the pores.

TMSN functionalized by post-synthesis and the 20%-TMSN material have been selected to complete the remaining steps and achieve the dual targeting system for treatment of bone metastasis. Subsequently the ability of both samples to produce selective killing of tumor cells will be evaluated. Despite the increased complexity, due to the great advantages of "smart systems", has been thought to improve nanocarriers by making the primary targeting sensitive to an internal stimulus (pH, enzymes) present in the environment of the metastasis bone area, thus promoting efficiency and internalization of nanosystems in cancer cells.

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Electrostatic doping of strongly correlated oxides

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Abstract. In this report we describe a field effect experiment that uses an electric double-layer transistor (EDLT) to electrostatically dope an ultrathin film, of the high temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO). Resistance versus temperature curves show a superconductor insulator transition at high doping levels, which demonstrates the ability of the EDL technique to control very large changes in the charge density of the cuprate.

Keywords: electric double layer transistor, electrostatic doping, superconductor complex oxides

1. Introduction

In strongly correlated electron systems the electrostatic interactions between valence band electrons give rise to a complex phase equilibrium that is delicately influenced by the charge carrier concentration and that strongly determine their electronic properties. Electrostatic doping experiments would allow the control of such charge density in a reversible manner avoiding the alteration of the level of disorder associated with conventional chemical substitution, which constitutes a very adequate tool to investigate the physics of these materials. [1]

A new type of field effect transistor is the so called electric double-layer transistor (EDLT), a device that uses a liquid electrolyte as the gate dielectric [2]. In the solid-liquid interface, between the liquid electrolyte and the drain-source channel, it is formed an electric double layer which can be considered as a capacitor composed of a sheet of ions in the electrolyte and another sheet of accumulated image charges on the surface of the solid. These two layers are separated by less than 1 nm, which allows to achieve electric fields of the order of 10^9 Vm^{-1} at the surface of the material under study and to obtain values of charge density (n_{2D}) as high as $8 \times 10^{14} \text{ cm}^{-2}$, several orders of magnitude above the conventional transistors.

The combination of this EDL technique, which allows high levels of induced charge, together with the nano-fabrication of ultrathin films of complex oxides, which provides with high quality 2D crystals, would give us the possibility to drastically change the electronic properties of these materials by the application of an external controlled electric field at the surface of the sample. This project aims to study the superconductor-insulator transistor in a thin film, 3 unit cell thick, of the high temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO) using the EDL configuration.

2. Methodology

We have grown 3 unit cells YBCO thin films on SrTiO_3 (STO) substrates. In order to avoid the presence of a dead layer at the substrate/thin film interface, we deposit a 5 unit cells buffer layer of $\text{PrBa}_2\text{Cu}_3\text{O}_{7-x}$ (PBCO) that ensures the expected superconducting properties of YBCO. The YBCO films were grown in a high O_2 pressure sputtering system (3,4mb) at 900°C . The device was patterned using a mechanical mask that produces an amorphous alumina template (see figure 1). This step of the process was done before the cuprate deposition to avoid the contact of the YBCO with chemicals that would degrade its properties. In situ annealing was done in 800mbar O_2 pressure and 500°C for 5 min. Both materials have been characterized with different techniques such as X-Ray diffraction, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM).

3. Results and Discussion

We studied the transport properties of the device by means of resistance versus temperature curves at different applied gate voltages (V_G) [see Fig. 2]. We observe superconducting behavior with decreasing T_C , while the V_G is increased from 0.2 to 2 V. This is in agreement with the accumulation of electrons at the YBCO layer [see Fig 1], and the corresponding decrease in the

density of holes, which are the charge carriers of the YBCO. At high enough V_G ($\sim 2.4V$) the superconductor- insulator transition is observed.

The reversibility of the process would evidence the electrostatic doping. By applying negative gate voltages we observed that the YBCO is able to recover its superconducting properties, although this process depends on the total amount of charge induced in the thin film.

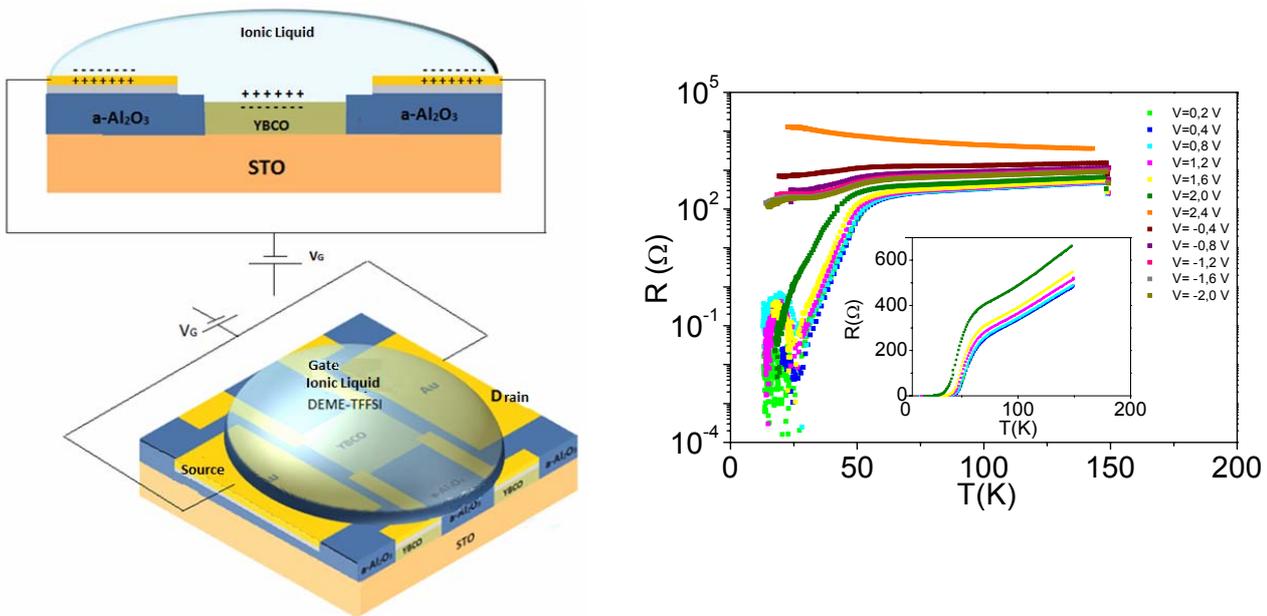


Figure 1. EDLT with the ionic liquid DEME-TFFSI as a gate dielectric. Device fabricated with high crystalline quality YBCO ultrathin films.

Figure 2. Resistance versus temperature curves of the YBCO sample for 12 different applied gate voltages using an EDL configuration.

4. Conclusions and Future research

We conclude that the use of the ionic liquid as gate dielectrics in EDLT configurations is an effective and reliable technique to induce high levels of charge density and thus, to modify the physical properties of complex oxides. In particular we have focused in the study of the superconductor-insulator transition of the complex oxide YBCO.

We have recently extended the use of EDL devices to study other interesting materials such as the well-known insulator PBCO which is isostructural to YBCO but without their superconductor properties. This technique is also being used to study colossal magnetoresistance phenomena exhibited in the manganites. Nanoscale control of electronic properties using field effects is an emerging area and the possibility of controlling the electronic properties of materials with nanometer resolution will allow the examination of fundamental issues underlying the behavior of strongly correlated electron systems.

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Hysteretic transport in oxide/graphene hybrid planar nanostructures

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Abstract. We report on the fabrication and magnetotransport characterization of innovative hybrid graphene-based spin valve nanodevices with epitaxial nanopatterned $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ manganite, grown on SrTiO_3 (100), as ferromagnetic current injector electrodes. The few layers graphene (FLG) was deposited onto the predefined manganite nanowires by using the PMMA transfer technique. These nanodevices exhibit hysteretic transport as measured by IV curves. The resistance can be reversibly switched between high and low states yielding a consistent non-volatile memory response.

Keywords: manganites, spintronics, graphene, nanolithography, memristor

1. Introduction

Since their discovery, colossal magnetoresistance manganites have focused a large research effort due to the interesting physics underlying the strong electronic correlations. In particular, the half metallic character of $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ (LCMO) or $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSMO) perovskite oxides has motivated their use as sources of spin polarized carriers in spintronic devices. Although many examples can be found in the literature where these oxides have been used as magnetic electrodes in multilayer devices for perpendicular transport along 3D pillars, planar devices involving nanostructured electrodes are to our knowledge very scarce [1]. This may be related to difficulties in nanostructuring these materials due to their mechanical hardness, or to the alteration of their electronic properties caused by etching processes. Yet, having access to single domain manganite wires or dots could be of interest for a wide variety of important experiments spanning from non local spin injection to artificial vortex pinning. In this communication we report on our recent effort on fabricating complex oxide nanostructures.

2. Materials and Methods

The 18 nm c-axis LSMO thin film samples were grown on (001)-oriented SrTiO_3 single crystals in a high- O_2 -pressure (3.4 mbar) r.f. sputtering system at 900 °C. In situ annealing was done in 800 mbar O_2 pressure and 550 °C for 30 min [2]. LSMO wires 200 and 500 nm wide were fabricated by using conventional Electron Beam Lithography and wet etching processes. In particular, 200nm thick ma-N2403 negative resist (from MicroResist GmbH) was spun on the LSMO thin film and 10 kV, 100 pA electron beam lithography parameters were used in order to define the manganite nanowires. The LSMO wet etching was done dipping the sample in a hydrochloridric acid solution for few seconds. The mechanically exfoliated FL-graphene on SiO_2/Si wafer was moved onto predefined $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ manganite nanowires by using the PMMA transfer technique (fig.1a).

3. Results and Discussion

The magnetic behaviour is examined by measurements of the anisotropic magnetoresistance AMR in magnetic fields with various orientations with the direction of the wire. In LSMO wires we find evidence for a magnetic state up to room temperature and resistivity values close to those found in large thin films, suggesting that the electronic state is little affected by the lithography process. Different coercive field values were found as function of the nanowire width. Abrupt resistance switching at coercivity is consistent with a single domain state. For magnetic fields oriented perpendicular to the wire AMR displays complex features suggesting domain wall resistivity. The resistivity vs temperature measurement shows a typical metal-insulator transition (MIT) accompanied with a strongly non linear transport with hysteretic IV curves characteristic.

particular, we find a typical memristive-like behaviour in the metallic regime and pinched-diode behaviour in the insulator regime (fig.1b). Interestingly, the bistable resistance states display a nonvolatile memory response.

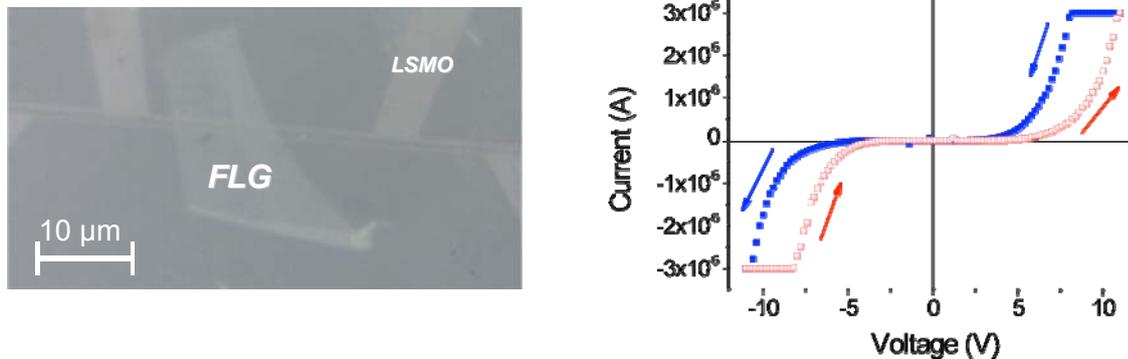


Figure 1: a) Micrograph showing a few layer graphene (FLG) on two LSMO wires of 500 and 200 nm thickness. b) Typical hysteretic IV curves measured at 140 K (inset resistance vs temperature curve of the FLG/LSMO device measured at $I=1\cdot 10^{-7}$ A).

4. Conclusions

New kind of hybrid LSMO/FLG nanodevices were fabricated and characterized. A peculiar hysteretic transport has been found at temperatures ranging from 10 to 300 K. This behaviour could be related to the contact resistance between the oxide and the graphene and could be used in the future as graphene-based non-volatile memory, in nanoelectronic applications. Further work will be necessary to identify the origin of such an intriguing response in these complex oxide/graphene nanostructures.

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Design and synthesis of two-dimensional magnetic and electric properties in perovskite materials

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Keywords: Mn perovskites, brownmillerite, electron microscopy, ferromagnetism, colossal magnetoresistance

1. Introduction

Looking for new ways to innovate and improve the materials properties constitute an intensive research area for technological development. The perovskite structure has traditionally attracted a great interest since properties such as colossal magnetoresistance (CMR) have been described in materials showing related structures.¹ Moved by the obvious technological interest of that property this project is focussed on the design, synthesis and characterization of new advanced functional materials related with perovskite materials for such application.

The brownmillerite structural type, a four-fold perovskite superstructure, is stabilised if the anionic vacancies in the cubic perovskite are ordered along $[101]_c$, leading to tetrahedral layers alternating with octahedral ones. The three-dimensional manganite brownmillerite configuration can provide the confinement of different interactions in the layers leading to exciting magnetic and transport effects similar to the two-dimensional systems. The design of the adequate compositional and structural requirements has allowed the stabilization of the $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_{2.5}$ polycrystalline brownmillerite material exhibiting magnetoresistance (MR) as a consequence of the presence of nanometric ferromagnetic (FM) clusters embedded in the octahedral layers of its antiferromagnetic structure.² In this sense, according to the structural configuration, MR could be related to the double exchange mechanism inside the octahedral layers leading to CMR and also, on the tunneling effect between them through the insulator tetrahedral ones, i.e., tunnel magnetoresistance (TMR). Previous studies suggest that new manganese brownmillerite materials having the required compositional conditions to exhibit confined FM interactions and, CMR and/or TMR could be stabilized by means of the introduction of cationic vacancies in a controlled way.³ Even more, the additional order/disorder phenomena between the layers related to cationic deficiency could lead to intriguing and unexplored magnetic and transport phenomena in oxygen deficient perovskite materials.

2. Materials and Methods

According to this project, our aim is studying the effect of the cationic vacancies in the polycrystalline $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_{2.5}$ material. For that purpose, the planning is the optimization of the thermodynamic conditions allowing the stabilization of new $(\text{La}_{1-x}\text{Sr}_x)_z\text{MnO}_{2.5}$ materials as well as the systematic study of their structural, magnetic and transport properties. Note that $(1-z)$ accounts for the % of cationic vacancies.

$(\text{La}_{1-x}\text{Sr}_x)_z\text{MnO}_3$ ($z = 1, 0.99, 0.98$) perovskite compositions, which was prepared by a conventional ceramic method, were selected in order to keep the same $\text{Mn}^{3+}/\text{Mn}^{4+}$ ratio respect to the $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$. $(\text{La}_{1-x}\text{Sr}_x)_z\text{MnO}_{2.5}$ materials were obtained by topotactic reduction of $(\text{La}_{1-x}\text{Sr}_x)_z\text{MnO}_3$ perovskite samples where the Mn oxidation state should be identical than in $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_{2.5}$. The reduction was performed in a CAHN D-200 electrobalance by heating the starting material at 560°C under an atmosphere containing 200 and 300 mbar of H_2 and He, respectively, at a rate of 0.15°C/min. Both oxidised and reduced samples were characterised by powder X-ray diffraction (XRD) with a Philips X'Pert diffractometer equipped with a $\text{CuK}\alpha$ radiation source. The cationic composition, as determined by X-ray energy dispersive spectroscopy (XEDS), was found to be in agreement with the nominal one. Selected area electron diffraction (SAED) was performed with a JEOL 2000FX electron microscope and high

resolution electron microscopy (HREM) was carried out with a JEOL 3000FEG electron microscope fitted with an Oxford LINK EDS analyzer and ARM 200 CFEG electron microscope equipped with aberration corrector in the condenser lens and a COLD-FEG gun. The magnetic properties were determined with a Quantum Design SQUID magnetometer in the temperature range from 5 to 300 K at applied fields of up to 5 T. The temperature dependent resistance measurements were performed using the standard four-probe method in the temperature range 5-300 K under 0 and 8.5 T applied magnetic fields.

3. Results and Discussion

The XRD study suggests a brownmillerite related structure for the above samples. Nevertheless, a clear orthorhombic distortion is observed as the percentage of cationic vacancies increases. At this point a technique able to provide information concerning the vacancy ordering is required. In this sense, a SAED and HRTEM study has been performed in $\text{La}_{0.52}\text{Sr}_{0.47}\text{MnO}_{2.5}$ ($z=0.99$) and $\text{La}_{0.54}\text{Sr}_{0.44}\text{MnO}_{2.5}$ ($z=0.98$) showing long and short ordering situations, respectively. Actually, for $z=0.99$ SAED patterns and corresponding HRTEM images are in agreement to the $\text{Ibm}2$ brownmillerite unit cell. Nevertheless, a more complex situation involving extended defects as a consequence of the disorder intergrowth between perovskite and rock salt blocks appears for higher cationic vacancy content as can be seen in figure 1 corresponding to a characteristic image and FFT along $[100]_c$ of $z=0.98$ sample. Magnetic and transport measurements indicate the presence of FM and MR in the $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_{2.5}$ brownmillerite related compound. Tunability of cationic vacancies in that composition leads to a new Mn oxide materials having the required compositional conditions to exhibit also FM and MR behaviour. The double exchange Mn^{3+} -O- Mn^{4+} interactions are confined in the octahedral layers leading to similar FM behaviour in all cases. However, MR behaviour seems more sensible to the cationic vacancy concentration as a consequence of different structural configuration.

4. Conclusions and Future research

Tunability of both cationic and anionic vacancies is a new strategy in perovskite related oxides to deal with new materials and promising associated properties such as FM and MR. Ionic conductivity measurements for these new materials are in due course. The analogous system with Ca, $(\text{La}_{1-x}\text{Ca}_x)_z\text{MnO}_{2.5}$, and Cu/Mn, $\text{LaMn}_{0.5}\text{Cu}_{0.5}\text{O}_{3-6}$, will also studied.

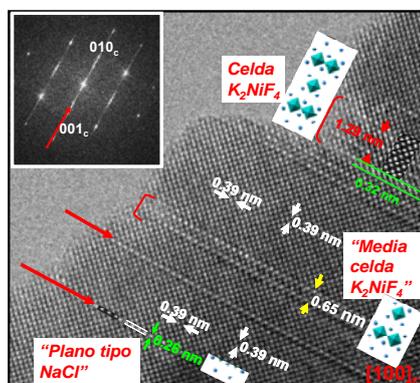


Figure 1. HREM image and FFT along $[100]_c$ corresponding to $\text{La}_{0.54}\text{Sr}_{0.44}\text{MnO}_{2.5}$. Extended defects are marked with arrows. Local ordering is showed at the top right of the image.

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Fabrication, characterization and testing of nanostructured W for nuclear power plants applications

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Abstract. The development of new materials able to resist in the hostile environment of a fusion reactor is one of the challenges in the design of the future nuclear power plant. In this project the capability of nanotungsten (nW) as a plasma facing material (PFM) are investigated. For this purpose, nW are deposited tuning their microstructure by changing the deposition parameters.

Keywords: plasma facing materials, first wall, nanostructures, light element diffusion

1. Introduction

The project is included within the HiPER (High Power Laser Energy Research Facility) EU project for energy generation. The aim of this work is to research and develops new materials capable of withstanding damage by irradiation and elevated temperatures for first wall applications.

Because of the low sputtering yield, low-activation with a high melting point, high thermal conductivity, and low thermal expansion, W is considered to be the best candidate to be located as PFM in both magnetic (MC) [1,2] and inertial confinement (IC) fusion reactors [3]. However, some limitations as the retention of light species which drives to material swelling and detriment, have to be defeated in order to fulfil specifications [4,5]. Nowadays, nW materials have been proposed to be very promising because of the large density of grain boundary. They show (i) a self-healing behaviour and moreover, (ii) the grain boundary act as effective diffusion channels for light species. Both things, contribute to delay the material swelling.

2. Methodology

The samples were grown by DC sputtering from a W commercial target (2" in diameter) in the presence of an Ar atmosphere on different substrates (Si, and steel) in a high vacuum chamber ($P_{base} \sim 10^{-8}$ mbar) at room temperature and 50 W of plasma power. The Ar gas pressure and the target-substrate distance were kept constant at $\sim 8 \times 10^{-3}$ mbar and 8 cm, respectively.

The transmission electron microscopy (TEM) characterization was done by using a JEOL JEM 2000FX microscope. The surface morphology was measured by field emission gun-scanning electron microscopy (FEG-SEM) using a JEOL JSM 6335F microscope applying different acceleration voltage from 10 to 30 kV. The chemical elemental analyses of microscopic regions of the samples were done with an energy-dispersive X-ray spectroscopy (EDS). Structural characterization was done ex-situ by X-ray diffraction (XRD) using a Philips X-PERT four-cycle diffractometer with a CuK_{α} radiation source in Bragg-Brentano geometry. In order to study the thermal stability of the nW, the samples were annealed under vacuum from RT to 400 °C for 30 and 240 min. The resonant nuclear reaction experiments were carried out by using the $H(^{15}N, \alpha)^{12}C$ nuclear reaction in samples implanted with (i) H at an energy of 170 keV, (ii) sequentially implanted with C at an energy of 665 keV and H at 170 keV and (iii) simultaneously implanted with C and H at the energies mentioned above. The nanoindentation tests were performed using a MTS Nanoindenter XP and the continuous stiffness measurement (CSM) technique together with a diamond Berkovich indenter.

3. Results and Discussion

W nanostructured with a thickness of $\sim 2 \mu m$ were successfully grown by DC magnetron sputtering on different substrates. Microstructural studies illustrate that coatings are pure α -phase and polycrystalline presenting quite low macro-stress and micro-strain, and good adhesion to the substrate even after annealing them at temperatures as high as 400 °C for long time (240 min). The morphology of the layers is shown in figure 2. All of them present the similar columnar morphology which grows perpendicular to the substrate as can be observed in Fig.2 c).

The TEM micrograph (Fig. 2a) in the dark field mode reveals that the grains present anisotropic shapes with sizes ranging from 50 to 150 nm. Those results are in agreement with the in-plane image obtained from SEM, Fig. 2b). In addition, the columns present an inverted pyramidal shape which is compatible with the zone T in the Thornton's morphology diagram [6].

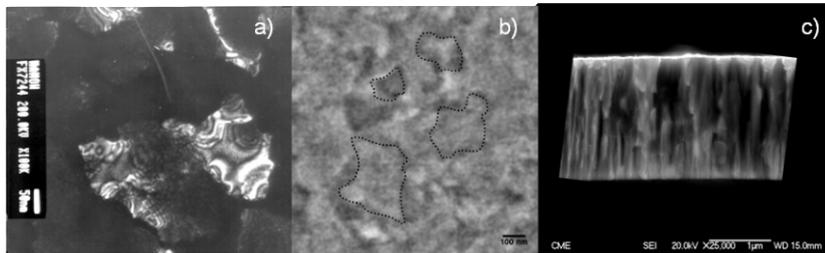


Figure 4. a) TEM dark field images of a W thin film, b) In plane and c) cross-section FEG images of a 1.89 μm W deposited on Si substrate [7].

No significant influence in the microstructure neither the morphology was observed for samples deposited on different substrates.

First experiments based on the implantation with H and co-implantation with H and C were performed in order to simulate operating conditions in nuclear reactor.

The H concentration for the nW is higher than for the massive W is. These results suggest that grain boundaries might act as pinning centres for H at room temperature what is in agreement with already reported secondary ion mass spectroscopy (SIMS) [8]. In principle, this is a very promising result because H accumulation at the grain boundaries will increase the H trapping area, thus reduce the local H density shifting the irradiation fluence threshold for blistering to happen to higher values. By comparing the H depth profiles for the nW and massive W samples sequentially implanted with C and H at RT (nW-H-CAI and massiveW-H-C-AI), it can be observed that the total H concentration for both samples is very much similar. The H concentration for H-implanted and sequentially implanted coatings is negligible at all depths.

4. Conclusions and Future research

Nanostructured W coatings, with a thickness of $\sim 2 \mu\text{m}$, were deposited by DC triode magnetron sputtering on different substrates (Si and steel). Microstructural studies illustrate that coatings are pure α -phase and polycrystalline presenting quite low macro-stress and micro-strain, and good adhesion to the substrate. The films consist of nanocolumns perpendicular to the surface substrate with a diameter in between 50 and 150 nm. No grains size evolution is observed after annealing.

From the implantation experiments preliminary conclude that grain boundaries dominate the H behaviour in nW.

In order to validate the coating for first wall applications further research has still to be carried out: (i) Study the interface properties of nW deposited on ODS, (ii) Co-implantation with triple beam, (iii) Thermal loads effects.

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Phase transitions in colloidal monolayers absorbed at flat interfaces

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Keywords: monolayer, interfase, crystal, melting, phase

1. Introduction

In this study, colloidal monolayers absorbed at different interfaces have been used as models for studying a rich variety of phase transitions in two dimensions (2D). Specifically, we focused on two different processes:

- a) How different phases develop on 2D dense binary colloidal monolayers as a function of the relative concentration of small/large particles [1].
- b) Melting/sublimation processes in 2D colloidal crystallites induced by a constant magnetic field perpendicularly applied to the flat interface.

2D colloidal systems are ideal model systems widely used for studying the universal properties of crystallization, glass formation, melting, sublimation... because of the easily accessible time and length scales and the unhampered access to structural information [2]. In our study, the temperature, the relative composition, the size ratio and the external applied magnetic field are the controlling parameters, and the final phase-behavior are mainly determined by the ratio of the interactions acting on the system. Translational, orientational distribution and other dynamical functions have been used systematically to monitor the continuous phase transitions through a detailed characterization of the kinetics and the global and local order.

2. Materials and Methods

Our binary system consists of different mixtures of small (s, $r_s = 1.45 \mu\text{m}$) and large (l, $r_l = 2.85 \mu\text{m}$) charged polystyrene microparticles absorbed at a flat interface made up of ultrapure Milli-Q water and octane. The magnetic crystals are made up by superparamagnetic polystyrene microspheres ($r_m = 1.95 \mu\text{m}$) absorbed at a flat water/air interface. In the latter case the inter-particle interaction strength is tuned from outside by an external magnetic field created by a coil, fed by a constant current power supply. We studied the dynamics and the structures of these systems using optical microscopy and digital imaging. Homemade software allows us to determine the area and the location of the center of mass of each spot in a sequence of binary frames. From these data, we evaluate several averaged statistical functions.

3. Results and Discussion

In octane/water interfaces, structured monolayers of microparticles are observed at relatively high surface coverages (Figure 1). The symmetry and structure of colloidal patterns are dictated by the repulsive colloidal pair interactions due to the presence of residual dissociated charges on the particle's surface. The presence of particles of different size hinders the global crystallization of the sample. For a relative small number of impurities, however, hexagonal structures persist in appearing in the binary mixture, leading to medium-range crystalline order. At near equimolarity, the hexagonal packing of the colloidal spheres is almost completely hindered: although slight short-range ordering is reported, no long-range order is observed, which is a clear feature of highly disorder glassy or dense liquid mixtures.

Capillary long-range attractive interaction, which originates from the deformation of the surface of a liquid caused by the presence of submerged particles, is probably the responsible of the self-assembled crystalline structures formed by superparamagnetic particles absorbed in the water/air interface. The magnetic repulsion of particles having parallel dipoles can break the

bonds that hold solids together. If the magnetic field is high enough small crystallites explodes into a gas of individual particles (Figure 2).

4. Conclusions and Future research

In dense binary colloidal monolayers we observed how a gradual enhancement in the number of particles of different sizes leads to a continuous vitrification process and how homogeneous binary glasses form in equimolar mixtures. We have performed a simple calculation that relates the structures found to the pair dipolar potential, allowing the forecast of local structures in other arbitrary binary mixtures. Finally, we have corroborated the goodness of the binary systems as a glass-forming model by comparing the established scenario with the structural features found in partially aggregated monolayers. On the other hand, we have studied by first time a field induced sublimation process in magnetic colloidal crystals. In “fast processes”, when the field induced repulsive magnetic interaction is the predominant interaction, the initial sublimation kinetics presents a scaling that only accounts for the effects of the field strength, being almost independent of the crystallite’s sizes and shapes.

In quite advanced researches we are studying field induced “slow processes”, more equivalent to thermal leading phase transitions, in polycrystalline assembly of particles (Figure 2). New transitions are expected under the application of tilted and oscillatory magnetic fields.

Figures

Figure 1

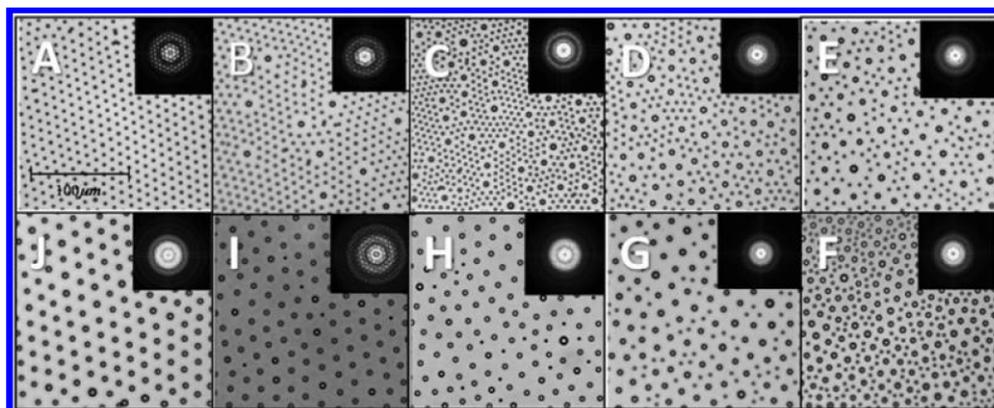
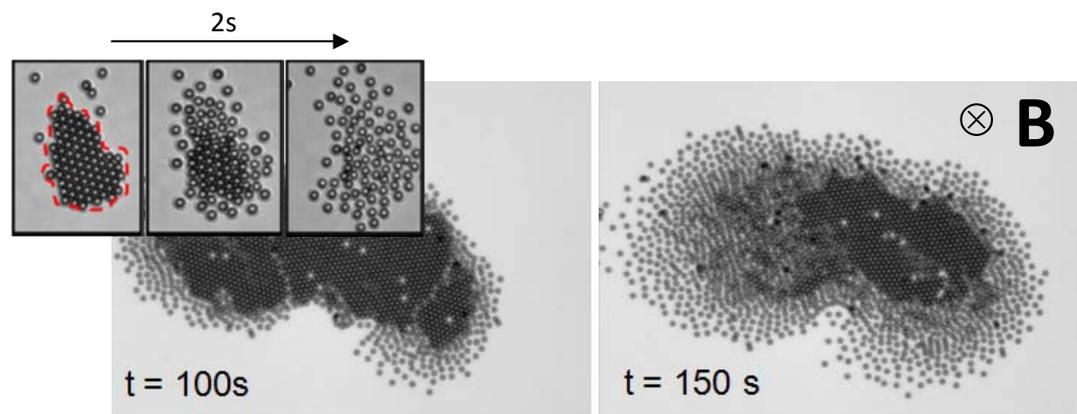


Figure 2



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Surface acoustic waves in graphene

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Abstract. The transfer of graphene to piezoelectric substrates with interdigital transducers allows generating surface acoustic waves (SAWs) that propagate across the graphene layer, modulating its properties. In particular, the dynamic strain field of the SAW is expected to create a grating in the graphene that permits the far-field coupling of light into plasmons without the need of any patterning. The dispersion of the plasmons hybridized with the phonons in the substrate has been calculated providing the required conditions for the experimental implementation of this novel technique in graphene.

Keywords: graphene, surface acoustic wave (SAW), plasmon

1. Introduction

The interaction of a SAW with graphene may allow not only to probe the material properties but also to develop new devices and functionalities induced or modulated by the SAWs. Graphene is an ideal two-dimensional electron gas (2DEG) with a huge electron mobility. The modulation of this 2DEG has been applied to the development of transistors and, more recently, the generation of plasmons. In comparison to standard noble-metal plasmons, those in graphene are of special interest because they are long lived, extend into the IR and THz domains, and can be tuned by means of the electrostatic modulation of the Fermi level. However, their generation requires either complex near-field coupling techniques [1,2] or the patterning of the graphene into nano- or micro-scaled arrays allowing standard far-field coupling techniques [3]. The latter implies the generation of a large amount of edge defects that modify the graphene properties. In this communication, we report on the generation of plasmons in graphene by means of standard laser techniques and without the need of any patterning using the modulation induced by the strain field of a SAW [4].

2. Materials and methods

Graphene on Cu foils, fabricated by chemical vapour deposition (CVD), has been transferred to piezoelectric substrates following the procedure described in Fig. 1(a). A layer of PMMA, spun on the graphene, allows to visualize and handle the graphene once the Cu foil is etched away. The quality of the graphene has been assessed by Raman spectroscopy, as shown for example in Fig. 1(b) for the case of graphene transferred to a quartz substrate. The absence of the defect-related D peak and the ratio of the intensities of peaks 2D and G, $I_{2D}/I_G=2$, indicate, respectively, the good quality and the single-layer character of the graphene.

3. Results and Discussion

Interdigital transducers (IDTs) have been fabricated on various piezoelectric substrates and the SAW characteristics have been evaluated. Fig. 2(b) shows the reflection and transmission spectra of two orthogonal SAW delay lines aligned along the Z and X directions of Y-cut LiNbO₃. The IDTs, fabricated by optical lithography, have a period of 8 μm, generating a SAW at a frequency $f \sim 430$ MHz with very low loss and a bulk acoustic wave (BAW) at higher f .

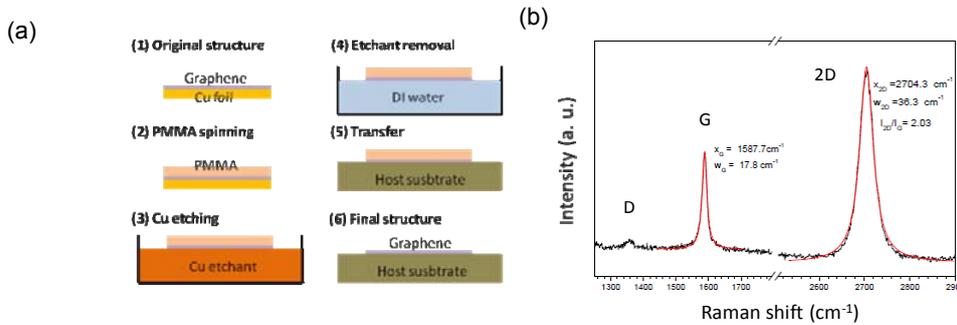


Figure 1. (a) Process for the transference of CVD graphene to a host substrate. (b) Raman spectrum of single-layer graphene transferred to a quartz substrate. The D, G, and 2D peaks are indicated.

The space between IDTs is aimed for the graphene, so that the SAW propagates across it. The plasmon dispersion and lifetime in graphene is affected by the substrate underneath due to the coupling to polar phonons. In the case of LiNbO_3 , the hybridized plasmon dispersion shows three branches, as shown in Fig. 2(b). The plasmon dispersion can be tuned by varying the Fermi energy of the graphene. The experimental generation of the plasmons is shown to be accessible for a range of SAW wavelengths and various standard mid-IR laser lines [5].

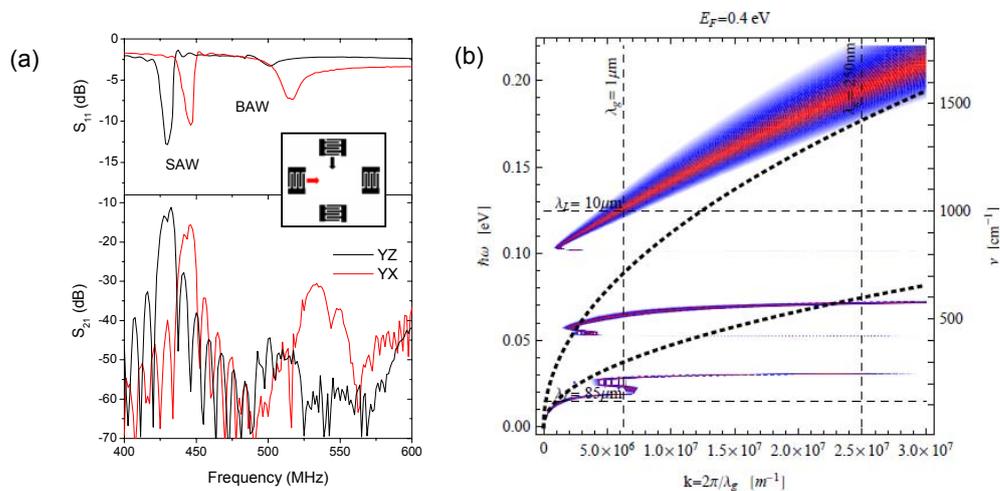


Figure 2. (a) Reflection and transmission spectra of the SAW and BAW propagating along the Z and X directions on Y-cut LiNbO_3 . The inset shows the schematic of the devices. (b) Hybridized plasmon-phonon dispersion in the graphene/ LiNbO_3 structure for a Fermi energy $E_F = 0.4 \text{ eV}$. The energy of the incident light ($\hbar\omega$) vs the plasmon wavevector (k) shows three branches accessible, for example, with the indicated grating periods (λ_g) and laser wavelengths (λ_L).

4. Conclusions and Future research

The modulation of the graphene properties by means of a SAW is being addressed and applied to the generation of plasmons. Different graphene/piezoelectric systems will be studied and the devised devices on the optimum structure will be fully tested for the generation of plasmons.

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Development of a Molecularly Imprinted Polymer (MIP) for the determination of Enrofloxacin in food samples

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Keywords: molecular imprinting, MIPs, polymer format, molecular recognition

1. Introduction

Molecular imprinting allows the design and preparation of tailor-made materials for selective recognition of chemical species. For polymer preparation the selected print molecule, that can be the analyte or a surrogate, interacts through covalent or non-covalent bonds with the functional monomers that are polymerized in the presence of a cross-linker to form a three dimensional structure [1]. After template removal the polymer will bear specific recognition sites with complementary size, geometry and arrangement of functional groups to the template molecule.

These materials are robust and resistant to harsh conditions during measurement (high temperatures, pressures, etc). In principle they can be used for sensing purposes both, in organic and aqueous media, and the cost of MIPs is lower and their preparation is easier than for antibodies. Thus, today's concept of molecular imprinting has been widely recognized as the most promising methodology for the preparation of tailor-made materials with selective molecular recognition properties.

MIPs can be prepared in different physical forms. The most widely applied approach for MIP preparation is bulk polymerization. The resulting monolithic structure is ground and sieved for the selection of particles in the right size range for a defined analytical application. This is an experimentally easy to handle approach however, part of the binding cavities may be destroyed during polymer processing, reduce the selective binding capacity and irregular particle shapes are obtained, which is a shortcoming for separation and sensing applications. Therefore, new polymer formats have emerged in the last years to overcome such limitations including, micro or nano beads [2], thin films or membranes, nanostructured MIPs or nanocomposites.

In this presentation we will describe several approaches for the preparation of MIPs in different formats for their application as solid phase extraction (SPE) sorbents in the preconcentration of fluoroquinolones (FQs) in food samples.

2. Materials and Methods

Polymers were prepared by a non-covalent imprinting approach using the antimicrobial enoxacin as template, methacrylic acid (MAA) and 2-trifluoromethacrylic acid (TFMAA) as functional monomers, trimethylolpropane trimethacrylate (TRIM) as cross-linker, a mixture of acetonitrile: dimethylsulfoxide as porogen and 2,2'-azobis (2,4-dimethylvaleronitrile) (ABDV) as initiator of the reaction. A non imprinted material (NIP) was synthesized using the same composition as the MIP but in the absence of the template. The polymers were prepared as monoliths or using silica beads, with a particle size of 40-75 μm , as sacrificial scaffolds for MIP preparation.

The binding capacity and the selectivity of the MIP/NIP sorbents were characterized by liquid chromatography. The morphology of the materials was evaluated by scanning electron microscopy (SEM). The BET surface area was calculated from the N_2 adsorption-desorption isotherms. MIP/NIPs were packed in SPE cartridges and applied to the analysis of FQs in chicken. The method has been validated by HPLC-MS/MS.

3. Results and Discussion

A polymer library was prepared using a set (10) of functional monomers; divinylbenzene, ethyleneglycol dimethacrylate or trimethylolpropane trimethacrylate as cross-linkers and acetonitrile or DMSO as porogens. The rebinding capacity of the MIP/NIP library was evaluated in batch mode by HPLC quantification of the free fraction of enrofloxacin at equilibrium. A polymer prepared using methacrylic acid (MAA) and 2-trifluoromethacrylic acid (TFMAA) as functional monomers and trimethylolpropane trimethacrylate (TRIM) as crosslinker, provided the highest selectivity and this composition was selected for further experiments. Polymer beads were prepared by pore filling silica beads that were dissolved after polymer preparation obtaining spherical MIP particles with improved binding properties (Figure 1).

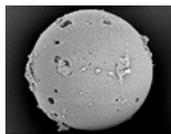


Figure 1. Scanning electron micrograph (SEM) of a MIP spherical bead prepared by pore filling silica.

Molecularly imprinted-based solid phase extraction (MISPE) conditions (loading, washing and elution solvents, and flow rates) have been optimized to allow multi-residue analysis of enrofloxacin, Sarafloxacin, ciprofloxacin, norfloxacin, lomefloxacin and Danofloxacin. The method has been validated by HPLC-MS/MS in collaboration with IRTA (Girona, Spain) according to EU's requirements (Commission Decision 2002/657/EC) and applied to the analysis of FQ antimicrobials in chicken tissue samples. Figure 2 shows a typical chromatogram corresponding to the analysis of a chicken sample extract spiked with the FQs and preconcentrated using the MIP/NIP cartridges.

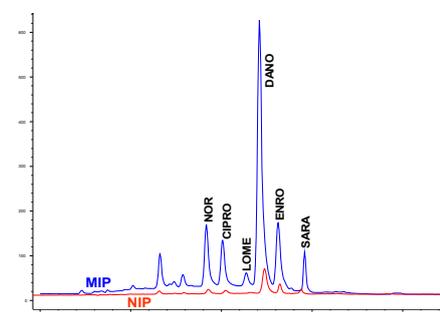


Figure 2. Representative LC-FLD chromatograms of a chicken tissue extract ($V = 10$ mL) spiked at 1.5 xLMR ($30\text{--}150 \mu\text{g Kg}^{-1}$) of FQs. After MIP (–) or NIP (–) preconcentration.

4. Conclusions and Future research

MIP composition and physical format can be tuned for selective multi-residue analysis of a class of antimicrobials in food samples. We are currently working on the synthesis of new materials for the selective recognition of biological molecules (peptides) using polymer beads. In parallel we are working on the optimization of a novel polymerization technique that allows the preparation of MIP nanostructures for sensing purposes as well as on the development of composite materials with magnetic properties.

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The background of the image is a stylized map of Europe, rendered in a dark blue color against a white background. The map is composed of solid blue shapes representing the continents and their coastlines, with a white background for the surrounding oceans and seas. The text is centered over the map.

1st Workshop
PICATA

Heritage Cluster

This Workshop included presentations by six interns from the Heritage Cluster. As requested, they gave the provisional results of their research projects, some of which are intended to form part of a doctoral thesis and others which are post-doctoral research. All six research projects were directed jointly by the UCM and UPM with one Director from each.

The lack of an initial contextual definition in this Cluster is evident in the diversity of aims and approaches, and in the absence of a homogeneous theoretical context or of interdisciplinary aims in these studies. Nevertheless, they can be brought together in the three research areas where the new coordination is currently working: Area 1. Basic or knowledge-based research; Area 2. Management-based research; Area 3. Applied research.

Half of the papers can be included in Area 3 (Applied research): the presentations by Inmaculada Martínez Garrido on preventive conservation; by Natalia Pérez Ema on the effects of different restoration processes on archaeological monuments; and by Luis Pablo Nuñez with a most original study, apparently not closely connected with Cultural Heritage, on a software development to facilitate annotations in digitalized works.

Two other presentations focused on Area 1, i.e. basic research designed to increase an understanding of cultural assets. Ainhoa Díez de Pablo gave an interesting presentation of her research carried out in Madrid, Paris and Berlin, on the rationale behind building social housing districts in these cities and their state of conservation. Manuel Rodrigo de la O Cabrera offered a completely different topic in his analysis of the land transformation resulting from the installation of energy industry-based infrastructure.

The last presentation, by Verónica Hernández Jiménez, is the only one which can be included in Area 2 (Heritage asset management-based research). Her study of the social participation in the evaluation of rural landscape introduced us to a very specialized area of forestry engineering which is her area of expertise and which is not normally dealt with in relation to Cultural Heritage, but more often in connection with sociology or even anthropology. Measuring opinions is a sensitive area, as has often been shown in a sociological context. However, the work of this research team, and of this researcher in particular, is certainly interesting, especially if the conclusions reached can be applied to improving the assets themselves or society's perception of them.

In each of these six cases taken individually, we were able to find connections with the themes of other Clusters, especially Global Change and New Energies. Each of these research projects certainly showed us how much still remains to be done in the field of basic and applied research in Cultural Heritage. On behalf of the Coordination of this Cluster we wish these six researchers every success in their future work and hope that it will enhance the assets of our common Cultural Heritage.

M^a Ángeles Querol Fernández

Juan Miguel Hernández León

Coordinators Heritage Cluster

Decay assessment, diagnosis and monitoring through wireless sensor networks and non destructive techniques for architectural heritage conservation

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Keywords: cultural heritage, wireless sensor networks, monitoring decay

1. Introduction and Contents

This research project aims to develop assessment, diagnosis and monitoring strategies of the materials decay which are part of the Cultural Heritage, and also environmental control to establish a preventive conservation proposal of them, using minimally invasive technologies such as wireless sensor networks.

Preventive conservation is one of the major goals in Cultural Heritage, understanding any actions or intervention that prevents or reduces damage risk, including environmental and anthropogenic decay. Continuous monitoring which is offered by emerging technologies such as wireless sensor networks lends the intervention through specific actions when an early stage damage is detected.

So far there are no protocols to address the problem of Architectural and Archaeological Heritage monitoring, where both its structure and content of artwork may suffer significant decay processes by cyclic outdoor and indoor variations. The research encompasses the development of wireless measurement techniques to suit the requirements in Heritage Conservation and also other non-destructive techniques (infrared thermography, hygrometric techniques, etc.) contributing to the knowledge and development of protocols for Preventive Conservation.

2. Methodology, Materials and Methods

Decay processes caused by indoor and/or outdoor conditions appear in many churches where heating systems can generate significant damage in Cultural Heritage, furthermore outdoor conditions exert a great influence on temperature and humidity behavior inside the walls. There are many aspects to consider for a complete monitoring [1] that will lead to decay modeling for prevention, since indoor microclimatic conditions depends not only on the thermal conditioning systems but also on the existing ventilation in the building, the presence of visitors, etc.

To address this task two wireless sensor networks with different technical characteristics have been developed, a fact which in turn has allowed establish the adequacy and performance of these technologies to the requirements marked on the scope of the Cultural Heritage. This research project was carried out in St John the Baptist Church at Talamanca de Jarama, it has its origins in the XII-XIII century, a Romanesque style, and it has undergone several expansions and restorations in its history, leaving only the stone apse of the original building. The bell tower is Baroque style and it was built during the XVII-XVIII century.

The monitoring system provides continuous monitoring through an outdoor and gases network which is working together with a temperature and relative humidity network measuring inside the walls. Furthermore, a number of button sensors used have been used for monitoring the indoor temperature and relative humidity, characterizing the operation of the heating system in the church of Talamanca, and studying the distribution of these parameters in both area and height. The distribution of the monitoring points has been strategically established after detecting the main decay problems through the use of other non-destructive techniques such as infrared thermography or hygrometric techniques. Monitored points are affected by salt crystallization, high moisture content, heating system operation, solar radiation, etc., being the solar radiation influence related to the orientation, materials are being studied (masonry, dolostone ...), etc.

3. Results and Discussion

Results of this work and continuous monitoring for one year period (1 December 2011 to 30 November 2012) have defined the first guidelines for monitoring decay and, after data studies by means of developed Matlab applications for the treatment of them, the main sources of deterioration such as solar radiation, presence of humidity due to capillary absorption, condensation, rainwater infiltration or leaking pipes, presence of public, heating system performance, ventilation, etc. have been characterized. The solar radiation influence has been the greatest decay agent in the walls, enabling to assess the relation between it and the orientation of the façades or the monitored materials [2].

From technological point of view the performance of each wireless sensors network have been analyzed, establishing communications comparisons to reduce error rate, taking careful monitoring every five minutes for outdoor conditions and every two minutes for indoor conditions and inside the walls.

4. Conclusions and Future research

By developing data processing and communications tools through Matlab, it is established Libelium technology (outdoor and gases wireless sensor network) provides fewer communication losses than MEMSIC (relative humidity and temperature sensor network), having better range due to its technical characteristics. For MEMSIC technology two different network topologies were tested, working Tree topology better than Mesh topology.

The building's construction history conditions the behavior in presence of solar radiation and water absorption of the walls processes affecting the indoor conditions. These conditions favor the materials decay by salt crystallization processes, capillary absorption or condensation.

There is also a relation between decay agents and the height where sensors inside wall have been placed, being the lowest heights the most affected by humidity problems. Solar radiation presents thermal cycles in the south façade and it has been possible to analyze heating/cooling processes depending on the solar radiation influence and material has been studied.

Future research tasks are established to extend studies to another scenario of action with different design features, materials and decay agents, indoor and outdoor, due to the existence of different heating system or variability in the number of visitors. This will validate the deployed monitoring method in St John the Baptist Church at Talamanca de Jarama, introducing technical developments for monitoring conditions inside walls which has been carried out so far. Likewise, it will be advanced in modeling tasks and characterization of materials for the extension and generalization of the guidelines established up to now.

Acknowledgments

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Comprehensive strategy of assessment of cultural landscapes related to Spanish energy industry: Stage of identification and catalog

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Keywords: cultural landscape of energy; energy production territorial systems; energy industry spatiality, conceptual model of landscape assessment; landscape transformation

1. Introduction and Contents

Cultural landscapes are considered a common European heritage and different European initiatives (planning schemes, landscape laws) are focused upon their conservation and promotion. However, governments have faced difficulties in the conservation and management of cultural landscapes, especially those with severe human modification (e.g. the 'Cultural Landscapes of Energy' -'Energyscapes'-). Energyscapes are shaped by processes related to the energy production industry and depend on the complex spatial and temporal combination of the supply, demand and infrastructure for energy.

This paper aims to reveal the main factors that have promoted the transformation of the territory with high presence of energy industry. This analysis allows to have an overview of the development, assessment, potential and some specific features of Spanish energyscapes, to rethink on which could be the interaction between 'energy landscape', 'society' and 'heritage' in the perspective of a spatial and economic development. Also, it provides a dynamic and comprehensive tool allowing the identification of agents, parameters and links that drive the transformation. The subsequent management of the landscape can be approached using the results obtained.

2. Methodology

Bernáldez's energetic methodology stands out and defends a two-fold dimension of landscape: on the one hand, there exists the "phenosystem", a perceivable dimension (vegetation, ground, town, factories, etc.) which is the appearance of the landscape that can be perceived. And on the other, there is also a hidden dimension, the "cryptosystem": a set of biophysical interactions and processes (an ecological system of energy and material flows) that are not directly perceived by the senses but which do create the landscape identity and architecture we perceive^{1,2}. Landscape transformation can make invisible elements appear and reveal describing features.

According to the basics of the energy systems theory, a comprehensive method with a significant scientific element has been developed. This method seeks to assess and appraise the dependence of natural and socio-economic processes upon the territory systems whilst including the notion of heritage. Based on this hypothesis, Spanish energyscapes are understood as a material organization arranging and regulating energy flows, and also as an energy arrangement that stabilizes and maintains material forms. That is, these structures are considered to be spatio-temporal manifestations of processes occurring in various scale domains³. These processes include fluxes of services, matter and energy, as well as interactions among companies and industries. Pattern and related processes are encapsulated in a cause-and-consequence relation, which is non-linear and, to certain degree, bi-directional. In other words, the observable pattern is often a product of spatially constrained processes (e.g. a mining deposit); on the contrary, prevailing structures influence process (e.g. a new transport infrastructure)⁴.

3. Results and Discussion

Research has identified and characterized the Spanish main areas which focused the transformation and processing of energy. Twenty-four regions that account 20% of Spanish territory and which contain 80% of the energy industry (in production parameters, including oil sector and electricity). Results included the evaluation of the spatial dimension of the national energy infrastructure through three groups of parameters: technological, political and cultural.

4. Conclusions and Future research

The notion of potentiality refers to the intrinsic ability of a place to become something different, to upgrade itself. Considering that any territory and land-use system can evolve in many ways, tracking potentialities becomes an innovative methodology intended to prevent social and ecological decay of the landscape, bypassing the ethical and aesthetical arguments raised by conservationism. From a spatial perspective, landscape planning of the energyscapes must respond to the adaptation to new situations in a perspective of instability or elasticity of landscape. The important tasks in landscape planning involve examining the cumulative spatial impacts and the effects of human intervention on processes and functions with the above mentioned consequences for their substance, matter and energy exchange. In other words, within an ecological context, we are referring to the resilience aspect of cultural landscapes. Comparing them with the present status will enable us to predict the question: How have land uses and landscape structure changed over historical time periods? How have these changes affected the system pattern?. And in this sense, "When does a heritage industrial landscape emerge? When does spatial imbalance exist? When does economic collapse occur? When new technologies are discovered, do the already existing ones automatically become obsolete?".

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Public action in social housing estates in Madrid, Paris, and Berlin. Identification, protection and intervention between 1979 and 2010

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Keywords: social housing estates, modern urban heritage, urban regeneration

1. Introduction

Since the late seventies social housing estates in Europe have joined the historic centres as main objects of public urban regeneration or renewal projects. However, while the preservation of architectural and urban heritage has become socially accepted in most interventions in the historical city, the transformation of social housing estates dating mostly from the second half of the twentieth century is often guided solely by economic and technical principles, which leads to a loss of the architectural, urban, technical and social values in many European social housing estates.

Social housing estates in Madrid show nevertheless a somehow different relationship between urban regeneration and heritage preservation policies.

2. Methodology

As a previous step to a possible preservation policy for social housing estates, this research aims to understand two main aspects. First of all, how social housing estates in Madrid have evolved and been transformed by public policies, and in which state of conservation they are now. Secondly, which are the main obstacles or conditions for their preservation, and how likely are they to be overcome.

The first goal results in an atlas of public interventions in social housing estates between 1979 and 2010, following and completing the thesis *Los Barrios de Promoción Oficial de Madrid*, published by professor Luis Moya in 1976, adding urban rehabilitation, renewal and regeneration to his study on the construction of social housing.

As for the obstacles or conditions regarding the social value given to existing social housing estates in a certain city, they can be divided between that coming from the municipal urban planning and protection system and tradition, and those particular to social housing. Regarding these last ones, Emmanuel Amougou¹ refers to the modernity of their architectural and urban conceptions and to their social status. To these two aspects, we should add their current state of physical or socio-economical decay. Four main obstacles are therefore considered: municipal role in heritage protection and urban regeneration; strength of the opposition between historical city centre and peripheral social housing estates; stigmatisation and perception of assistance and dependence in the social housing sector; and evolution of the concept of habitability and of the statistical methods for its territorialisation.

The particular configuration of these conditions in the city of Madrid can only be understood through adding to the atlas the study of the evolution of a estate that has been included both in protection and in urban regeneration programs, and its comparison with similar estates in other major European cities. For this study, the Poblado Dirigido de Caño Roto has been chosen, and it is compared with the estates of Les Courtilières in Paris, and Fennpfuhl in Berlin.

Both the atlas and the case study are based on the analysis of primary sources, including more than thirty individual and group interviews with urban regeneration managers and experts, as well as with current inhabitants. In the case study, testimonies have a crucial role, both those originally dating from the construction, evolution and regeneration of the estate, and those based on remembrance. The particular configuration of the obstacles in the comparison cases, Les Courtilières and Fennpfuhl, is extracted mainly from secondary sources, although a certain number of primary sources and individual interviews has been necessary in order to clarify or complete them.

3. Results and Discussion

The elaboration of the atlas of public interventions in social housing estates in Madrid has been completed to a large extent, includes information regarding all areas which have been the object of urban renewal or regeneration since the late seventies, and collects information regarding their construction, evolution and transformation by public policies, as well as their eventual protection. The analysis of the data compiled so far allows us to conclude the following:

- Regarding the current state of social housing estates, we have observed that there is a greater degree of transformation of the buildings than of public spaces and urban structure; the transformations occurred are mostly partial and reversible, with a limited number of demolished estates, most of them included in the *Operación de Barrios en Remodelación*, and the *Programa de Renovación de Barrios*; and that those estates included in the protection catalogue have not been treated in a significantly different way, which shows the insufficiency and inadequacy of existing protection tools.

- Regarding the municipal protection and urban regeneration tradition, we have noted that the first intervention projects were undertaken in the 1980's by the municipal and regional public housing institutions, setting a early example; the initial laws, programs and projects and actual realisations did not establish a distinction, neither methodological nor legal, between interventions in the historical city centre and in modern social housing estates; protection tools that could be applied to social housing estates were early developed and included in the Plan General de Ordenación Urbana de Madrid dating from 1997; technicians have had an important role in the maintenance of the municipal tradition, shown by the continuity of their professional activity and the singularity of the realisations in Madrid, which cannot be derived directly from the content of plans and programs; a later distinction between historical centre and modern estates originated with the establishment of a national public founding system for urban renewal and regeneration at the beginning of the 1990's influenced by international experiences coming mainly from France, United Kingdom and the United States.

- The opposition between historical city centre and modern peripheral estates seems to be in Madrid particularly weak. We have noted that there is no correspondence, neither temporal nor spatial, between great urban renewal projects in the centre of Madrid, developed mainly in residential areas at the end of the 20th century, and in industrial and residential areas in the seventies, and the construction of social housing estates in the outskirts of the city in the fifties and sixties.

- As to the stigmatisation of social housing, the predominance of ownership explains partially why social housing estates have mostly profited from the social promotion of their original inhabitants and their children, and not suffered pauperisation in such a degree as, for example, most social housing estates in Paris. Socioeconomic indexes have therefore remained mostly stable, or become slightly better, since their construction, compared to the district averages.

- Regarding habitability, and more particularly statistical territorialisation of physical and socio-economical decay, it has only been recently and limitedly adopted, based on foreign examples such as the French *Zones Urbaines Sensibles*, and vulnerability indexes and perimeters have not yet been used to determine or prioritize regeneration areas.

Due to the development of a research period in the *Institut d'Urbanisme de Paris* between the 12th of September and the 13th of December 2012, the study of Les Courtilières has been given preference to that of Caño Roto, and is now been completed by the analysis of the collected data.

4. Conclusions and Future research

The compilation of primary data and testimonies regarding Caño Roto, as well of mainly secondary data on Fennpfuhl will complete the necessary information for the analysis, and allow to verify and complete the hypothesis not only by the general data included in the atlas, but also through the study of the evolution of a particular estate, and its comparison with similar European examples.

The atlas, the case study of Caño Roto and its comparison with Les Courtilières and Fennpfuhl are expected to show the particularity of Madrid social housing estates, both regarding their current state of conservation and the conditions for their wider social appreciation, which make their recognition and protection as modern heritage particularly viable, in comparison with other

European examples, and recommend a continuity with the municipal tradition dating from the first democratic local governments.

Effects of conservation and restoration treatments on porous inorganic materials in archaeological sites. Case study: Mérida

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Abstract. The evaluation of past, and recent, restoration interventions is a crucial task when considering future preservation of cultural heritage. In the case of archaeological sites monitoring and assessment of the effectiveness of treatments are complex studies and often inexistent. In this sense this project explores the effects of different restoration treatments, in terms of efficacy, durability and alteration processes (when damage has been caused), on the archaeological city of Merida.

Keywords: conservation, treatments, stone, archaeology, Merida, restoration

1. Introduction

Research on the assessment of effectiveness and durability of restoration treatments on archaeological sites is an open field that needs to be explored, where the mid and long-term effects of these interventions are still poorly known [1]. The particular features of archaeological stone material preserved on site preclude the extrapolation of results from other disciplines such as sculpture or historic buildings, as well as outcomes from laboratory artificial aging tests, and deserve an exhaustive analysis of materials treated and preserved in its own environment. Some of these treatments have become an alteration source and there is no clearly information about degradation mechanisms and, consequently, possible solutions.

General goals:

- Review of restoration treatments applied to the archaeological heritage.
- Physic-chemical analysis to determine the effects of the interaction of restoration products on the original substrate.
- Validation, or dismiss, of treatments and establishment of standard operating protocols.
- Encourage monitoring measures of interventions throughout the use of portable field devices, and NDT of analysis.
- Analysis of compatibility between old and new treatments applied on same substrate.

The project is supported by two R&D groups:

- Analysis and Intervention in Architectural Heritage; AIPA (ETSAM, UPM)
- Applied Petrology for Heritage Conservation Research Group, Instituto de Geociencias (CSIC,UCM)

2. Methodology

Work is being developed in three phases:

1. Documentation and bibliographical research: conservation and restoration actions have been executed from the beginning of archaeological excavations in 1911 until today, showing an evolution of criteria a methodology of intervention. All these interventions have been registered, with special focus on the exact location, products and concentrations used, methodology of application and state of conservation previous to the treatment. All this information allowed us to select and limit our case studies and materials.
2. Field research: the study of the onsite state of conservation of archaeological sites selected (Roman Theater and House of Mitreo) is crucial in order to distinguish all

variables that affect the stone material. In this sense former restorations are one more alteration agent within the group of anthropic agents.

3. Characterization and analysis of materials: both in situ and in laboratory. The use of portable devices and NDT of analysis is one of the principles of these projects. The aim is to compare parameters such as color, permeability to water, internal cohesion, thermal changes, alterability related to natural agents and other changes derived from the application of restoration treatments, measuring values and comparing between treated and untreated areas. On the other hand, measuring interaction between the restorative product and the original substrate by applying the treatment on laboratory and monitoring evolution and changes derived. Some of the available techniques are: DRX, Raman Spectroscopy, NMR, Spectrophotometry, DRMS, Ultrasounds, SEM+EDS, IT, among others.

3. Results and Discussion

The initial examination regarding the state of conservation of selected archaeological sites allowed us to assess important alteration processes related to past interventions:

- Problems arising from use of synthetic resins: the exposition of these products to weathering, particularly to solar radiation, involves loss of mechanical and adhesive properties [2]. In this regard it has been documented the fall of fragments from ornamental marble elements in the front stage of the theater.
- Problems arising from the use of cement or concrete: different physico-chemical properties between cement and original stone [3] cause mechanical and chemical alteration, like cracking and salt efflorescence.
- The use of metal elements as a fixing system has caused bursting due to corrosion of a metal fixing, as well as rust stains.

Regarding recent measurements carried out onsite we can verify different values comparing treated and untreated areas with techniques such as ultrasound (which indicates different degrees of internal cohesion) or spectrophotometer (which indicates color and brightness changes), as well as changes in superficial texture with the roughnessmeter [4].

4. Conclusions and Future research

It is necessary to get deeper knowledge about the long-term effects of conservation treatments, especially in archaeological sites, because on one hand this is a task traditionally neglected, on the other taking into account its particular conservation features, in extreme weathering conditions.

Results from this study will allow high guarantees of preservation and real knowledge about pathology and deterioration processes in Mérida's sites. In this sense it will also permit the design of realistic and pragmatic preventive conservation measurements.

Experimental research with nanoconsolidants has been considered within this project in order to include, not only past treatments, but also future possibilities for archaeological stone material.

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Participatory processes for valuing cultural landscapes in rural areas

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Abstract. Is landscape interpretation necessarily partial and subjective? We claim it is, and it depends on who is looking at the landscape. People's perceptions, preferences or understandings are tightly related to the different elements in the landscape which are sources of knowledge, and thus, shape the people's memories. We will focus on specific cultural elements such as public works, which make an enormous contribution to shaping the territory and generating landscape [1] in order to look for pathways to enhance local awareness in rural landscapes. Discursive and analytical approaches have been combined to carry out the participatory process of action research. People ought to be the central core of any attempt to value our landscapes, as people act as agents to model their surrounding landscape [2].

Keywords: landscape, cultural heritage, participatory processes, rural areas

1. Introduction and Objectives

The European Landscape Convention (ELC) provides the appropriate scope to understand landscape as a place where society was, is, and, will be. The ELC recognized this dimension defining landscape as "an area, as perceived by people, whose character is the result of the action and interaction of natural and/or human factors" [3]. This landscape policy framework reinforces the need to maintain and value the rich diversity in the relationship between nature and society associated with heritage, identity and values, building on an approach emphasized two decades earlier [4]. However, people observe the landscape from a point of view, with a collective memory, a past, which acts to characterize what we are looking at. In this communication, we address the soft equilibrium among cultural landscapes, uses, and protection within society to enhance the social appreciation over the cultural heritage in rural areas. Participatory processes in rural land planning [5] are discussed in order to implement mechanisms for knowledge transfer of cultural heritage as well as building social capital in rural areas.

Rural areas have a rich, diverse and scattered cultural heritage that remains largely unacknowledged. Two *comarcas* from Cantabria and Caceres were the regions chosen to study. Specifically, we have been looking at public works, as one of the cultural elements which shape territory. Public works (roads, dams, reservoirs, channels, bridges, mills, railways) are developed under the basis of social demand and benefit. However, the landscape that emerges following a civil engineering project has been little considered and poorly regarded [6].

2. Methodological Approach

The combination of quantitative and qualitative analysis as part of an iterative and adaptive design and validation process (See Figure 1) has achieved a successful involvement of stakeholders to enhance value of cultural heritage in rural areas. This perspective of collaborative land planning with local communities applies Participatory Action Research (PAR) techniques [7] enabling the research team to develop trust networks among them and local population to better understand social context and, as a consequence, develop actions to value the cultural elements through consensus. Preliminary phases of identification and characterization of public works in both regions were followed initially by mapping of stakeholders. Interviews and dialogues were held to acquire robust information about different perceptions and interpretations. Validation of quantitative information was carried out in situ with

groups of stakeholders. SWOT analysis allowed weaknesses to be defined and so, future strategies to enhance cultural heritage in the regions. Focus groups and workshops were established to encourage and lead action plans from the bottom level of the decision-making process.

3. Results and Discussion

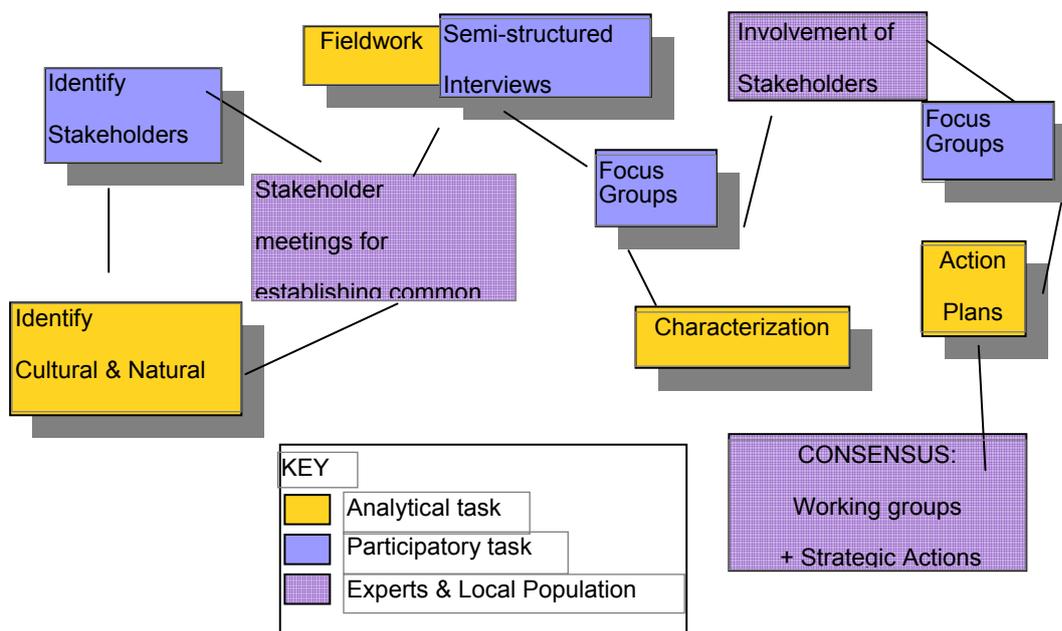
Public works in rural areas have always been valued on the basis of their use (water supply, irrigation channels, communication, etc). Once the purely functional character disappears, they are usually forgotten and isolated. This cultural heritage often appeared sparsely distributed in the territory. Some elements have passed into private ownership, thus losing their public character which may generate several problems in the process of valuing this cultural heritage for the insider and outsider population. However, these facts could be considered as opportunities under this participatory process, in which society from rural communities would play a role enhancing their own cultural values. We have shown that geographical location or local political agreements are not the only criteria in deciding what to value regarding cultural heritage, but also local knowledge could have a relevant role.

4. Conclusions and Future pathways for research

Perception of the territory comes from the social network which builds and maintains the landscape as a whole socio-ecosystem. "Transhumance cattle used to cross these bridges every season. They travel from Caceres to higher pasture lands in the North of Spain". These old recollections from a peasant bring interpretations linked to background and place in society. Innovative developments of action research to involve stakeholders in landscape interpretation would increase the level of knowledge and public awareness about their cultural heritage in rural areas.

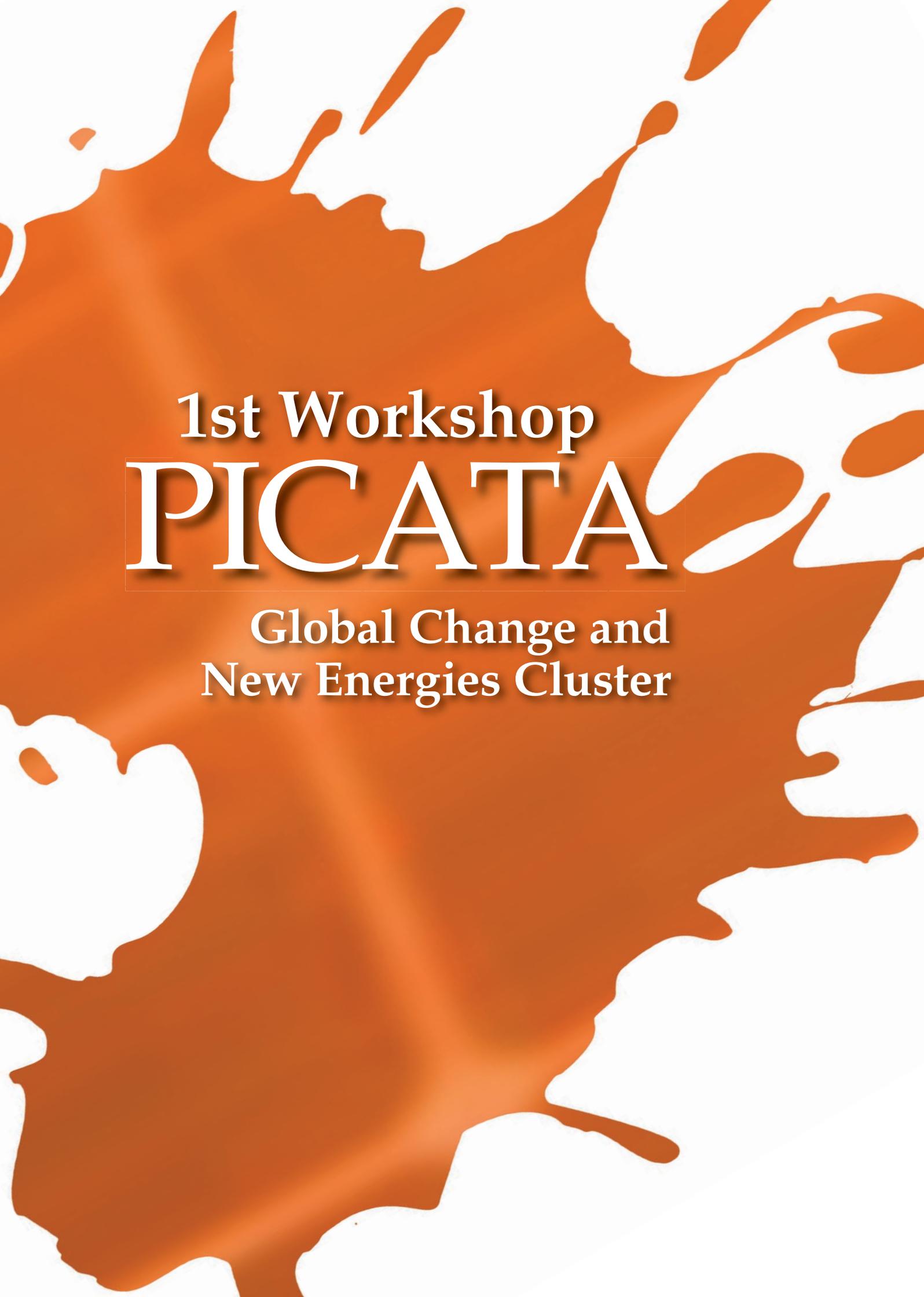
Figures

Figure 1. Methodological approach: an integrative perspective for participatory land planning



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1st Workshop
PICATA

Global Change and
New Energies Cluster

“The power of diversity” is the *motto* of the Moncloa Campus of Excellence Project. We believe that the presentations we had during the PICATA workshop from the Global Change and New Energies Cluster certainly show proof of diversity, and of its power. Pluridisciplinary and interdisciplinary approaches make it possible translational research in every area, and also in this cluster. The combination of basic knowledge with applied goals has been conspicuous in the PICATA presentations. Most of the collaborative projects shown blossomed thanks to the CIE Moncloa Campus, and some of the projects outstand because of its originality.

Thus, for instance, we have the study of links between weather and crops, perfectly suited to a mixed team of researchers displaying both agronomic and meteorology expertise. In the presentation of Miriam Cappa we realized that there may strong correlation among large scale climatic phenomena, like El Niño, and crop yields at far distances as in Spain. While the direct relation with the potential to predict near future crop yields is already interesting, the inverse use of this relationship, that is, trying to infer on El Niño status when direct data is not available but historical crop records exist, it is at least intriguing. Sustainability of large computation centers, of foreseen growing importance, size and number, was dealt in a very original way, as explained by Marina Zapater, just via optimized policies for computing job assignments taking into account power consumption of each computer task. Also in the sustainability battlefield, helping to develop more energy-efficient building techniques thanks to a better understanding of the thermal properties of glass walls in buildings, the collaboration of physicist and architects was exemplified by Juan Miguel Lirola project.

With regard to New Energies, we witnessed Ovidio Peña-Rodríguez quest for revolutionary materials that can help sustaining the radiation damage experienced by nuclear fusion containers. He is coordinating the efforts of teams at UCM developing plasmonic nanostructures, and the ones of expert nuclear fusion engineers at UPM in testing how these materials react when bombarded by nuclear radiation that will be found in nuclear fusion reactors. Again, a pristine example of the kind of collaborative research the Moncloa Campus longs to foster.

We hope you will find the Global Change and New Energies contributions to the PICATA workshop as inspiring and as we felt them after watching the energetic presentations made by the young PICATA researchers. Their enthusiasm was an example for all of us as it helped us to cope with the difficult times for research we are experience and to believe in a better tomorrow for research.

José Manuel Udías Moinelo

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Development of new efficient materials for carbon capture technology

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Keywords: carbon capture, supercritical CO₂, SBA-15, surface modification

1. Introduction

The capture and storage of carbon dioxide (CCS) is one of the most important options for reducing the CO₂ emissions to atmosphere and preventing climate change. There are three main steps in the CCS process: capture (separation plus compression), transport, and storage. One of the main approaches to capturing the CO₂ generated from the fossil fuel combustion is the adsorption using solid sorbents. [1] A wide variety of sorbents can be used for CO₂ capture such as zeolites, active carbon, metal-organic frameworks etc. Each class has its own advantages and disadvantages. [2] Therefore, it is necessary to continue the development of more efficient new materials.

Supercritical fluids (SCFs) have been attracting much attention in the synthesis of materials. SCFs show properties intermediate between those of liquids and gases. They have transport properties close to gases: low viscosity, high diffusivity and zero surface tension but their solvating power is similar to that of the liquids. The synthesis of materials in SCFs overcomes some of the limitations of liquid phase techniques, being a faster method of synthesis as well as resulting in materials of unique properties. [3] Moreover, supercritical carbon dioxide (scCO₂) is considered to be a green solvent because it is non-toxic, non-flammable, inexpensive, naturally abundant and relatively inert.

The aim of this work is to modify the surface of mesoporous materials with amine-organosilane precursors, which capture CO₂ via chemical adsorption, using supercritical CO₂ (scCO₂) as a solvent in order to improve the selectivity to CO₂ adsorption. In particular, we have carried out for the first time the surface modification of mesoporous silica SBA-15 with (N,N-Dimethylaminopropyl)trimethoxysilane (DMAPTS) in scCO₂. The effects of the reaction conditions (pressure, temperature and time) on the surface modification have been studied.

2. Methodology

An important factor in the surface modification of materials in SFCs is that the precursor, in this case DMAPTS, has to be soluble at a certain pressure and temperature in the SFCs. The solubility measurements were carried out using a high-pressure variable volume view cell [4].

After phase equilibria measurements, the mesoporous silica SBA_15 was synthesized using the method reported by Zhao et al. [5] Sol-gel chemical reaction was used for the surface modifications of SBA-15 and the conditions for surface modification were optimized. The experiments were performed in high pressure batch reactors between 40 and 50 °C and 100 and 200 bar. The reactor was loaded with the mesoporous SiO₂ SBA-15 and DMAPTS. After that, the reactor was placed into a thermostatic bath and filled with scCO₂ using a high-pressure syringe pump at the reaction temperature up to a given pressure. At the end of the reaction, the reactor was depressurized using a needle valve and the sample was recovered. Finally, the materials prepared in scCO₂ were compared with SBA-15 functionalized with the DMAPTS following a conventional method using toluene as solvent. [6]

Materials were characterized using standard analytical techniques such as X-ray diffraction data (XRD), IR spectroscopy, N₂ adsorption experiments, differential thermal analysis (TGA/DTA,TRP) and elemental analysis.

3. Results and Discussion

The phase behavior of DMAPTS and CO₂ was measured at 40, 50 and 60°C in the 80.0-120 bar pressure range. Analysis of the phase equilibria measurements reveals that the DMAPTS is quite soluble in scCO₂ and its solubility increases as the temperature decrease or the pressure increase. For example, the solubility at 40°C and 85 bar is about 1.5 % DMAPTS in CO₂.

The presence of the organosilane coating in the prepared samples was confirmed by FTIR. Characteristic bands of the organic molecule appear in the 2820 - 2940 cm⁻¹ range and are assigned to the C-H stretching vibration of the organic part of the molecule.

The thermal behavior of the silane treated samples as well as the amount of impregnated silane was studied by TGA (Figure 1). The main weight loss appears between 325 and 650°C. This is mainly due to the thermal decomposition of strongly bounded species (highly crossed-linked and/or chemisorbed silanes) by breaking of C-C and Si-C bonds [6]. The effects of pressure and temperature on the amount of DMAPTS loaded into the samples were very weak. As can be seen in the figure, the amount of DMAPTS covalently attached in the supercritical method increases with time. The supercritical method for surface modification was more efficient than the conventional method in toluene.

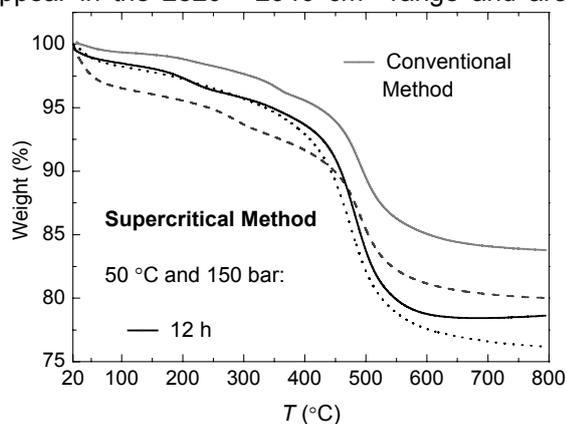


Figure 1. TGA curves of surface modified SiO₂ SBA-15 with DMAPTS.

The CO₂ adsorption capacity of the modified SBA-15 is governed by formation of carbamates with the tertiary amine of the DMAPTS. The nitrogen amount loaded on SBA-15 using scCO₂ was found to be higher than that obtained in toluene [6] due to the better transport properties of scCO₂. On the other hand, the CO₂ adsorption capacity in the modified SBA-15 in scCO₂ was around 0.4 mmol g⁻¹ sample at 25-60°C. Similar values for CO₂ adsorption capacity have been obtained by other authors using other tertiary amines. [6,2]

4. Conclusions and Future research

The surface modification of SBA-15 with DMAPTS has been carried out for the first time in scCO₂. The amount of DMAPTS loaded can be tuned with the reaction time. In comparison to the conventional process using liquid organic solvents, the surface modification of mesoporous materials in scCO₂ is faster and yields larger loads of DMAPTS. Further experiments to control the degree of surface coverage by DMAPTS in scCO₂ are currently in progress in our group.

In the future, the amino group will be attached to other mesoporous materials such carbon, Al₂O₃, graphene or renewable materials source. In order to increase the CO₂ adsorption capacity, other amine-organo silane precursors which contain primary and secondary amines will be used.

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New generation nano-structured membranes for solar-driven micro/ultra filtration systems

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Keywords: electrospinning, nano-structured membranes, micro/ultra filtration, interfacial polymerization, fouling

1. Introduction and Contents

The main objective of the proposed research study is the preparation and characterization of novel nano-structured polymeric membranes for different separation processes (microfiltration, MF and ultrafiltration, UF) and their subsequent applications in solar systems for the treatment of contaminated waters.

2. Materials and Methods

Polysulfone (PSU) nano-fibrous membranes were prepared by electro-spinning using the solvent mixture (tetrahydrofuran, THF and NN-dimethylformamide, DMF). Electro-spinning technique consists on the application of a high voltage, in the range of kilovolts, to form charges of a certain polarity in a polymer solution, which are then accelerated towards a metallic collector of opposite polarity. In this technique, a polymer solution held by its surface tension at the edge of a metallic needle is subjected to an electric field that is induced between the needle and the collector. When the applied electric field reaches a critical value, repulsive electrical forces overcome the surface tension forces and a Taylor cone is formed. A charged jet of the polymer solution is ejected from the tip of the Taylor cone and an unstable and rapid whipping of the jet occurs through the distance between the needle tip and the collector. Finally, the nano-fibers are randomly deposited over the collector [1].

In this study the effects of different involved electro-spinning parameters (voltage, polymer solution flow rate and distance between the needle and the collector) on the final structure of the PSU electro-spun membranes have been investigated and the optimum parameters were identified. The effects of post-heat treatment on the integrability and structural morphology of the nano-fibrous membranes were also studied.

The prepared nano-fibrous membranes were characterized by means of different techniques such as scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and contact angle measurements. Permeation tests of the PSU nano-fibrous membranes were carried out first with distilled water as feed under different transmembrane pressures and then with humic acid (HA) feed aqueous solutions (15 mg/L of HA at different pH values: 3 and 11). Turbidity measurements of both the feed and permeate solutions were carried out to determine the separation factor of the PSU nano-fibrous membranes. Permeate fluxes of both HA solution and distilled water before and after each HA test were measured and the irreversible membrane fouling factor was evaluated [2].

The surface of the PSU nano-fibrous membranes was modified to improve their filtration performance and decrease the irreversible fouling effect. Interfacial polymerization (IP) technique was applied in this case to form a polyester layer over the PSU nano-fibrous membranes [3].

3. Results and Discussion

The obtained optimum conditions for the polymer solution (20% w/v PSU, 64% w/v DMF and 16% w/v THF) are: 2.5 mL/h polymer solution flow rate (F), 16 kV voltage (V), 10 cm distance between the needle and the collector (G), 45 min electro-spinning time and 220°C post-treatment temperature.

Permeation results of the nano-structured membranes were compared to those of the commercial membrane (0,22 μm GVHP, Millipore). These preliminary results indicated that the PSU nano-fibrous membranes can be used in microfiltration (MF) process.

It was observed that the post-heat treatment favored the connections between nano-fibers with a more compact network (see Figure 1 (A) and (B)). Moreover, the interfiber space decreased after the post-heat treatment without altering the hydrophobicity of the nano-fibrous membranes (i.e. water contact angles above 120°). Furthermore, with the increase of the post-heat treatment time maintaining the same temperature, the permeate flux of the PSU membrane decreased while the HA separation factor increased.

It was found that filtration should be performed at pH 11 in order to improve the HA separation factor and decrease the irreversible fouling of the PSU nano-fibrous membranes.

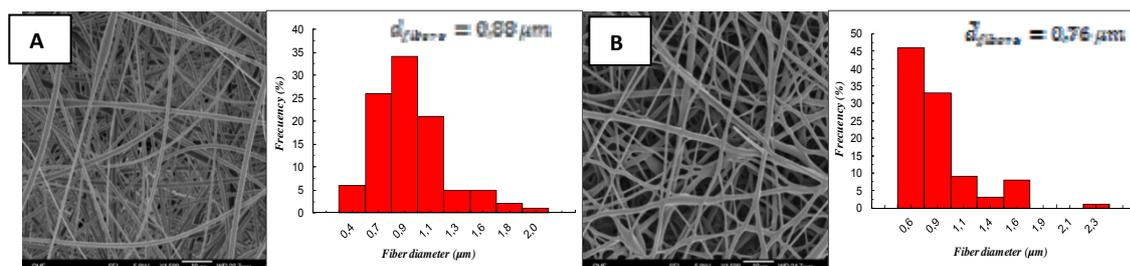


Figure 1: SEM images of a nano-fibrous membrane ($V = 18 \text{ kV}$, $F = 1.5 \text{ mL / h}$, $G = 15 \text{ cm}$): A) without post-treatment, B) with post-treatment and their respective nano-fiber diameter distribution.

The polyester layer formed on the nano-fibrous membrane surface (Figure 2) is hydrophilic (i.e. water contact angles less than 90°). The permeate flux of the composite PSU nano-fibrous membranes increased while the irreversible fouling factor was reduced.

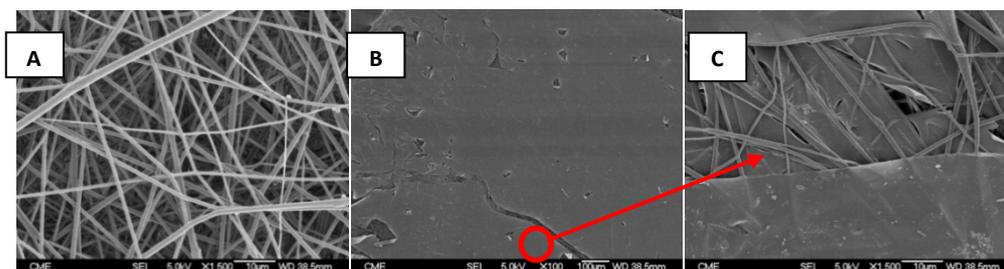


Figure 2: SEM images of unmodified (A) and modified nano-fibrous membrane (B, C) by interfacial polymerization at different magnifications, $\times 100$ and $\times 1500$, respectively.

4. Conclusions and Future research

Some of the main conclusions of the present study are:

- PSU nano-structure membranes prepared using the polymer solution (20%PSU+64%DMF+16%THF) exhibit an inter-fiber space smaller than the pore size of the commercial membrane GVHP (0.22 μm).
- The application of a post-heat treatment resulted in a better connection between nano-fibers and a small inter-fiber space of the PSU nano-fibrous membranes.
- The modified PSU nano-fibrous membranes by interfacial polymerization are more hydrophilic than the un-modified ones due to the thin polyester layer formed on its surface.
- The irreversible fouling factor was reduced while the permeate flux was increased after modification of the PSU nano-fibrous membranes.

Some of the future objectives proposed in this research are:

- Fabrication of mixed matrix nano-fibrous membranes using different nano-charges such as titanium dioxide (TiO_2) in order to reduce fouling phenomena and improve membrane performance.
- Develop a theoretical model based on response surface methodology (RSM) in order to determine the optimum heat-treatment method.
- Coupling the filtration systems with optimal designed photovoltaic panels (PV).

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Intermediate band materials for a new generation of solar cells

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Keywords: solar cell, intermediate band materials, ion implantation, pulsed laser melting

1. Introduction and Contents

Our current energy model based on the massive consumption of fossil fuels has proved once and again to be incompatible with a sustainable development of our society. The scientific community is devoting a tremendous effort in the development of new energetic alternatives based on renewable energy sources. Specifically in the field of photovoltaic solar energy a new concept called intermediate band (IB) solar cell was proposed in 1997 to overcome the theoretical limits of solar energy conversion [1]. Based on this concept, the main objectives of this work are to obtain new IB materials based on silicon and to integrate it on heterojunction with intrinsic thin layer (HIT) solar cells [2].

2. Methodology

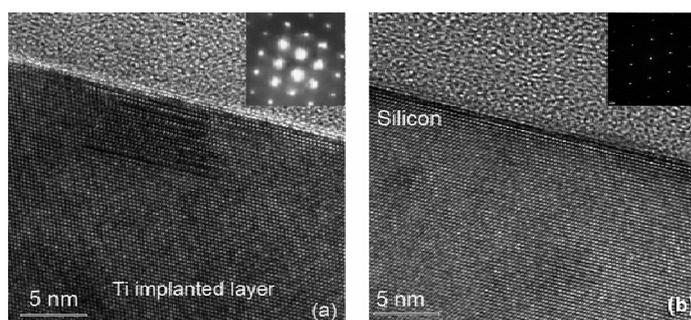
Samples 1x1 cm² in size of n-type Si (111) with a thickness of 300 μm ($\rho \approx 200 \Omega \text{cm}$; $\mu \approx 1500 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$; $n \approx 2 \times 10^{13} \text{ cm}^{-3}$ at RT) were implanted with Titanium (Ti) and Vanadium (V) in a refurbished VARIAN CF3000 Ion Implanter. Different implantation dose in the range of 10^{13} - 10^{16} cm^{-2} and energies in the range of 35-150 keV were used. After implantation, all the samples were pulsed laser melted (PLM) with one 20 ns long pulse at an energy density in the range of 0.6-1.8 J/cm². The system was a KrF excimer laser (248 nm) at IPG Photonics (New Hampshire, USA).

Cross sectional transmission electron microscopy (TEM) images were obtained by a JEOL JEM-2000FX working at 200 keV at C.A.I. de Microscopía (Madrid, Spain). Simultaneously with the TEM measurements, electron diffraction (ED) patterns with a selected area of diffraction of about 50 nm were obtained.

Photoconductivity measurements were carried out with a set up formed by a TMc300 Bentham monochromator (halogen lamp source) and a SR830 digital signal processing lock-in amplifier manufactured by Stanford Research Systems (California).

3. Results and Discussion

Regarding the structural characterizations, Fig. 1 shows a high resolution TEM images of the Ti implanted sample (a) and of a silicon reference substrate (b). We can observe in Fig. 1a that we have obtained an almost perfect crystalline structure after the PLM process, and only some stacking faults defects are observed. No differences are observed if we compare the ED pattern of the silicon reference sample with the corresponding to the Ti implanted layer, concluding that we have obtained a Ti supersaturated Si layer with a single crystalline structure.



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Figure 1 Transmission electron microscopy and electron diffraction pattern of a Ti implanted and PLM processed sample (a) and a silicon reference sample (b).

measurements for a set of Ti and V implanted samples with different implantation doses and PLM energy densities. Also an unimplanted reference Si sample is measured for comparative purposes.

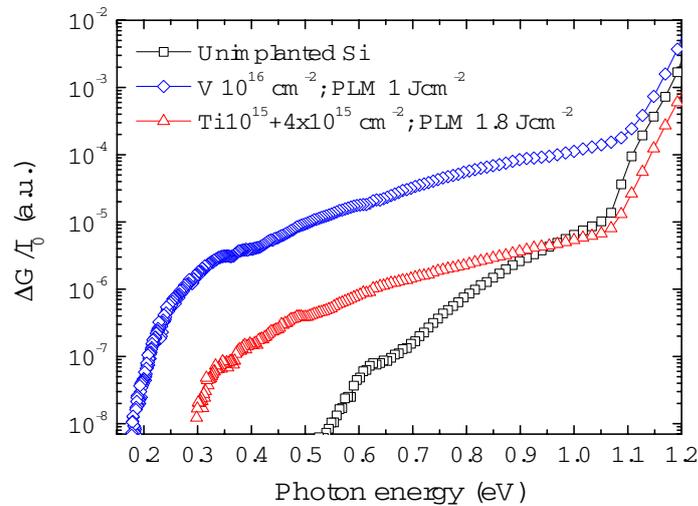


Figure 2 Variation the spectral photo-response normalized to the impinging light power as a function of the incident photon energy for the Si unimplanted reference sample, and for the V and Ti implanted samples at different doses and PLM process. Measurements were carried out at 90 K.

We can observe a remarkable increase of the photoconductivity for the Ti and V implanted samples over the unimplanted Si. An abrupt photoconductivity front is observed at different energy position as a function of the implanted element. These features are related with an increase of the photogenerated carriers lifetime which is an experimental proof of the formation of an IB material based on Si supersaturated with Ti or V.

4. Conclusions and Future research

In this work we have shown a structural and optoelectronic characterization of Si samples supersaturated with Ti and V. These results suggest the formation of an IB material with a single crystalline structure which will be positives features in order to implement this new material in a solar cell [3].

Future works are in progress. We are exploring three different impurities that are well known to form deep levels in silicon: vanadium, zirconium and chromium. We have fabricated the new materials and the characterization has begun in the Universidad Complutense de Madrid under the supervision of Professor I. Mártil. Parallel with the experimental studies, a fundamental theoretical study of these new elements is performed in the Universidad Politécnica de Madrid under the supervision of Professor P. Wahnón. We expect that our efforts will give us a complete understanding of the physical process that describe these new materials and allow us to engineer a new high efficient generation of solar cells.

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Plasmonic nanoparticles for the protection of the final optics in inertial-confinement fusion facilities

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Abstract. In this project we are exploring the feasibility of using plasmonic nanoparticles (NPs) for the protection of final lenses in inertial fusion facilities. During the past year we have deposited silver NPs by means of femtosecond laser pulses, attaining NPs with sizes around 50 nm and a narrow size distribution. Simultaneously, we have studied the deformation kinetics of silver NPs embedded in silica during the irradiation with swift heavy ions. Several experiments are planned for the remaining year, aiming to achieve significant progresses in both, the synthesis of metallic NPs and the study of their geometrical variations during irradiation.

Keywords: inertial fusion, final lenses, plasmonic nanoparticles, fano resonances

1. Introduction

Inertial-confinement fusion facilities (ICFF) are very promising for the development of new energy sources but some elements need to be improved to fulfill specifications. One of them is the final optics assemblies (FOA) and, particularly, the final lenses, which are exposed to intense radiation pulses. There are currently no materials capable to withstand ICFF's harsh conditions for a reasonable chamber size [1]; hence, the development of new materials is a very important topic. Any suitable material should have (i) a very high transparency to the laser's third harmonic (351 nm) and (ii) a high resistance to the radiation. Absorbing the remaining of the laser's first (1053 nm) and second (526.5 nm) harmonics is desirable, as well. Nanostructured materials (NSM) can be a good choice for this task because they behave as self-healing materials [2]. This property arises because the mean free path of the vacancies on NSM is greater than the size of the (nano) grains, which leads to effective annihilation of vacancies at grain boundaries and produces a high resistance to the radiation-induced damage. Plasmonic nanostructures have some specific added advantages. Firstly, they can absorb some energy from the incoming ions and release it to the embedding medium in larger times (reducing somewhat the thermal spike). Moreover, their optical properties, dominated by the Surface Plasmon Resonance (SPR), can be tailored to exhibit a very low optical density at 351 nm while, at the same time, absorbing strongly the first and second harmonics, simply by varying the NP's geometrical parameters. The goal of this work is to study the suitability of plasmonic NPs for protecting final lenses, focusing on their controlled synthesis and the effects of the ion irradiation on their optical and structural properties.

2. Methodology

Plasmonic NPs used in this work were deposited on Si (111) and silica substrates, using femtosecond Pulsed Laser Deposition (fs PLD) The experimental setup consists of a stainless steel chamber operating at 2×10^{-4} Pa. Silver targets (provided by Heraeus) were placed on a rotating sample holder to avoid crater formation by repetitive laser irradiation. Pulses of 45 fs were produced by a Ti:Sapphire amplified laser system (Spectra Physics) centered at 800 nm and operating at a repetition rate of 1 kHz.

In a parallel experiment, a different set of silica samples containing embedded silver nanoparticles were irradiated in a 5 MV tandem accelerator with Br^{5+} ions at 30 MeV. Optical absorption spectra were measured in real time using a compact spectrometer QE6500 (Ocean Optics Inc.) configured with a multichannel array detector for measuring simultaneously the whole spectrum in the range 200-850 nm. The final goal is to irradiate the NPs prepared by PLD but this preparatory experiment was used to test the experimental setup developed for the measurement and to study the deformation process.

3. Results and Discussion

Exploratory deposits of silver NPs were done using fs PLD; these NPs were then characterized by means of optical absorption and scanning electron microscopy (SEM). As it can be seen, the obtained NPs exhibit an intense SPR (Fig. 1) and have diameters around 50 nm and a narrow size distribution (Fig. 2). Thus, in principle, they are suitable for the intended applications.

Now, we are conducting a detailed study for determining the dependence of the NPs' properties as a function of the deposition parameters (e.g., laser power, target-substrate distance, etc.) Moreover, we have developed an experimental setup for measuring in-situ (i.e., during the deposition) the reflectance of the layer containing the NPs. These measurements reveal detailed information about the deposition kinetics.

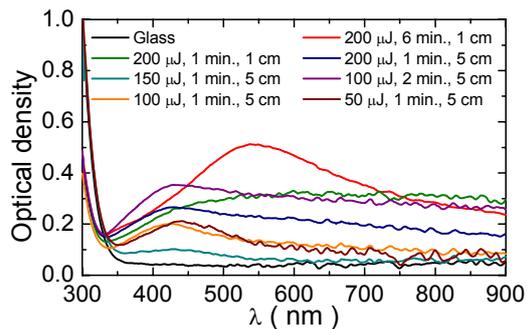


Fig. 1: Optical absorption spectra for some samples with silver NPs deposited on glass using fs PLD.

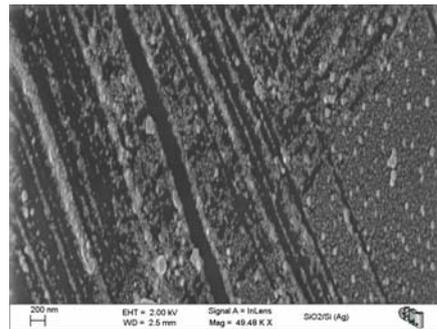
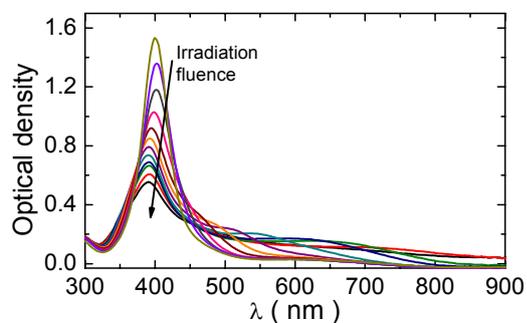


Fig. 2: SEM images obtained for a sample with silver NPs deposited on Si (111).

Simultaneously, we studied the effects of swift heavy ions (SHI) on silver NPs embedded in silica. It is well known that metal nanoparticles are deformed when irradiated with SHI, but there is little information on the deformation kinetics. We used a home-made optical setup to measure in real time the optical (i.e., plasmonic) response of metallic NPs during irradiation. Then, we calculated the aspect ratio of the deformed NPs as a function of the irradiation fluence, taking advantage of the strong dependence of the optical response on the NP's geometry. This gave us an unprecedented level of information about the deformation process. Some selected spectra from a typical sample are shown in Fig. 3 to illustrate these variations.



the strong dependence of the optical response on the NP's geometry. This gave us an unprecedented level of information about the deformation process. Some selected spectra from a typical sample are shown in Fig. 3 to illustrate these variations.

Fig. 3: Some representative optical absorption spectra, illustrating the evolution of the optical response (i.e., the NPs' geometry) as a function of the irradiation fluence.

Finally, we have explored two additional topics that might be interesting for this project. First, we have performed a theoretical study about plasmonic Fano resonances (FRs) in multilayered metal structures [3]. Plasmonic FRs [4] can be used to enhance the transparency in selected spectral regions. We have also collaborated in a work on the modification of the optical properties of silica (the final lens' material and the embedding media for our NPs) under irradiation with SHI [5].

4. Conclusions and Future research

The development of this PICATA project is proceeding as planned. So far we have made important advances on the synthesis and study of plasmonic NPs for applications in ICFF. Namely, we have (i) successfully deposited silver NPs by means of femtosecond laser pulses, attaining good sizes and concentrations and (ii) studied the deformation kinetics of silver NPs embedded in silica during the irradiation with swift heavy ions. We will not likely solve the problem in the remaining year of the project, but we aim to achieve significant progresses in both, the synthesis of metallic NPs and the study of their modifications during irradiation.

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Simulation of thermal performance of glazing in architecture using scale models

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Abstract. The research and applicability of energy efficiency in buildings, and especially in almost zero-energy buildings, is one of the current priorities of sustainability. Compared to others, research in energy by undistorted glazed scale models of real prototype buildings exhibits the advantage that, in them, it is possible the exposition of the model to climate conditions for collecting direct data. Furthermore, the construction of models leads also to costs reduction. This research is developed both experimentally and analytically. The experimental research has been carried out by means of comparison between real and reduced scale models while the analytical research has been conducted by simulations based on mathematical-physics theories. The applicability of the conclusions is expected to improve energy consumption in buildings by strategic modifications done in virtual and scale models.

Keywords: energy efficiency, thermal transport, scale model, reduced model

1. Introduction

The research by scale models provides valuable data over their correspondent real building prototypes. Mainly the use of scale models in research is based in manipulation of the scale model for finding a specific search value [1]. These proceedings cause grave distortions in its form and in its thermal conditions, so that the scale model under these circumstances is, in most cases, doubtfully a scaled architectural space. Our main aim is to develop a methodology for testing scale models, avoiding form or temperature distortions, at weather conditions in order to predict its correspondent prototype temperature.

2. Methodology

The research of scale models is based on the following parts:

- Testing basic models at different scales [2] under climate conditions. (Fig.1)
- Undistorted scale models of experimental buildings pretending to be tested (Fig.2)
- Data collection of real prototypes [3] to be compared to building scale models (Fig. 3)



Fig. 1



Fig. 2



Fig. 3

- Laboratory tests [4] (with thermography control (Fig. 4 -5))



Fig. 4

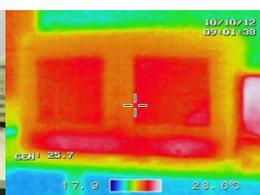


Fig. 5

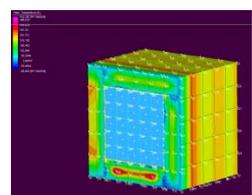


Fig. 6

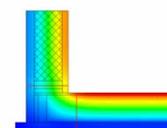


Fig. 7

- Analytical development: The analysis by means known mathematicians and physicists theories.
 - Comparison of results with computer simulations (Energy+, Strauss and ZUB-Argos) (Fig. 6-7)
- Other part of the research is the elaboration of patents in renewable energy field in order to reach the almost zero-energy cell [5]

3. Results and Discussion

The results collected by experimentation between undistorted models at different scales in climate conditions present relatively different temperature behavior between them.

The first experiments were conducted with simple cubic space models for predicting temperature of the correspondent scaled-up boxes. The following graphics 8 and 9 show two approximations, one by simulation and the other by undistorted scale model of a 60 cm box.

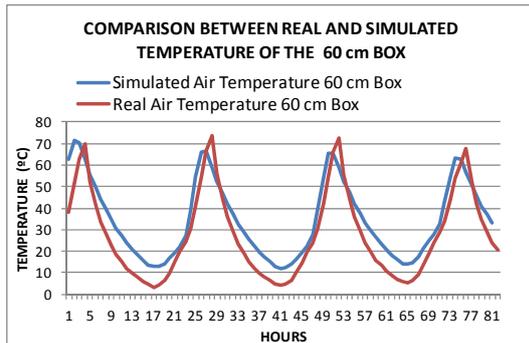


Fig. 8

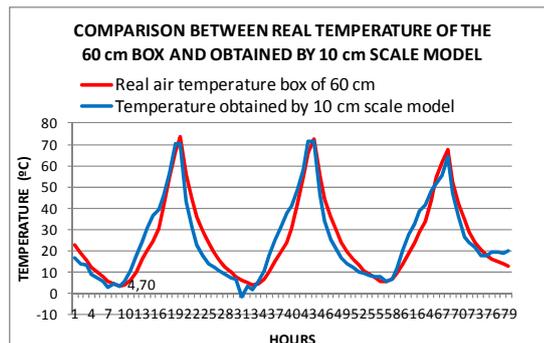


Fig. 9

4. Conclusions and Future research

Through experimentation conducted so far, we can say that the use of scale models for predicting temperature's prototypes provides more specialized and concrete data based on real behavior model compared with correspondent simulation with real weather data file.

Theoretical analyzes performed so far, and not yet definitive, permit to affirm that depending on the methodology of analysis to be performed some specific limits are recognizable when comparing reduced models and their respective prototype.

The short-term future development of this research involves both the extension of the findings with simple models to more complex forms of space and comparison of a reduced model with an existing building fully constructed and operational.

The long-term development will be the temperature's forecast of a real prototype.

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Proactive and reactive thermal optimization techniques to improve energy efficiency in data centers

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Keywords: energy efficiency, data centers, green computing

1. Introduction

Reducing the energy consumption of data centers is nowadays a critical objective because of its dramatic environmental and economic impact. By 2000 data centers used 0.53% of the world's total electricity consumption. By 2010, data centers consumed approximately 235.5 BkWh, representing 1.3% of worldwide electricity used [1].

Today's data centers need to take into account many different aspects at the same time in order to minimize the total energy consumption [2]. Energy consumption and peak power need to be decreased to avoid power outages.

Our work proposes mechanisms of reactive and proactive optimization to leverage energy efficiency at data centers, placing them on a more scalable and sustainable energy-efficiency curve.

2. Methodology and Methods

Our research focuses on optimizing the energy consumption at the data center from a holistic approach, taking into account the thermal state of the data center, workload energy requirements, thermal and energy characteristics of the cooling and computing resources and recent execution history.

We profile the workload executed in the data center, and then use that knowledge to anticipate the energy requirements and develop proactive strategies. Profiling is performed by taking data from the server sensors (CPU temperature, power, fan speed, active cores), performance counters and from a wireless sensor network deployed in the data center that gathers environmental data (air room temperature and humidity and differential pressure in the raised floor). We also take advantage of the heterogeneity in the IT resources, which is typical in most data centers, to execute the workload in the nodes where they perform better in terms of energy efficiency.

Traditional data centers use resource management software for the efficient and effective deployment of workload among the computational nodes in a spatio-temporal way. Our work broadens the scope of resource management techniques by applying our methodologies and algorithms in a real resource manager (SLURM) so that our solutions can be tested in a real environment.

3. Results and Discussion

At the resource management level, our research has shown that usage of heterogeneity to execute a particular workload can yield up to 30% energy savings [3]. These results are based on the fact that different workloads perform differently in terms of power consumption depending on the machine where they are allocated (see Figure 1). By using the information provided by the workload profiling tools we can predict the dynamic power consumption of servers and apply proactive resource management policies based on MILP optimizations, genetic algorithms and other techniques.

Resource management techniques can be extended from the data center framework to globally distributed computation frameworks. We have developed extensions of our data center algorithms to minimize the overall energy consumption in sensor deployments for Smart Cities [4] as well as in new computational paradigms of distributed computation [5].

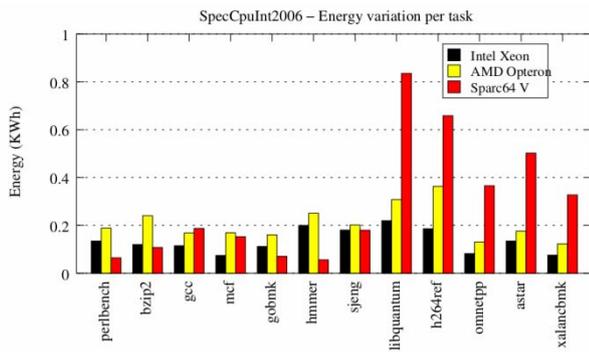


Fig. 1. Variation on energy consumption of SPEC CPU2006 benchmark

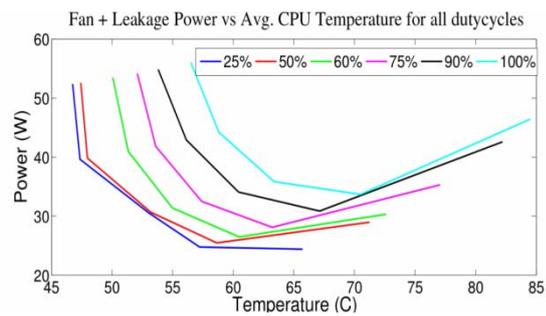


Fig. 2. Leakage-cooling tradeoff at the server level for different CPU utilization

Recent work also shows that as technology shrieks, leakage plays an important role in the energy consumption of servers and, thus, it must be taken into account. We have demonstrated that leakage and fan power describe a convex-like curve (see Figure 2), that can be used to develop leakage-aware fan control policies. Our fan controllers bring up to 10% energy savings in the overall power consumption of a server [6].

After studying the contributions of both dynamic and static power to the overall energy problem, we are currently focussing on the development of a thermal model for the data room based on genetic programming. Our solution aims to provide runtime spatio-temporal allocation algorithms that take into account not only the computational resources but also the cooling infrastructure of the data room.

4. Conclusions and Future research

Energy consumption in data centers is a major concern today. Our work proposes to address this problem from a holistic approach, jointly optimizing computation and cooling at the resource management level. Results obtained so far show very promising results in the holistic optimization approach proposed by this research. However, it is important to extend these results to a real environment, proving that they can be applied to real data centers.

We are currently collaborating with the “Centro de Supercomputación y Visualización de Madrid” (CeSViMa) and we envision the deployment of our techniques in this data room in the near future, as part of the LPCLOUD project in which our research group is currently involved.

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Design and characterization of cryogenic low noise amplifiers at the CDT-Observatorio de Yebes

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Keywords: cryogenic low noise amplifiers, radio astronomy, noise measurement

1. Introduction

The aim this work is to contribute to novel cryogenic low noise amplifier (LNA) development and testing. The LNA design is mainly focused on the implementation of intermediate frequency (IF) amplifiers for superconductor-insulator-superconductor (SIS) mixers to be used in focal plane array (FPA) receivers as well as for kinetic inductance detectors (KIDs). These developments are to be applied in future radio astronomy instruments. In relation to the contributions for LNA testing a new concept of noise source module for accurate cryogenic noise measurements has been fabricated and characterized.

There is great interest in developing FPA receivers since they will greatly improve the observational efficiency of present single dish observations. The problem addressed is simple: in a great number of radio telescopes the receivers observe a single point in the sky which logically makes mapping celestial sources a time consuming task. The basic idea behind a FPA system is to integrate an array of detectors in the space where now only one is placed, therefore multiplying the observational capabilities of the radio telescope. The complications in this type of developments are mainly concentrated in reducing the volume and power dissipation of the cryogenic electronics used to collect and process the extremely faint signals that are received from the sky. In single pixel applications, normally additional components are placed between the mixer and the LNA to improve coupling. In a multipixel receiver this extra hardware would add mass and increase the size to a point that would make practical implementation of the receiver unfeasible. The aim of this work is to trade off and improve amplifier performance to be able to adequately eliminate the need for any extra hardware not essential for signal detection.

Several interesting developments have been made directly connecting SIS mixers to LNAs, like the design made by Pan et al [1] where independent mixer and amplifier units were fabricated to allow for 50Ω reference testing. Other interesting results in this area have been recently obtained by Damon S. Russell [2] with Monolithic Microwave Integrated Circuits (MMICs) based in SiGe.

KIDs constitute one of the most ingenious detectors conceived in the 21st century and have a direct application in fabricating multipixel receiver systems. These detectors are based in the very subtle impedance variations which take place when some superconducting materials are exposed to photons. The idea is to exploit these impedance variations in an array of resonators placed in the focal plane of an antenna. Each element is designed for a different frequency so the special information can be recovered in the frequency domain (frequency multiplexation). These designs require state of the art LNAs to fully exploit the level of sensitivity which this technology can deliver.

KID detectors have been a raging topic since they were introduced in 2003 by Day et al [3]. Proof of this is the high number of laboratories developing detectors based in this technology, as for tests that have been made using physical implementations on radio telescopes [4].

2. Methodology

Several advances have been made in cryogenic LNAs with improved input reflection to be directly connected to SIS detectors. In particular, two functional amplifier prototypes have been designed, built and tested to study how to satisfy the design constraints of the project. Transistor technology employed for these amplifiers is InP HEMT with 100nm gate length. Also different strategies are being proposed to interconnect SIS mixer and LNA.

An important contribution has been made in the fabrication, characterization and demonstration of an ingenious noise source module adequate for accurate cryogenic LNAs measurement. This contribution has consisted in the assembly for measurement of a MMIC fabricated in Fraunhofer-IAF (Institut für Angewandte Festkörperphysik, Germany) and its calibration. Finally a rigorous study of the thermal properties was conducted to justify the use of this system versus other traditional noise measuring schemes. The module has been successfully used for several noise measurements and is currently employed in a regular basis to measure noise in our laboratory. These results have been published in December 2012 [5].

3. Results and Discussion

Experimental results agree quite well with those of the theoretical model for the final simplified LNA design. In particular the input reflection levels are very promising and set a new milestone in this development since these levels have never been achieved by our lab in a broadband hybrid amplifier design at these frequencies. These input reflection results appear in figure 1.

As for the noise source module, several LNA noise measurements have been made and compared to results obtained using other methods. One of such measurements is depicted in figure 2.

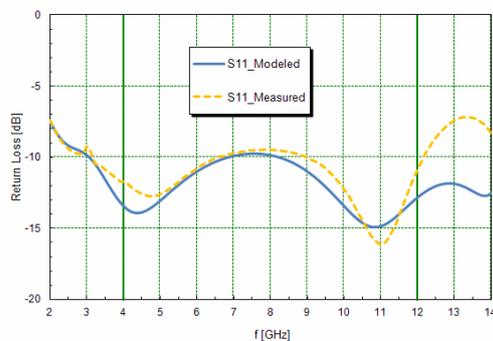


Fig. 1. Modeled and experimental input reflection data at 300K. for the YXR2002 amplifier.

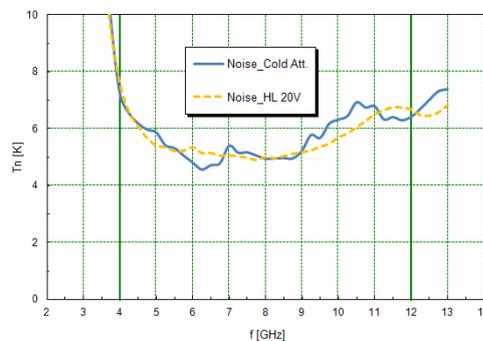


Fig. 2. MCX6003 amplifier noise measurements comparing cold attenuator and noise source module results at 15K.

4. Conclusions and Future research

Our intent is to proceed in the current line of work of developing cryogenic LNAs for a FPA receiver. Knowledge gained from the implementation of the simplified amplifiers is to be used to produce a complete LNA design that satisfies design goals. Also a decision will be made on the way to interconnect the LNA and SIS that suits the necessities of all implicated laboratories. All this work will finally converge with the physical implementation of a full working pixel of a prototype FPA.

Also, the data acquired from the experimental measurements of thermal behavior of the noise source module will be used to model and understand heat transfer between transistor terminals and other components used in cryogenic LNAs. This study will contribute to a better understanding of the effect of power dissipations in cryogenically cooled transistors which could give way to new advances in cryogenic LNA design.

Design constrains of LNAs for KIDs are yet to be determined but initial contacts have been established with some groups involved in the design of this type of detectors.

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Development of high precision FPGA-based noise reduction techniques for infrared interferometers fusion diagnostics

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Abstract. An FPGA-based processing system is currently being used in the TJ-II infrared interferometer to compute the electron density. This type of measurement requires the implementation of highly precise phase meters. When implemented in FPGAs, high performance Digital Signal Processing (DSP) algorithms typically use fixed-point arithmetic, where fractional precision is limited. This introduces numerical deviations that must be modelled and considered during the implementation process to generate high quality architectures with reduced noise levels. To this end, a fully automated quantization tool that includes noise propagation analysis and optimized solution search is being developed.

Keywords: wordlength optimization, quantization, FPGA, interferometry, fusion diagnostics

1. Introduction

The flexible Helic TJ-II is an experimental fusion reactor that ranks among Spain's Large Scientific Installations. The reactor holds plasma through magnetic confinement by means of various sets of coils that create bean-shaped magnetic surfaces to guide plasma particles in trajectories that avoid collisions with the vessel walls. Confined plasma is variable with time, so several working parameters of the reactor should be adjusted during operation time in order to maintain the nuclear fusion for long periods of time. One of the properties to study is the electron density of plasma. But up to now, this analysis is performed off-line after short times of operation of the reactor. Recently FPGA-based platforms have been installed in the infrared interferometry system of the TJ-II to extract the properties of the plasma and feed them to the control systems of the reactor so working parameters can be adjusted in real time.

The present project deals with the problem of optimizing the numerical format of the operators involved in the fusion diagnostics algorithms to ensure high performance and accuracy, both of them strong constraints for this application. High-level description tools, where systems are designed, use floating-point (FIP) data types. It guarantees high fractional precision, but in the final implementations on FPGAs custom fixed-point (FxP) is used to ensure the cost, power consumption and operational speed constrains are met. Thus, an exhaustive analysis of the integer and fractional sizes (wordlength) of each variable is required to optimize the hardware cost while complying with the allowed error constraint. But classical methodologies, based on Monte-Carlo simulations, are too slow. Consequently new analytical models need to be developed. Also, due to the continuous evolution of the fusion diagnostics, an automated toolchain to do the wordlength optimization (WLO) process is to be developed.

2. Methodology

The analytical model known as Polynomial Chaos Expansion (PCE) [1] has already been studied and applied for the quantization of a phase measuring algorithm for the infrared interferometer of the TJ-II [2]. Results are promising, but its accuracy with systems with discontinuities is low. To deal with this, a dynamically adaptive method called Multi-Element generalized Polynomial Chaos (ME-gPC) [3] will be implemented. This task will require to address specific problems derived from the increasingly complexity of the mathematical models, such as scalability of the solution and simplification of the resulting equations.

New WLO search algorithms will be developed. WLO is a NP-complete problem and, as the complexity of the systems grows, the solution space to explore increments exponentially. It is necessary to develop new heuristics to guide the search towards optimized solutions and use HPC architectures to accelerate the process. For this, several scenarios will be considered.

Simulation and analytical-based models will be studied, as well as specific information about target architectures.

Afterwards, the developed algorithms and analytical models will be integrated in a fully automated quantization workflow. The objective is to design a modular software architecture capable of running all the steps of the WLO process with minimal intervention of the designer.

Finally, the workflow will be used to quantize and optimize the infrared interferometry algorithms being developed at the Laboratorio Nacional de Fusión of the CIEMAT. The implementation of these algorithms on the FPGA platforms will be used for verifying both the measurement approaches and the correction of the ME-gPC analysis and the used heuristics.

3. Results and Discussion

Research initially focused on search algorithms and heuristics to find optimized wordlength combinations. Two different strategies have been developed, both of them using Monte-Carlo simulations [4, 5]. Experiments show speedups that range from 1.95 to 5.38 in the case of [5] and from 1.59 to 11.86 in [4] when compared to classical algorithms of the WLO literature.

Afterwards, the signal and noise modelling problem has been addressed. A first non-automated prototype of ME-gPC has been implemented in Matlab. The first results of this prototype will be presented in [6]. Also a partially functional version of the WLO tool has been developed in C++. Input interfaces with LLVM and an XML grammar have been developed.

When implementing the ME-gPC prototype, one of the main issues that arises is the problem of scalability. When representing a model of uncertainty as a summation of weighted polynomials and propagating it through a series of operators the number of terms grows quickly and, even in modern computers, memory and computation power limits are reached. To deal with this, an automated hierarchical partitioning algorithm was developed [7]. It generates system decompositions under imposed design constraints where ME-gPC can be applied.

4. Conclusions and Future research

Results up-to-date show promising perspectives for the completely functional quantization workflow. The developed search algorithms have demonstrated that the possibilities of improvement are high, and the prototype of the ME-gPC demonstrates the suitability of this approach. In addition, the fact that this solution is dynamically adaptive is beneficial for the objective of minimizing the interaction of the designer. The scalability problem has also been partially solved thanks to the developed hierarchical partitioner.

The next step to be carried out is the recomposition and simplification of the ME-gPC models obtained in each of the subsystems obtained in the partitioning stage. Afterwards, the functional ME-gPC prototype will be integrated in the framework and the process will be automated. Once the complete system is ready, the analysis, quantization and implementation of DSP infrared interferometry algorithms will be performed and tested.

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Software developments and astronomical researchs for integral field instruments at LICA (Laboratorio de Instrumentación Científica Avanzada)

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Abstract. Here I summarize the main goals achieved during the first 2 years of my Ph.D. Thesis “Software developments and astronomical researchs for integral field instruments at LICA” at University Complutense of Madrid (UCM) and University Politecnica of Madrid (UPM) funded by the spanish programme of PICATA-International Campus of Excellence Moncloa (CEI). The objective of my thesis is twofold. First, I am working within the MEGARA Control System (MCS) Team, composed by the groups GUAIX at UCM and CICLOPE at UPM, for the preparation of the different aspects of the Control system hardware and software for MEGARA (Multi-Espectrógrafo en GTC de Alta Resolución para Astronomía), the future optical IFU and multi-object spectrograph for the 10.4m GTC Telescope. We are responsible for moving all the mechanisms of the instrument along with the necessary tools to optimally prepare and process the observations, as the Exposure Time Calculator, the Image Simulator, the Fiber-Mos Positioning Tool and MEGARA reduction pipeline. Secondly, I am working within the CALIFA collaboration to make the preparatory science cases for MEGARA. In particular, I am involved in the reduction data and data-quality procedures along with the scientific analysis of a sample of spiral galaxies within the CALIFA survey (Calar Alto Legacy Integral Field Area Survey). The efforts of my PhD Thesis are devoted to add another dimension to the study of nearby disk galaxies thanks to the use of 3D data and to improve our understanding of the mechanisms that drive the evolution and the formation of disk galaxies looking into the detailed information contained in the stellar populations, stellar and gas kinematics, and chemical (both stellar and ionized-gas) abundances.

Keywords: instrumentation: spectrographs, techniques: spectroscopy, galaxies: local, spirals

1. Introduction and contents

The evolution of galactic disks is one of the most important and yet not fully understood topics in extragalactic astronomy. Despite significant progress in the recent past regarding our understanding of the baryonic physics of galaxy evolution, important questions remain unanswered due especially to the telescopes limitations. A new generation of telescopes and instruments such as MEGARA at GTC are needed to explore the questions that the present generation of space and ground telescopes has opened. MEGARA is an integral-field unit (IFU) and multi-object spectrograph (MOS) that is able to work in the entire optical window at high spectral resolutions. MEGARA (first light on 2015) is being built by a Consortium of public research institutions led by the UCM that also includes INAOE (Mexico), IAA-CSIC (Spain) and UPM. In this context, the UCM (and its LICA laboratory) and UPM play the most important role in the design and development of MEGARA. Within the MCS our principal tasks are to provide the capabilities to move the different mechanisms, to readout the data from the detector controller and the necessary routines for the Inspector Panels, the Observing Program Manager tools, the Data Factory and the Sequencer strategies. At LICA we are focusing our efforts on the MEGARA Data Factory Pipeline that shall provide the necessary routines for reduction, archiving and quality assessment of the calibration and scientific data taken with the instrument. In addition, as preparatory science for MEGARA, we are analyzing similar IFU data coming from the ongoing

CALIFA survey that is a statistically well-defined sample of ~ 600 galaxies with the PMAS/PPAK at Calar Alto 3.5m telescope. The preparatory science made with CALIFA allows us to study both the integrated and spatially resolved spectroscopic properties of galaxies with enough resolution but with MEGARA@GTC we would obtain the potential to provide observational evidence to constrain many outstanding questions of the galaxy evolution.

2. Methodology

In order to facilitate the definition and assessment of the MEGARA Science Cases and using our experience on the reduction of PPAK data we have developed at LICA different packages necessary for the MCS. Joining the experience of the GUAIX and CICLOPE groups we developed several softwares able to fully control and monitor the internal activities of the instrument like the Exposure Time Calculator, the Image Simulator and a set of Data Reduction Pipeline components implemented to reduce and analyze the acquired data that runs integrated in the GTC Control System. As a pilot study for the MEGARA science cases we also analyze the full bi-dimensional spectral cube of the nearby spiral galaxy NGC5668. We investigate the properties of 62 HII regions and 18 annuli within NGC5668. We combine the IFU data with panchromatic broad-band images to obtain radial profiles and colors and compare them with the chemospectrophotometric evolutionary models.

3. Results and Discussion

The first MCS result was obtained on March 2012, due to impressively advanced and detailed status of the MEGARA project we successfully passed the first milestone of the PDR contract.

The exhaustive study on NGC5668 was published on July 2012 in a refereed paper on The Astrophysical Journal [1]. The main result that we find is the discovery of a bar in its formative stages that produce an unusual flattening in metallicity gradient (Fig.1) suggesting that not all galaxies follow the growth prediction of the inside-out scenario for the formation of disks. Other scientific results on which I have contributed are listed in the references list ([2],[3],[4],[5],[6]).

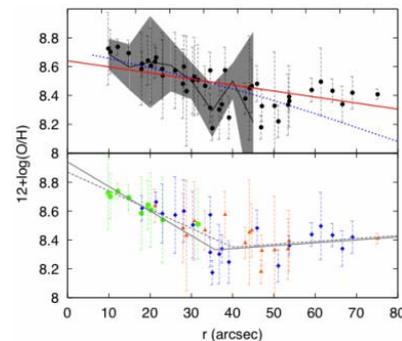


Fig. 1. Radial abundance gradient in NGC 5668 (for details see [1]).

4. Conclusions and Future research

Thanks to the published paper on NGC5668 and the successful PDR of the MEGARA instrument I should conclude that these 2 last years of Ph.D. have been highly productive. The next milestone to be passed will be on May 2013 during the Critical Design Review of the instrument. In the framework of the preparatory science for MEGARA, we have carried out a new study on new empirical single line-ratio metallicity calibrators based on the CALIFA data and a compilation of Te-based measurements from the literature. This novel study makes use of an unprecedented set (~ 4000) of HII regions and will address important clues for understanding the chemical evolution of different types of galaxies. Once finished the internal review phase, I will submit it to the journal Astronomy and Astrophysics. Currently, I'm visiting Dr. Alessandro Boselli at the Laboratoire de Astrophysique de Marseille for a short stay of three months with the aim of working on the comparative study of the bidimensional distribution of ionized-gas and dust and their properties using a sample of galaxies extracted from the Herschel Galaxy Reference Survey and that have been observed by our group at UCM using the IFU PPAK at the CAHA 3.5m telescope. This visit represents an excellent opportunity to share our respective expertise on the analysis and interpretation of the optical 3D and Herschel far-infrared data.

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Soil bacteria adaptive stress-response to the presence of Nanoscale Zero Valent Iron

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Abstract. Nanoscale Zero Valent Iron (NZVI) is emerging as a new option for treating contaminated soil and groundwater even though the potentially toxic impact exerted by NZVI on soil microorganisms remains uncertain. We focused on nanotoxicological studies performed *in vitro* using commercial NZVI and soil bacteria. Cellular viability was affected depending on NZVI concentrations, exposure time and bacterial strain. Microscopy analysis showed the cells entrance in sporulation phase or NZVI location around the cell membrane. Despite no changes at transcriptional level were detected using five genes as treatment-related markers (*narG*, *nirS*, *pykA*, *gyrA* and *katB*), a proteomic approach highlighted differentially expressed proteins under NZVI exposure. We demonstrated that proteins involved in oxidative stress-response and TCA cycle modulation were overexpressed; moreover proteins involved in motility and wall biosynthesis were repressed. Our results enabled to detect a molecular-level response as early warning signal, providing new insight into first line defense response of a soil bacterium after NZVI exposure. These early indicators of alterations on soil biota may be considered promising endpoints to assess environmental safety.

Keywords: nano zero-valent iron, soil bacteria, cytotoxicity, biomarker, proteomics

1. Introduction and Contents

Nanoparticles (NPs) are generally defined as particles with at least one dimension <100 nm, which gives them unique chemical properties. Among NPs, NZVI represent a new generation of environmental remediation strategies but there is no specific regulation on their use and the lack of health and environmental risks research is a barrier to their commercialization. To evaluate toxicological effects of nanomaterials on microorganisms, multiple toxic endpoints (proteomic stress-response, gene expression, morphology or growth) could be considered.

Genes considered as treatment-related biomarkers might provide an understanding of the impact of iron nanotechnology on microbial functionality. Thereby, genes encoding functional enzymes involved in key biogeochemical processes, such as *narG* (nitrate reductase) and *nirS* (cytochrome cd1-containing nitrite reductase) involved in the nitrogen cycle are of particular interest. Other genes such as *gyrA* (encoding gyrase involved in DNA replication) and *pykA* (encoding pyruvate kinase a key enzyme in glycolysis) can be considered broad-spectrum indicators of biological activity. On the other hand, catalase encoded by *katB* gene, is an enzyme actively involved in cellular oxidative stress response. Proteomics has become a useful complement to functional genomics. Proteins are promising alternative markers, because they reflect the actual functionality with respect to metabolic reactions and regulatory cascades, and give complementary and more direct information about microbial activity than functional genes and even the corresponding messenger RNAs.

In this project, we performed nanotoxicological studies using commercial NZVI and ubiquitous widespread soil bacteria, which can serve as models of sensitive bacterial strains for ecotoxicological purposes. We have considered a) the potential cytotoxicity induced (cellular viability, morphological changes) and b) the molecular-level changes in its gene-expression profile and in its proteomic profile after NZVI exposure.

2. Methodology

- NZVI were commercially synthesized and supplied by NANOIRON s.r.o.
- The effect of NZVI on bacterial viability was evaluated by CFU count method.
- Bacterial strain morphology was examined by transmission electron microscopy (TEM).

- Expression analysis of treatment-related biomarkers was evaluated by qRT-PCR.
- Proteomic assay was conducted by Differential In-Gel Electrophoresis (DIGE) analysis and identification of protein spots by MALDI-TOF MS.

3. Results and Discussion

Bacterial cells viability varied according to NZVI exposure time, concentration and bacterial strain. TEM revealed that cells exposed to NZVI responded by entering in an early sporulation stage (Fig.1), by entering inside the cell or by displaying around the cellular membrane.

In this study, we proposed five genes as treatment-related molecular markers to examine the impact of NZVI on bacteria at the molecular level. The expression level (by RT-qPCR) of the target genes showed a poor treatment-related response of soil bacteria. This is consistent with the early spore-state and thus the low cellular activity that characterizes it.

The proteomic approach highlighted differentially expressed proteins involved in stress-response and oxidative stress-response, providing an understanding of the molecular mechanisms involved in a first-line cellular response to this environmental stressor.

4. Conclusions and Future research

In conclusion, comparison of gene expression and protein profiles, in combination with assessment of morphological characteristics, has contributed to a better understanding of the soil bacteria cellular stress-response after NZVI exposure.

Our results indicate that under NZVI exposure, cells rapidly set up a molecular response, entering in an early sporulation stage to survive under the stressful conditions and modulating the expression ratio of specific proteins; this strategy provides to the cell a first line of defense against oxidative stress. The proteomic approach enables us to detect the molecular-level response as an early warning signal. Because there is a temporal shift between the transcriptome response of cells and the development to the corresponding phenotype, further analyses considering long-term exposure will provide new insight to answer the following question: How long can the cell maintain the adaptive stress-response?

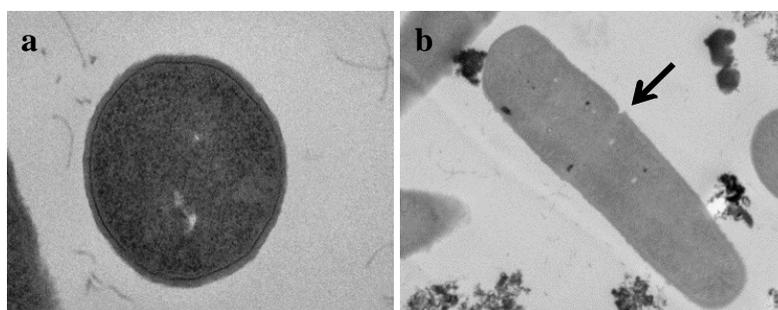


Figure 1. TEM micrographs showing *Bacillus cereus* control cells (a), cells exposed to NZVI (b).

Stridulation variability in dung beetles: An examination of the species *Geotrupes mutator* (Marsham, 1802) (Coleoptera, Scarabaeoidea)

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Abstract. We analyzed Stridulation sounds produced by the dung beetle *Geotrupes mutator* (Marsham, 1802) to check for intraspecific variation and to determine to what extent bioacoustic parameters depend on the morphology of the stridulatory organ, environmental conditions and geographic location. The analyses show that there are differences in the stridulatory apparatus between males and females. It also shows the spatial variation of sound production, allowing speculate on the existence of intraspecific dialects, as well as the possible influence of environmental and morphological characteristics of some features of the wave.

Keywords: Geotrupidae, stridulation, bioacoustic, morphology

1. Introduction and Contents

The insect exoskeleton, sclerotized and articulated in different parts, is prepared to produce sounds [1]. It is possible that different evolutionary pressures have acted on sound production to make this tool a mechanism for recognizing potential intraspecific and interspecific differentiation.

The dung beetles are considered sporadic stridulators. In the genus *Geotrupes* Latreille, 1796, the stridulation is produced by a rubbing motion of a stridulatory part (*pars stridens*) in the coxa against a plectrum in the the abdomen (coxo-abdomnal apparatus). The stridulation includes syllables. Each Stridulation is composed with two pulses repeated: hemisílabas A and B, separated by a very short interval, the silence between A and B. Although for some species there are descriptions of stridulatory apparatus [2], studies attempting to delineate the behavioral and evolutionary implications of this character are limited [3].

The aim of this paper is to analyze the sound produced by *G. mutator* in relation to the circumstances that attend its variation can be internal, such as morphological and relating to sex, or external such as geographic and environmental.

2. Methodology

Samplings were performed weekly in spring-summer period at the community of Madrid and Galicia, for the live capture of species Geotrupidos. The study was carried out both by analysis of sound signals and the morphological study the stridulatory apparatus.

Bioacoustic

The animals collected were recorded in the laboratory of the Department of Zoology bioacoustics and Evolutionary Anthropology at the Complutense University using the SAS program Avisoft-Lab Pro. For each individual we have analyzed 100 syllables. In total we have considered the following 15 variables from bioacoustic sound recording. From the oscillogram: DurA (duration of syllable A); durB (duration of B); Silab (Silence Between A and B), from the spectrogram: Apfmax (maximum peak frequency of A); Amfmax (mean frequency at maximum amplitude of A); Apfmean (mean frequency peak of A); Amfmean (mean frequency at mean amplitude of A); Aq25mean (mean of quartile measured at 25% of A); Aq75mean (mean of quartile measured at 75% of A); Bpfmax (peak maximum frequency of B); Bmfmax (mean frequency at maximum amplitude of A); Bpfmean (mean frequency peak of B); Bmfmean (mean frequency at mean amplitude of A); Bq25mean (mean of quartile measured at 25% of B); Bq75mean (mean of quartile measured at 75% of A).

Morphometry

We have made morphological measures of the body and the stridulatory apparatus. To describe body size were taken seven different measures: LP (length of pronotum), LE (length of elytra), AWP (apical width of pronotum), MWP (maximum pronotum width), BWP (basal pronotum width), BWE (basal width elytra), MWE (maximum width elytra) and WC (maximum width coxa). For stridulatory apparatus 3: La (length stridulatory apparatus), n (number of crests) and La / n (density of crests). Once recorded measured specimens were prepared and stored in the collection of the "Recognition of bioacoustic characters in Scarabaeoidea Laparosticti" (CGL2010-16944).

Statistic

The set of variables has been organized into four groups useful for carrying out the analysis: morphological (M: body and stridulatory apparatus), sex (S), environmental (A: in reference to the recording conditions), space (E: coordinates geographical). Differences were analyzed using analysis of variance (one-way ANOVA), the possible relationships between the four groups of variables by Spearman correlation. General models were linearized (GLM) to explain the effects of environmental and spatial morphological variables on the sound produced.

3. Results and Discussion

The ANOVAs show significant difference between genders in the stridulatory apparatus (La n). The correlations indicate the significant relationship between the size and number of crests. The GLM for the acoustic variables of the hemi-syllables A and B against the morphological, environmental and spatial effects demonstrate that the pure effects affect more than the combined effects. In particular, there are significant differences between males and females in B descriptors while hemi-syllable A is more influenced by the geographic area (Table 1).

4. Conclusions and Future research

The difference between sex in stridulatory apparatus is evident in the density of crests of the pars stridens. While in the female the number of crests is proportional to the body size, the male tends to keep a fixed number of crests (Figure 1). This makes us to suppose that stridulation participates in courtship. Females describe themselves through the stridulation (higher stridulatory apparatus, larger size); males make them recognizable as co-specific. A sound level these differences are expressed predominantly in the hemisilaba B. The study also shows that the geographical relationships influence the stridulation, especially in hemisilaba A, which suggests the existence of dialects population.

variables		apf	amf	apf	amf	aq25	aq75		
		durA	max	max	mean	mean	mean	mean	
efectos puros	M			*	***		*		
	S	*							
	A		**	*	**	**	**	**	**
	E	**	*	*		**	***	***	
variables		durB	bpf	bmf	bpf	bmf	bq25	bq75	silAB
		max	max	mean	mean	mean	mean	mean	
efectos puros	M						*		
	S	*	*		*				
	A					*			
	E	**			**		**	**	*

Table1

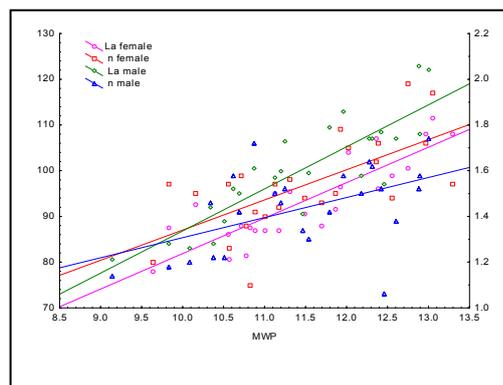


Figure 1

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Alpine lizards in Mediterranean mountains: Distribution patterns and prospective evolution under conditions of global change

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1. Introduction and Contents

Alpine lizards are adapted to cold environments in order to have a successful reproduction, and life histories and reproductive strategies may change along the altitudinal gradient to adjust for environmental variation (e.g. changes in temperature). If populations do not cope with new local conditions as descending in elevation, some environmental factors may act as a barriers and therefore limit dispersal of these alpine species. This is particularly relevant given that plasticity to environmental change at a local scale can also help us to improve predictions of environmental change at a global scale. Thus, if organisms are unable to respond to temperature increase along the elevational gradient, alpine populations might be particularly sensitive and/or vulnerable to the impacts of global change.

To study plasticity to temperature, of lizards that occur in mountains, regarding their life history traits, we used two approaches:

A) Green lizard *Lacerta schreiberi*: eurosiberian species, with its populations presumably in decline. Its incubation thermal requirements are not known (neither temperature nor moisture), and hence there is no information about how these requirements could be affecting their distribution limits. In this project we investigated the effects of both incubation temperature and moisture effects in reproductive traits providing an ecological context of modelled soil temperatures in the field.

B) Iberian rock lizard *Iberolacerta cyreni*: alpine endemism, for which has been found a connection between incubation conditions and distributional limits. Nevertheless, adjustment of reproductive strategies along the elevational gradient is unknown. In this project we explored if populations located at different elevations (ca 2000 m y ca 1800 m) in two mountain areas (Gredos and Guadarrama) present different life history traits regarding reproductive embryonic development.

2. Materials and Methods

We performed captivity breeding experiments, where eggs were incubated at different temperature and/or moisture treatments. Juveniles were kept and monitored for one month. We tested the effects of temperature on the following traits: incubation time, hatching success, size, mass and body condition at hatching and at the age of one month, size and mass specific growth rates. In the A section results were combined with data on available soil temperature in the field and with data on the species presence in the whole study area.

3. Results

Green lizard *Lacerta schreiberi*

Temperature affected negatively hatching success while moisture did not. Analogously, temperature, but not moisture, affected incubation time, this period being shorter for eggs incubated at higher temperatures. Size, mass and body conditions were also affected negatively by increasing incubation temperatures, both at the time of hatching and at the age on one month. Moisture only affected size of juveniles at hatching, which was larger for the neonates incubated at the higher moisture treatment (80% moisture). Postnatal growth rates were similarly negatively affected by increasing incubation temperatures.

We found that the species was present in areas where soil temperature under shrubs was equal or less than 24°C (coinciding with what we found in the experiment, where this temperature yielded the maximum reproductive success in the traits measured).

Iberian Rock lizard *Iberolacerta cyreni*

We found that populations located at lower altitude (at the lower elevation distribution limit) presented lower hatching success, as well as those populations from Guadarrama. Although temperature had a strong effect accelerating egg development, we did not find differences in incubation times between populations at different elevation. Moreover, increasing temperature reduced juvenile viability (n° of surviving juveniles at the end of the experiment). On the other hand, postnatal effects of temperature were not as clear: individuals incubated at higher temperatures although presented a worse hatching body condition at hatching, experienced much faster growth rates and ended up the experiment being larger, heavier and with better body condition than those who came for colder incubation treatments.

4. Main conclusions

Green lizard *Lacerta schreiberi*

This species showed to be very sensitive to incubation temperature changes, its reproductive traits being strongly affected by thermal treatments. On the other hand, under the reasonable assumption that females may use shrubby substrate to lay their eggs, there could be a connection between distributional limits and thermal embryonic requirements. This species might be, therefore, sensitive to climate changes, although more data on maternal behaviour and natural nests are needed.

Iberian Rock lizard *Iberolacerta cyreni*

Hatching success was lower in marginal populations (located at lower altitudes) and that increase incubation temperature reduces juvenile viability. In addition, there is not an adjustment of developmental rate to temperature (i.e. there are no differences in incubation time between treatments). This all suggests the species may not be locally adapting to changing conditions encountered along the elevational gradient. Our results suggest the species might be having difficulties to adapt to warmer locations at lower elevation. Nevertheless more studies on the potentiality of behaviour to buffer this physiological constrains (e.g. nest site selection) are needed.

5. Future research

Our results point out that environmental conditions changing along with elevation, may pose a barrier for lizards inhabiting mountains through its effects on reproductive traits associated with incubation conditions. This may have implications in the vulnerability of these species to increasing temperature as it has been predicted under climate change. It would be very interesting to expand research to more populations located at different elevations, which sometimes (such as the case of *Iberolacerta monticola*) can be very contrasted. It seems particularly relevant to monitor eggs in the field and add information of nest site selection to address the real actual temperature eggs are exposed to, and to assess how females may be buffering physiological constrains through behaviour.

Impact of climate variability on Iberian Peninsula summer cropping systems

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Keywords: yield variability, crop models, climate impacts, climate variability, agroclimatology

1. Introduction and Contents

Climate variability and changes in the frequency of extremes events have a direct impact on crop damages and yields. Crop yield variations have obvious impacts on farm economies, agricultural markets and food security. Thus, improvements in the knowledge of climate anomalies projections at monthly and yearly timescales are essential for early warning systems and adaptation of crop management (insurance coverage, changes in sowing dates, choice of species and varieties) to take advantage of favorable conditions or reduce the effect of adverse conditions. This knowledge will favour a better forecasting of cropping seasons. In this way, the variability of the Ocean surface temperature has been shown to be crucial for predictability issues. For this reason, the general objective of this work is to identify interannual and decadal climate variability patterns affecting summer cropping systems of representative places of the Iberian Peninsula (IP), through relationships between yield and ocean thermal anomalies.

2. Methodology

Time series of simulated maize yields were computed with CERES-maize model [1], included in DSSAT v.4.5 Decision Support System for Agrotechnology Transfer [2]. Last version of the model was re-calibrated and validated in three representative agricultural locations in Spain with contrasting temperature and precipitation regimes: Lugo (northwestern), Getafe (centre) and Albacete (southeastern Spain) for specific maize varieties currently used at each location, with observed climate and crop data from existing field experiments. Simulations used daily data of radiation, maximum (Tmax) and minimum temperature (Tmin) and precipitation data.

Once validated, crop simulations were done for irrigated maize with different climate data sets and different periods depending on data available for each location. Climate data sets were: 1) Observed climate data obtained from the State Meteorological Agency of Spain (AEMET); 2) Climate data from NCEP/NCAR 40-year reanalysis project (NOAA National Center for Environmental Prediction) [3] and ECMWF reanalysis (European Centre for Medium-Range Weather Forecasts: ERA 40 and ERA Interim); and 3) Sea Surface temperature (SST) obtained from Reynolds database [4] and different indices (Niño, PDO) obtained from the Climate Prediction Center of the NOAA.

To obtain the dominant modes of variability of maximum and minimum temperature in the Iberian Peninsula, Principal Components [5] were calculated and their relationships with oceanic teleconnection patterns were done using regression and correlation analysis.

Crop simulations obtained with observed data were used to analyze the evolution of maize yield anomalies and its relationships with the evolution of different patterns of climate variability. Crop simulations done with reanalysis (ERA40, ERA Interim, NCEP) were evaluated by comparison of results with those obtained with observed climate (AEMET), and then used to generate longer times series of simulated yield. Longer series helped to explain the mechanism of the influence of El Niño and Pacific Decadal Oscillation (PDO).

3. Results and Discussion

Results of crop simulations obtained with observed data showed that there was a significant correlation between maize yield and El Niño and PDO Indices. El Niño affects differently depending on the location in the Iberian Peninsula: for the northwest (represented by Lugo) there is a significant linear negative correlation, being the maximum correlation - 0.62 in Niño 3 region in July (Fig.1). For the southeast (represented by Albacete and Getafe) there is a non linear correlation, because only low yields are negatively correlated with El Niño but high yields are not associated with El Niño events. Also, yield anomalies presents a decadal variability, being positive from the 70's to the 80's and negative onwards, coinciding with the change of phase of the PDO (Fig. 2). Results of crop simulations obtained with reanalysis confirm the preliminary relationships obtained with observed data. Also, these simulations reveal that there is a non stationary relationship between maize yield in Spain and El Niño 3 Index.

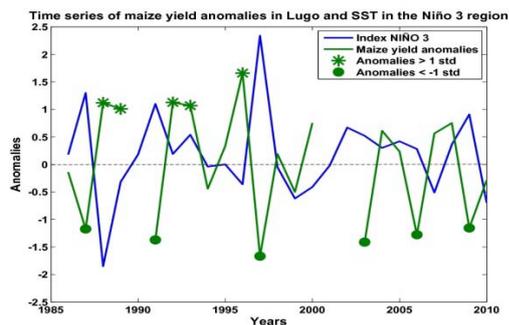


Figure 1. Time series of yield anomalies of irrigated maize in Lugo (simulated with observed data) and sea surface temperatures in the Niño 3 region (July)

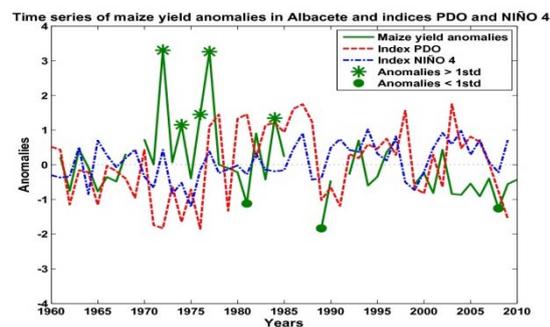


Figure 2. Time series of yield anomalies of irrigated maize in Albacete (simulated with observed data) and Indices Niño 4 of August (previous year of crop cycle) and PDO in February (previous year of crop cycle)

Correlations of anomalies of observed and reanalysis climate variables for Lugo (Tmax, Tmin, radiation and precipitation) with El Niño 3 for the month of maximum correlation with yield (July) are lower than correlations with the corresponding simulated yield. This result indicates that crop yield is acting as an integrated bioclimatic indicator that captures better the existing teleconnections than the atmospheric variables that feed the crop model.

Correlation analysis reveals a strong relationship between first Principal Component (PC1) of Tmax and Tmin of May in IP and PDO (0.56 and 0.57 respectively, significant at 95%). First Principal Component explains 77% and 75% of the variability of Tmax and Tmin of May over IP, respectively. However, these relationships are not found for El Niño Index. Thus, it is suggested that a large part of decadal yield variability in Iberian Peninsula is induced by PDO.

4. Conclusions and Future research

This work is developing a new methodology to analyze the effects of current and future climate variability on Iberian cropping systems. One potential application would be crop forecasting. Results can also be useful for climate change impact assessment, providing a scientific basis for selection of climate change scenarios where combined natural and forced variability represent a hazard for agricultural production. Furthermore, we will extend this methodology to irrigated/rainfed winter crops (wheat or barley).

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Contributions of active faults in El Salvador to the seismic hazard

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Keywords: earthquake geology, seismic hazard, geomorphological index, active tectonics, El Salvador

1. Introduction

El Salvador is located in northern Central America, in the western margin of the Caribbean plate. The SW part of the country forms part of the forearc sliver of the Caribbean plate. The NE part of this country belongs to Chortís Block, a continental block which is composed by a paleozoic basement, mesozoic marine sediments and volcanic material associated to the Coco's plate subduction beneath this block.

El Salvador Fault Zone (ESFZ) is a deformation band of 150 km long and 20 km wide within the Salvadorian volcanic arc [1]. This shear band distributes the deformation between main strike-slip faults trending N90°-100°E and around 30 km long, and secondary normal faults trending between N120°E and N170°E. The ESFZ continues westward and is relieved by the Jalpatagua Fault in Guatemala. Eastward ESFZ becomes less clear disappearing at Golfo de Fonseca. Five segments have been proposed for the whole fault zone, from the Jalpatagua Fault to the Golfo de Fonseca. From west to east these segments are: Western segment, San Vicente Segment, Lempa Segment (also named inter-segment Lempa), Berlin Segment and San Miguel Segment.

The high activity rate of the ESFZ, the important amount of new GPS and paleoseismic data, the extremely high vulnerability of the region and the seismogenic potential of the faults within salvadorian volcanic arc, makes this place an interesting place in order analyze the influence of the introduction of geological parameters of faults in the seismic hazard values.

The ESFZ has been studied by many authors (i.e. [1][2][3]). There are important results in the paleoseismic studies of the San Vicente Segment, from which some authors have conclude that ESFZ is a seismic source capable of produce Mw 7.6 earthquakes with a recurrence interval of 800 yr, implying ruptures of around 50 km length and therefore more than one segments have been implicated in paleo-events [3]. The seismic potential of ESFZ has been underestimated up to now.

In this study we have characterized the seismic potential of the ESFZ, throughout paleoseismological and morphotectonic and we contribute new geological data applicable to seismic hazard assessment.

2. Methodology

We have excavated four paleoseismological trenches in the Berlin segment of the ESFZ. Deformation of quaternary deposits identified in the trenches have been quantified by nine samples dated in Rafter Radiocarbon Laboratory of New Zeland (¹⁴C dating).

To analyze the lateral distribution of the vertical displacement within ESFZ, in the overlapping zones between segments and the interaction of different strands and segments of the ESFZ we have done a morphometric analysis. This analysis includes the calculation of hypsometric curves, hypsometric integral and the analysis of the orientations of the fluvial basins.

The whole morphometric study is developed from a 10 m resolution Digital Terrain Model (DTM), obtained by the digitalization of 1:25.000 topographical maps and supplied by the MARN (Ministerio de Medio Ambiente y Recursos Naturales de El Salvador). The software used have been Geographical Information System free software tools (GRASS, GDAL and Qgis) as well as scripts in Bash environment using AWK and GMT [4] for the data process and the graphic representation.

3. Results and Discussion

The paleoseismological analysis of the Berlin segment reveals a preliminary recurrence interval for large $M_w > 6.5$ earthquakes of 2160 ± 270 years. Also, we have found paleo-events that could be correlated with events identified in the adjacent San Vicente Segment. Considering ruptures implying these segments at the same event (San Vicente, Berlin and Lempa) would considerably increase the seismic hazard in the region.

From the morphometric analysis we have identified 29 seismic sources. Maximum magnitudes of these sources vary from $M_w 6.49$ to 7.11 (Table 1).

Segment number	Name	Length (m)	Max. $M_w \pm 0.30$ (Stirling empiric law)	M_w (W&C, empiric law)	Strike	Dip	Rake	SR (mm/yr)	RI (yr)
1	Falla Intipuca	25652	7.01	6.74±0.28	290	70	-133		
2	Falla Olomega	12627	6.76	6.39±0.28	140	70	-23		
3	Falla La Quesadilla	10987	6.71	6.33±0.28	140	70	-23		
4	Falla El Zapote	11177	6.72	6.33±0.28	190	70	9.75		
5	Falla Conchagua	13490	6.78	6.43±0.28	200	70	25		
6	Falla Chilanguera	5832	6.49	5.87±0.34	120	70	-84		
7	Falla Rio Grande	19108	6.9	6.59±0.28	310	70	-41		
8	Falla El Espino	11016	6.71	6.33±0.28	280	80	-167		
9	Falla Chirilagua	14460	6.81	6.46±0.28	160	70	-7		
10	Falla Guachipilin	19764	6.92	6.57±0.34	120	70	-84		
11	Falla El Tecomatal	15369	6.83	6.43±0.34	130	70	-41		
13	Guaycume	23665	6.98	6.67±0.34	110	70	-133		
14	Falla Comecayo	19670	6.92	6.61±0.28	100	80	-167		
15	Santa Ana W	14638	6.81	6.47±0.28	340	70	-7		
16	Santa Ana E	13443	6.78	6.42±0.28	160	70	-7		
17	Falla Apaneca	14384	6.81	6.46±0.28	130	70	-41		
18	Falla Teotepeque	6761	6.54	6.09±0.28	280	80	-167		
19	Falla El Zacamil	12066	6.75	6.37±0.28	350	70	-2.6		
20	Sesuntepeque E	14820	6.82	6.47±0.28	200	70	25		
21	Sesuntepeque W	13121	6.77	6.41±0.28	355	70	-0.6		
22	Falla Victoria	12294	6.75	6.38±0.28	200	80	12		
12	Falla El Pulguero	23096	6.97	6.66±0.34	110	80	-133		
23	Falla San Vicente	18774	6.9	6.59±0.28	90	70	-164	4	800
24	Falla Berlin	28251	7.04	6.79±0.28	100	70	-154	11	2160±270
25	Falla Coatepeque	17891	6.88	6.56±0.28	95	85	-175		
26	Falla San Miguel	34152	7.11	6.88±0.28	90	85	-176		
27	Falla Lempa Sur	10411	6.69	6.30±0.28	280	70	-154		
28	Falla La Joya	12391	6.75	6.38±0.28	280	70	-154		
29	Falla El Caracol	12595	6.76	6.39±0.28	285	70	-146		

Table 1. Main features of the identified seismic source in El Salvador. W&C: Wells and Coopesmith, 1994, SR: Slip-Rate; RI: Recurrence Interval.

The Lempa inter-segment region is specifically interesting because the deformation is distributed in this area in a large set of $N120^\circ-170^\circ E$ trending normal faults that seems to connect San Vicente and Berlin segments increasing the rupture length capability of the ESFZ and then the seismic hazard (faults 12+23+24 highlighted in Table 1).

4. Conclusions and Future research

The morphometric analysis carried out contributes to a better understanding of the seismic behavior of the ESFZ. This study supports the hypothesis of a recent rotation of the maximum shortening direction, and the accommodation of the current deformation through the reactivation of pre-existing structures inherited from previous tectonic phases. To answer this question we are going to analyze the ESFZ structure and evolution using 4D analogue modeling in the Institute of Geological Sciences of Bern. We will carry out several experiments using brittle analogue materials (quartz sand and Corundum as upper crust) and viscous analogue material (Polidimethyl-siloxane as lower crust) under computerized tomography to control the 3D real time development of structures.

The data obtained are still preliminary results, but they will be useful to future seismic hazard assessment studies following deterministic and probabilistic methods.

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Next-generation materials and devices for energy-efficient systems

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Abstract. Novel materials and electronic devices for energy applications are presented.

Keywords: gallium nitride (GaN), silicon carbide (SiC), diamond, graphene, carbon

1. Introduction

Materials and devices addressing new energy needs for global change are presented below. GaN transistors with diamond heat spreaders are expected to improve efficiency in high voltage converters, which regulate about half of the generated power in the world. Silicon Carbide is a material closely matching GaN in terms of commercial development. For energy storage applications, graphene and carbon have also been studied: graphene for electrical contact properties and Manganese Oxide deposition on carbon for energy storage.

2. Gallium Nitride and Diamond

We focused on essential aspects of top-side nanocrystalline diamond (NCD) integration in III-Nitride transistors that lead to measurable improvement in thermal and electrical performance. NCD was grown on GaN-based wafers on Si substrates using chemical vapor deposition techniques. A key aspect to achieving good thermal performance was growth of diamond mid-process, rather than capping a finished device [1, 2].

3. Silicon Carbide

4H-SiC properties such as wide energy gap and high critical field, and the resulting devices with low capacitance and high blocking voltage, have enabled fast switching and high power applications in harsh environments. This study addresses the potential of SiC as a high temperature material for MOS devices by demonstrating stable operation at 300°C [3].

4. Graphene

Vertically conducting diode structures of epitaxial graphene (EG) on n-type 4H-SiC were characterized by Raman spectroscopy, electroluminescence, and electrical techniques. Vertical current and capacitance measurements revealed a rectifying property, which improved at cryogenic temperatures as the reverse leakage decreased over six orders of magnitude without freeze-out in either material [4].

5. MnO₂ / Carbon

There is an increasing need for supercapacitors as they are unique in their ability to deliver high power levels over a time span unattainable by a traditional capacitor. We present a low-cost MnO₂-based chemistry on large area sheets of carbon aerogel paper. The specific capacitance of manganese oxide is typically lower than the best in class of ruthenium oxide; however, the much lower cost and available supply of manganese makes this material much more attractive. Specific capacitance of MnO₂ (C_{SP,MnO_2}) and series resistance (R_S) at 1 mA and 5 mA of galvanostatic charging current (I_{CH}) were calculated. Specific capacitance for sample B at 1 mA charging current was increased from 47 F/g to 64 F/g, a 36% improvement over a bare carbon paper surface [5].

6. Conclusions and Future research

In this paper, we have demonstrated results on novel materials such as GaN, SiC, diamond, graphene, and carbon.

Figures

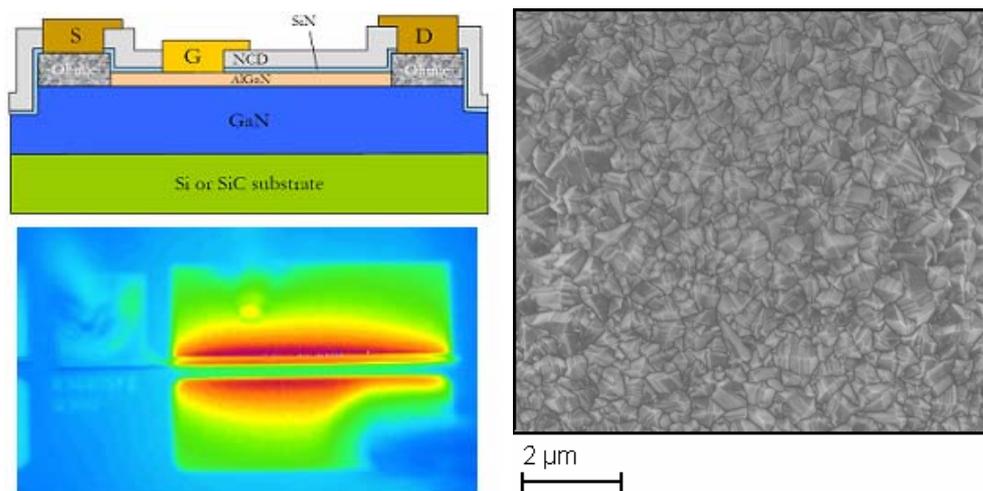


Figure 1: Schematic (top left) and infrared image (bottom left) of diamond-capped transistor and a scanning electron micrograph of the nanocrystalline diamond surface (right).

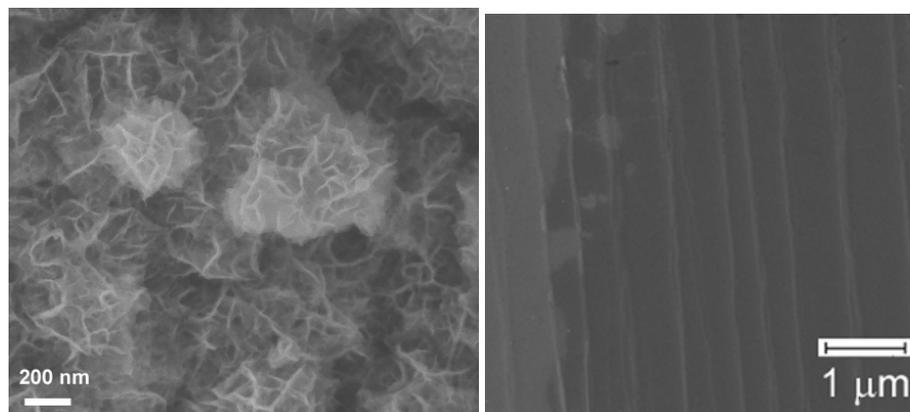


Figure 2: Scanning electron micrograph of nanoflowers of MnO₂ on carbon paper (left). Epitaxially grown graphene over the steps of a SiC substrate (right).

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Iceberg discharges of the last glacial period driven by oceanic circulation changes

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Abstract. Ice core data and marine and continental records reveal the existence of pronounced millennial time-scale climate variability during the last glacial cycle. Greenland ice core records show abrupt transitions known as Dansgaard-Oeschger (DO; Dansgaard et al., 1993) events within decades from cold (stadial) to relatively warm (interstadial) conditions, followed by a slow cooling lasting several centuries and a more rapid fall through stadial conditions. Two types of explanation have been suggested: periodic external forcing (e.g. Braun et al, 2005) and internal oscillations in the climate system, for which ocean circulation is the main candidate (e.g. Alvarez-Solas et al, 2010a; Banderas et al, 2012). On the other hand, six periods of extreme cooling registered in the Northern Hemisphere, known as Heinrich events (Heinrich, 1988), have been found to be coeval with increased deposition of ice-rafted debris, which is interpreted as enhanced discharge of icebergs into the North Atlantic Ocean. Recently, the coupled effects between ocean circulation and ice-sheets dynamics have been suggested to play a major role in triggering Heinrich events (Alvarez-Solas et al, 2011; Alvarez-Solas and Ramstein, 2011; Alvarez-Solas et al, 2012). This interpretation of Heinrich events being responding to changes in the oceanic patterns (or at least not being a pure internal and spontaneous manifestation of ice sheets), takes the advantage to provide an explicit relationship between DO events and the periodic iceberg surges. In particular, Alvarez-Solas et al, (2010b) showed in a box model that a series of DO events favors the occurrence of a Heinrich event through a resonance phenomenon, giving an explanation to the denominated Bond cycle. This hypothesis has been reassessed here within a more realistic modeling framework by forcing a 3D state-of-the-art ice-sheet model with the output of abrupt climate change simulations carried out with a coupled climate model of intermediate complexity. These show the main expected characteristics of such events: an abrupt warming of the North Atlantic and Atlantic Meridional Overturning Circulation (AMOC) intensification followed by a progressive cooling and AMOC reduction and a more drastic fall into a stadial condition. Interestingly, stadial periods are characterized by the occurrence of a subsurface warming up to 3 K in regions where deep water formation takes place (Nordic and Labrador Seas). These results show that subsurface warming is a crucial mechanism to destabilize the Labrador Sea ice shelves favoring the acceleration of the Laurentide ice streams (Figure 1). Iceberg production is then enhanced during stadial periods. However, this pattern is not monotonically present through all DO events: the combination of both a characteristic ice-shelf break-up and re-developing time larger than the DO forcing period and the fact that ice-streams need to flow extremely fast to create major calving rates explains the different magnitude of iceberg discharge during different stadial periods. We propose that Heinrich events were triggered by warm by North Atlantic subsurface waters resulting from reduced NADW formation. Under this new mechanism, the dynamic ocean–ice-sheet interaction leads to both cold surface conditions and warm subsurface waters, which are crucial for ice shelf breakup. Reducing their buttressing effect induces a large iceberg discharge and an ice-stream acceleration that translates into up to 2 m of sea level rise, with a maximum rate of 4 mm/yr (the same order of magnitude as the present-day anthropically-induced rise, with all effects included) only by dynamical reaction of the Laurentide ice sheet.

Keywords: abrupt climate change, ice sheets, ice shelves, oceanic circulation, iceberg discharges

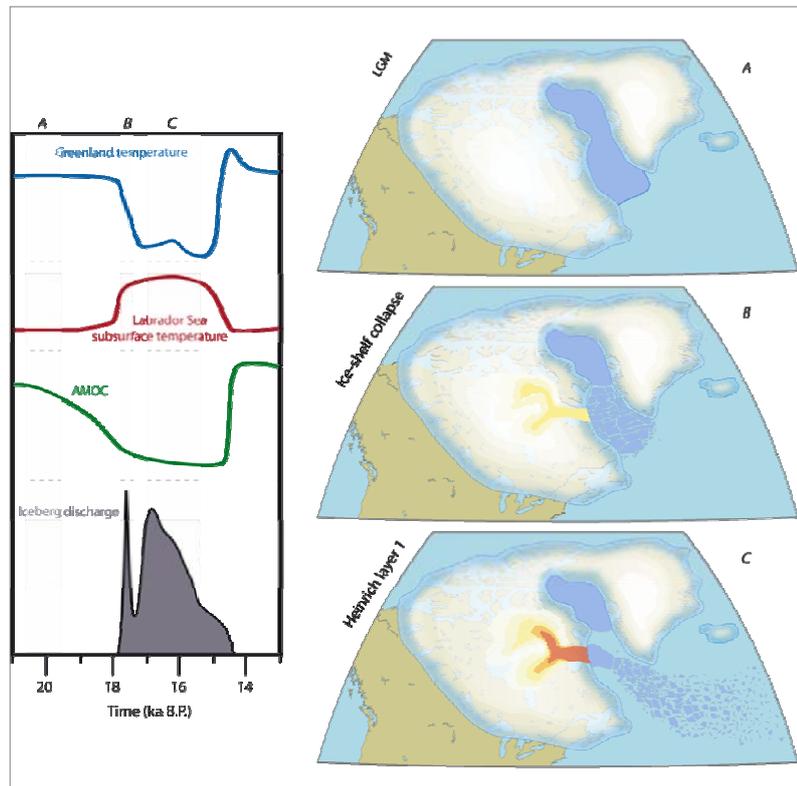


Figure 1. Schematics of the Heinrich event 1. Left: Time series illustrate the evolution of the main variables involved with the triggering mechanism. A, B, and C indicate critical steps in the Laurentide ice sheet around Heinrich event 1. Right: Warm colors in B and C represent acceleration and thinning in ice streams of the Hudson Bay and Hudson Strait area. Source: Alvarez-Solas and Ramstein, 2011.

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