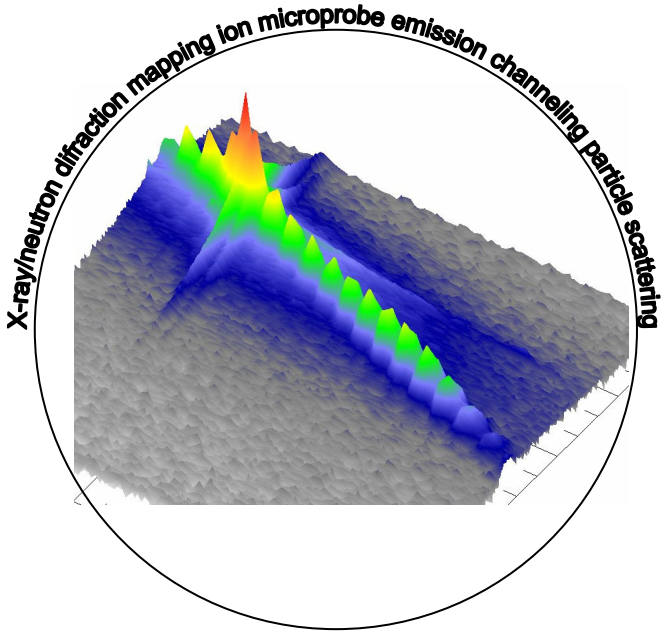
Physics Sector



Physics

Eduardo Alves

The activities developed in the Physics Department are mainly oriented to Applied and Fundamental Research in Materials Science. The research groups in the sector have a long tradition of combining High level Education (M.Sc., Ph.D.) with their own research projects making the department an active scientific Centre. The Physics department owns unique research facilities in Portugal grouped in the following laboratories:

1 - Ion Beam Laboratory (IBL) has a 2.5 MV Van de Graaff Accelerator with an ion microprobe end-station and a 210 kV high fluence ion implanter. This infra-structure is open to external users and the experimental studies cover the fields of material science, environment, health, biomedical, atomic and nuclear physics (cross--section measurements).
The research highlights will appear in the following pages under the headings *Advanced Materials Research, Biomedical Studies, Elemental Characterization and Speciation, Materials Characterization with Radioactive Nuclear Techniques, and Nuclear Reactions.*

2 - High Temperature Materials Laboratory (MA^3T) is equipped with a high-resolution, high-temperature diffractometer (*Hotbird*). The *Hotbird* owing to its high specificity and extended capabilities is used to solve difficult problems in advanced materials used in the electronic industry, high-temperature alloys for fusion applications and superconductors. The research activity in the laboratory is merged with that of the Advanced Materials Research Group.

3 - Neutron Spectrometers at the ITN nuclear research reactor RPI comprise a 2-axis diffractometer, DIDE, one SANS instrument, EPA, and one TOF diffractometer for educational purposes. A new detector assembly for DIDE is projected and awaits a funding decision. Tests to improve signal-to-noise ratios are currently under way at the EPA facility. R&D on the characterization of new materials and instrument optimization currently involves collaboration with groups in Aveiro, Saclay, Budapest and Sofia. Design and fabrication of neutron spectrometer components under contract, was carried out for the Greek research reactor at Demokritos NRC. Activities are presented under *Condensed Matter Physics.*

4 - Ionising Radiation Facilities – The Co-60 unit (UTR) with a semi-industrial dimension, has been running to develop applied research for Industrial purposes. In order to develop new radiation technology applications, the upgrading and renewal of the equipment is being carried out by the "Radiation Technologies: Processes and Products Group". This project implies the use of ionizing radiation equipment (e.g. accelerator and gamma experimental facilities), a multidisciplinary laboratory with controlled environment and application of automated-robotic systems in the facilities. The main R&D activities for the application of ionising radiation are described under the heading *Radiation Technologies: Processes and Products.*

5 – Nuclear instruments and Methods activities focus in modelling of radiation fields, calculation of neutron physics parameters, measurement of neutron cross-sections; development of software for control, design of electronic instrumentation for nuclear applications, instrumentation and technical assistance. Activities are presented under *Nuclear Instruments and Methods.*

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J.G. CORREIA, Invited Aux.
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L. FERREIRA, Aux.
M.L. BOTELHO, Aux.
M.T. PINHEIRO, Aux.
M. REIS, Aux.
N. PINHÃO, Aux. (20%)
R.C. da SILVA, Aux.

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M.T. COSTA
H. MARCOS

Advanced Materials Research

Eduardo Alves

The Advanced Materials Research Group (GIMA) is responsible for the major infrastructures installed in the Ion Beam Laboratory (IBL). The laboratory is equipped with a 2.5 MV Van de Graaff accelerator, a 210 kV high fluence Ion Implanter, and an ion microprobe attached to the accelerator.

The work carried out during the last two decades allowed the group to achieve a large expertise on the field of applications of ion beams to Materials Science. The group activities are centred on the processing and characterisation of advanced materials using ion beam based techniques. The large number of National and International collaborations allows a permanent change of experiences and mobility of researchers. This is a condition to keep the scientific activity in the group at the forefront of research.

The current research activities of the group were focused in two kinds of materials: Wide Band Gap Semiconductors and Nanostructures and Insulators. Studies in semiconductors include the doping of GaN and ZnO with optically and electrically active ions. These two wide band gap semiconductors are under intense research all over the world due to the possibility of developing optoelectronic devices working in the visible wavelength range of the electromagnetic spectrum. Our work aims at the optimization of the implantation conditions of the dopants. Other relevant research work is being carried out in quantum well structures. An intense study of the structural properties of GaN/InGaN structures is under way in collaboration with the University of Aveiro and Strathclyd.

The work in insulators is a continuation of ongoing projects or bilateral collaborations. Some of these comprise the modification of the optical and electrical properties of α-Al_2O_3 and laser materials (KTP and RTP), as well as the study of nanoaggregates formed in MgO and rutile by high fluence implantation doping with transition metals. Besides this and due to the potential of ion beam techniques to study thin films and multilayers, important work continued in the characterisation of magnetic thin films for magnetic spin valves and tunnel junctions.

The activity in the technology programme of the European Fusion Development Agreement (EFDA), in association with the Centro de Fusão Nuclear of the Instituto Superior Técnico continued with studies on the oxidation behaviour of beryllides, and on the characterization of the new Eurofer (ODS) steel.

Besides these research activities the group has also been strongly engaged in training graduate and undergraduate students, through the supervision of M.Sc. and Ph.D. thesis.

All these works were financially supported by a large number of projects, both European and National (FCT), in collaboration with other Institutions or led by members of the group.

The scientific activity of the group in 2005 materialized in:

Publications (peer review journals): 50

Conference and workshop contributions: 8 invited talks, 17 talks and 46 posters.

Running projects: 23

Research Team

Researchers (*)

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(*) Also members of CFNUL.
(**) High Temperature Materials Lab.
(***) Technician, Dep. Cons. & Rest., UNL

Characterization and Modification of Group-III-Nitrides with Ion Beams

K. Lorenz, E. Alves, E. Nogales, K. Wang, R. W. Martin, K. P. O'Donnell, R. Nédélec, J. Penner, R. Vianden, S. Ruffenach, O. Briot, and the RENiBEl network

During the last decade the group III nitride semiconductors GaN, AlN and InN as well as their ternary alloys InGaN, AlGaN and AlInN with their wide and direct band gaps have attracted much attention in research and industry due to the wide variety of applications in (opto-) electronic devices, such as light emitters, transistors and sensors.
Doping GaN with optically active rare earth (RE) elements allows the production of electroluminescent emitters that cover the entire visible spectral range. Ion implantation is a powerful technique to introduce electrically or optically active ions in a reproducible way with a defined concentration profile. However, for GaN this method still suffers from the incomplete annealing of the resultant lattice damage and the dissociation of the surface at high temperatures.
Within the frame of the European Research and Training Network RENiBEl the damage built-up during rare earth implantation into GaN as well as post-implant annealing was studied in great detail. The effect of substrate temperature, implantation angle, energy and fluence were investigated. Main emphasis of this year research was put on high temperature annealing. Very significant improvements have been achieved by depositing AlN capping layers on GaN prior to RE implantation.

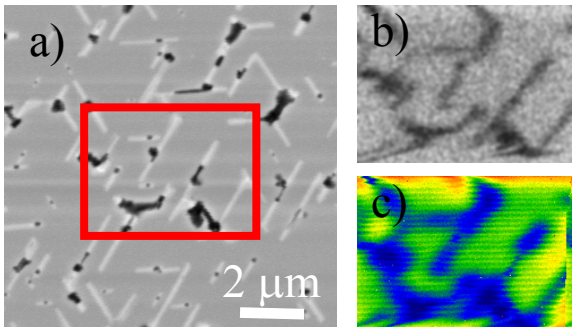

Figure 1: a) BSE image of a Eu-implanted GaN sample after annealing at 1200 ºC; b) the corresponding N-compositional mapping obtained with WDX and c) CL mapping of the integrated intensity from the $^5D_0$-$^7F_2$ transition corresponding to the same area showing decreased N-content and CL intensity within the cracks.

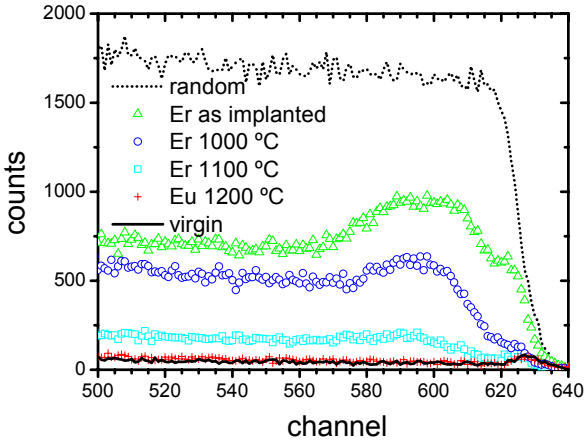

Figure 2: Typical random and <0001> aligned RBS spectra of Er and Eu implanted GaN after annealing at different temperatures.

These lead to greatly increased RE-luminescence efficiency, both as a result of the ability to withstand higher temperature annealing (up to 1300 °C) and as a consequence of reduced damage due to a suppression of implantation induced nanocrystallisation and/or amorphisation. However, small cracks due to the lattice mismatch of AlN and GaN can lead to localized failure due to the out-diffusion of N and the formation of holes (Fig. 1).

In collaboration with the University of Bonn (bilateral project funded by DAAD/GRICES) the influence of the annealing ambient on defect recovery at high temperatures was studied. Samples annealed in N_2 and vacuum show surface damage after annealing at 1000 ºC and are completely destroyed by annealing at 1100 ºC. Annealing in a NH_3+N_2 atmosphere stabilizes the GaN surface which stays smooth up to higher temperatures. After annealing at 1200 ºC in NH_3+N_2 the crystalline quality of the unimplanted GaN material was restored showing only very superficial damage (Fig. 2).

Transparent thin film transistors based on indium oxide semiconductor

A. R. Ramos, E. Alves, G. Lavareda[1,2] , C. Nunes de Carvalho[1,2], E. Fortunato[1], O. Conde[4], A. Amaral[2,3]

Recent work in transparent electronics based on ZnO proved that transparent oxides can be used as semiconductor layer on TFTs. Indium oxide (InO_x) material presents similar properties and therefore can be used in the same way. Several studies and application of InO_x can be found in the literature either as a conductor (TCO) when doped with Sn (ITO) or Ti, or as a semiconductor in gas sensors. In this work, field-effect devices (Thin Film Transistors, TFTs) were made with InO_x deposited by a rf plasma enhanced reactive thermal evaporation (rf-PERTE). InO_x properties were controlled by changing the deposition conditions, in particular the O_2 partial pressure, substrate temperature and rf-power. For TFT production, silicon nitride (a SiN_x) deposited by rf-PECVD was used as gate dielectric. The combined use of rf power and substrate temperature allows the control of the oxygen contents in the film, changing the optical and electrical properties. The films obtained have electrical resistivity ranging from 13.7 to 1.7×10^7 Ωcm. Transparent TFTs made with those films as semiconducting and conducting layers, respectively, present threshold voltages near 2 V and on/off ratios of 104.

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[4] ICEM/Dep. de Física, FC-UL, 1749-016 Lisboa, Portugal

Development of external analytical microbeam at the ITN nuclear microprobe[1]

A. Rodrigues, L.C. Alves, R.C. da Silva

The project started in the last quarter of 2005 and aims to develop and install an external microbeam analytical end-station at the nuclear microprobe facility and fit it with the ion beam techniques of PIXE and RBS, with the intention of applying it mainly to the field of patrimonial studies, particularly in artwork and archaeology.
At this stage, planning and project of the installation of the external microbeam analytical end-station is well underway. This first task comprises the design of the end-station, overall and component parts, and fine trimming the chosen technical solutions. Structural parts and supports, line end and beam extraction window cases have been machined, assembled and vacuum tested. The beam transfer end-section is ready to be included in the analytical end-station.

[1] Project POCTI/CTM/60685/2004

Structural, optical and magnetic properties of ion implanted ZnO

U. Wahl, E. Rita, K. Lorenz, E. Alves, J.G. Correia, T. Monteiro[1],T. Trindade[2], J.P. Araújo[3] E. Wendler[4], W. Wesch[4]

This research topic concerns the structural, optical and magnetic characterisation of ion implanted ZnO, a wide band gap semiconductor which is of particular interest for optoelectronic applications and as a base material for diluted magnetic semiconductors. While ITN is carrying out the ion implantation itself and structural characterisations using RBS and emission channelling, the optical properties of virgin and implanted samples are investigated by means of photoluminescence (PL) at the University of Aveiro. In the case of Mn implanted and annealed ZnO, while RBS revealed a similar lattice recovery as previously observed for Fe implanted samples, no Mn $3d^n$-related optical emission was observed, in contrast to ZnO:Fe. Low temperature (15 K) implantations of N, Ar and Er ions within a large fluence range were performed to study the damage recovery kinetics. Annealing measurements below room temperature show a significant recovery of the lattice starting at temperatures between 80 and 130 K for a sample implanted with low Er fluence. Samples with higher damage levels do not reveal any damage recovery up to room temperature, pointing to the formation of stable defect complexes. Zinc oxide single crystals were implanted with Fe and Mn ions at doses around $1\text{-}5\times10^{15}$ cm^{-2} and supplied to the University of Porto for measurements of their magnetic moment by means of a SQUID. While the investigations of ZnO:Mn are still under way, the Fe implanted sample revealed a clear ferromagnetic signature at room temperature, showing that it is possible to produce ZnO-based diluted magnetic semiconductors by means of ion implantation.

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[3] Departamento de Física, Universidade do Porto
[4] Department of Physics, University of Jena

Structural and Magnetic properties of oxides implanted with transition metals

J.V. Pinto, M.M. Cruz[1], M. Godinho[1], E. Alves, R.C. da Silva

We continued the study of the behaviour of the transition ions Co, Ni and Fe implanted into MgO and TiO_2 single-crystals. Both these oxides are good candidates for future spintronics applications, e.g. through the formation of diluted magnetic semiconductor structures. Our main goal is to fully characterize the behaviour of the implanted ions in such lattices: formation of nanoaggregates with magnetic behaviour and subsequently control the cluster size by thermal treatments. In both cases magnetic characterization as well as structural (RBS and XRD) were used to study these systems. Previous results showed evidence for the formation of nano-clusters of Co, Ni and Fe, having orientation correlation with the MgO host lattice.
In TiO_2, clusters have also been found in the as implanted state as evidenced by their superparamagnetic behaviour. Annealings induce an enhancement of the magnetic moment and a tendency for ferromagnetic behaviour. RBS-channelling shows that these ions have preferred locations in the host. The possibility that a magnetic compound have been formed is being investigated. The electric behaviour of these samples is also being analysed.

[1] Physics Department, Faculdade de Ciências da Universidade de Lisboa.

Characterization of potash-glass corrosion in aqueous solution

M. Vilarigues[1], R.C. da Silva

We continued to study the corrosion processes of potash-glass surfaces in contact with aqueous solutions, using Ion Beam Analysis techniques, Optical Microscopy and Fourier Transform Infra-Red (FTIR) spectroscopy.

Glass samples with base compositions of 56 mol.% SiO_2, 24 mol.% CaO and 20 mol.% K_2O, and added with CuO and MnO as colorants, were prepared.

In order to characterise the corrosion progress these surface studies were combined with the evaluation of the changes taking place in the aqueous solution. In particular, hydrogen profiles obtained from the attacked surface region of glass are compared against the pH changes of the aqueous solutions, in order to extract information about the ion exchange processes. It has been shown that the pH may be a good parameter for studying corrosion kinetics under high humidity conditions.

Finally, two testing conditions, with and without stirring of the aqueous solutions, continued to be investigated as they lead to different surface morphologies.

Colour characterization is in progress making use of Optical Absorption measurements and Ion Beam Induced Luminescence analysis. The application of the late technique for corrosion assessment is also under study.

[1] Department of Conservation and Restoration, Universidade Nova de Lisboa.

Microstructural Studies of PZT Thick Films Directly Deposited on Cu Foils

E. Alves, A. R. Ramos, Aiying Wu[1], P. M. Vilarinho[1], S. Srinivasan[2], A. I. Kingon[2], I. M. Reaney[3]

In this work ferroelectric PZT thick films in the thickness range from 5 to 20 micron were deposited on metal foils by EPD. Flexible copper foils with the thickness of 20 micron were used as substrates. The deposited films were sintered at different temperatures from 900 to 1050ºC. The effect of adding a PbO coating on the film surface was studied with the aim of improving the sintering and producing dense films. Compared with PZT thick films deposited on Pt foils, PZT films deposited under the same conditions on Cu foils showed inferior properties. To understand the influence of the substrate, the phase purity was analysed by x-ray diffraction (XRD). The microstructure of the deposited films and the interface reaction region were inspected by transmission electron microscopy (TEM) and Rutherford backscattering spectrometry (RBS). Although the sintering density and the electrical properties were improved by introducing a PbO coating on the EPD deposited films, the dielectric and ferroelectric properties were worse than those observed on samples deposited on Pt foils. Microstructure studies by TEM and RBS revealed the formation of a Cu-Pb alloy when sintering above 950ºC. The electrical properties of the films were correlated with the reaction region and the density of the films. This undesired reaction can be avoided by depositing a buffer layer and decreasing the sintering temperature in further studies.

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Ge-SiGe heterostructures on relaxed SiGe graded buffers grown by hybrid epitaxy on Si(001) substrates

N. Franco, N.P. Barradas, E. Alves, A.M. Vallêra[1], R.J.H. Morris[2], T.J. Grasby[2], O.A. Mironov[2], E.H.C. Parker[2]

The introduction of SiGe to standard Si-MOSFET technology allows band gap engineering for enhanced performance of HMOS transistors. High hole mobility can be realized using p-type modulation doped $Ge/Si_{1-x}Ge_x$ heterostructures, in which a $Si_{1-x}Ge_x$ buffer layer is used as a virtual substrate (VS) and the Ge layer acts as the active channel. This can be achieved using a fully relaxed VS and a fully strained Ge channel, since the axial strain in the channel leads to an increased hole mobility.
In this work $Ge/Si_{1-x}Ge_x$ inverted modulation doped heterostructures with different nominal Ge channel thickness were grown. Post-growth furnace thermal annealing (FTA) was performed to study the effect on structural properties, such as the strain and composition of the VS and Ge channel. The study was performed by XRD using both symmetric and asymmetric reciprocal space maps (RSMs) so as to accurately determine the Ge composition and strain of the channel, as well similar information for the other layers within the structure. Layer thickness and diffusion was determined with complementary high-resolution Rutherford backscattering (RBS) experiments.

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[2] Department of Physics, University of Warwick, Coventry

Ge islands grown on Si(001) through Vollmer-Weber growth mode

A. Fonseca, E. Alves, J. Leitão[1], N. A. Sobolev[2], M.C. Carmo[2], A. Nikiforov[3]

Si/Ge low-dimensional structures have attracted the attention of the scientific community in last years due to their potential interest in electronic and optoelectronic devices. Among the different ways to produce Ge islands on Si substrates, a technique was recently developed that is based on the Wollmer-Weber growth mode, which relies on the growth of the Ge islands on top of a SiO_2 interlayer. Through this mode, we may obtain smaller Ge islands with extremely high density.
In this work different thicknesses of Ge (3, 6 and 9 Å) were deposited on top of an ultrathin SiO_2 layers with nominal thicknesses of 0.5, 0.75 and 1 ML. Structural and optical characterization were performed by scanning tunnelling microscopy (STM), RBS/Channelling and photoluminescence, respectively. PL results reveal the existence of a broad emission at 0.8-0.9 eV owing to a superposition of the dislocation D1 band (0.81 eV) with another band centered at ~0.85 eV that we attribute to the Ge islands, for thicker Ge sample. For thinner Ge layer sample PL emission is essentially due to dislocation D1 band. RBS/Channelling results show an increase of the minimum yield for the Ge curve as the Ge thickness layer is increased. An increasing of the asymmetry of the angular curves of the Ge with increase of SiO_2 interlayer is observed. These results in conjunction with PL indicate a presence of Ge islands for thicker sample and the inexistence of the islands for thinner sample.

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Damage behaviour of multilayer structures

S. Magalhães, A. Fonseca, N. Franco, N. P. Barradas, N. A. Sobolev[1], E. Alves

In this project we studied the implantation damage formation into GaAs/AlAs multilayers with different periods. The superlattices (S_i) were implanted with 150 keV Ar^+ ions at 77 K with fluences in the range (1-10)× 10^{13} cm^{-2}. The samples were studied with Rutherford Backscattering (RBS)/Channelling and X-ray diffraction techniques and it was found that, even for the thicker GaAs (68 nm)/AlAs (82 nm) period, the higher fluence (10^{14} cm^{-2}) was not enough to amorphize the implanted region. Since the same fluence renders pure GaAs amorphous this is a clear evidence for the influence of the multistructure nature of the samples on the damage production. The X-ray results reveal a new peak shifted to lower angles indicating the formation of a region with higher lattice parameters. Software based on Takagy's solution of the wave equation was created that turn possible the XRR (X-ray reflectometry) spectra analysis. Reciprocal Space Maps were also used to analyse diffuse intensity in the Bragg reflection XRD (X-ray Diffraction) and XRR geometry.

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Production and characterization of nanocolloidal compounds created by ion implantation on α-Al_2O_3

C. Marques, E. Alves, R.C. da Silva, A. Kozaneck[1] C. McHargue[2],

Nanoparticles embedded in dielectric matrixes are of great interest, from both the theoretical and application points of view. The physical properties exhibited by these particles are intriguingly different from those of the respective bulk material. Sapphire is an exceptional host matrix for its unique physical and chemical properties. After implantation of high fluences, well above the solubility limit, the formation of metallic nanoparticles dispersions on the radiation amorphized substrate is observed. Subsequent annealings lead to the stabilization of the systems into colloidal dispersions of precipitates embedded on crystalline sapphire, the composition and size of the precipitates depending on the annealing atmosphere and temperature. Since the optical response is related with the morphology and nature of the precipitates it is thus possible to control and tailor the optical properties of the final systems. On the other hand, low fluences are needed to produce optically active rare-earth dispersions and subsequent annealing tends to redistribute these rare-earths onto lattice regular sites.
The implantation fluence, the temperature and type of annealing atmosphere affects both the emission and absorption/reflection bands of these systems in a controllable way, and are being studied.

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Studies of compositional and structural changes in ZrO_xN_y films depending on growth conditions

E. Alves, A. R. Ramos, N. P. Barradas, L. Rebouta[1], F. Vaz[1], U. Kreissig[2]

The work focuses on the analysis of ZrO_xN_y thin films, the composition evolution with changing growth conditions and its relation with the structural and morphological properties of the films. The films were prepared by rf reactive magnetron sputtering, using different reactive gas flows. Composition and structure were measured combining ion beam analysis (IBA) and X-ray diffraction (XRD) techniques. The depth profiles of nitrogen and oxygen have been obtained by elastic recoil detection analysis (ERDA).
Results showed that the oxygen fraction in the films increases with gas flow, reaching a value of $x \sim 0.33$ for a reactive gas flow mixture of 6.25 sccm. During growth mixed zirconium nitride and oxide phases form. Furthermore, the deposition rate correlates with the oxygen content variations, showing a continuous decrease with reactive gas flow.

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Friction and wear mechanisms in orthopaedic prostheses: influence of the composition of the periprosthetic fluid[1]

E. Alves, R.C. da Silva, B. Saramago[2]

The most common cause of failure and lack of durability of total hip prostheses is related with the generation of wear debris of ultra high molecular weight polyethylene (UHMWPE) from the acetabular part, when sliding against the ceramic or the metallic ball which substitutes the femoral head. Surface treatments and coatings, both on the polymeric and metallic parts, are some of the solutions proposed to improve the tribological performance of UHMWPE components. Titanium nitride (TiN) is one of the most studied ceramic coatings due to its biocompatibility. This material leads to a significant increase in the metallic surface hardness, helps in the protection against corrosion and reduces the bacterial colonization. It is also responsible for a significant decrease of the metal ion release to the biological fluids.
In the present work we have been studying Cl-implanted TiN coating as a potential solution to protect the metallic components of prostheses. Characterisation of the coatings in the as-implanted state and after tribological tests performed by rubbing against UHMWPE in lubricating conditions (the lubricants used were the biological model fluid Hanks' Balanced Salt Solution, HBSS, and solutions of albumin in HBSS) are under way in order to understand the role played by the chlorine ion in the mechanism of lubrication. Comparison studies were made with Ar-implanted TiN coatings to elucidate the specificity of the chlorine ion.

[1] Project POCI/SAU-BMA/55493/2004
[2] Chemistry Department, Instituto Superior Técnico

Optical doping of AlN by Er implantation

K. Lorenz, E. Alves, T. Monteiro[1], M.J. Soares[1], M. Peres[1], S. Pereira[1]

Emissions from optically active rare earth (RE) ions span a wide range of the electromagnetic spectrum from UV to IR including the whole visible spectrum. Due to the large band gap of AlN (~6 eV), energetically high lying RE levels can be incorporated in the AlN gap and a minimal thermal quenching of the intra-4f emitting centres is expected. First RE implantation studies were performed in AlN in the frame of a bilateral project with the University of Aveiro (funded by FCT contract POCI/FIS/57550/2004). AlN is more resistant against implantation damage than GaN but little damage recovery was observed for annealing temperatures up to 1300 ºC. Lattice site location studies show that in thin AlN films Er occupies a site slightly displaced from the substitutional Al-site along a preferential direction while it was found substitutional in thicker films. This displacement from the perfect substitutional site in thin films is probably related to the larger elastic strain. The photoluminescence study showed Er related emission in the IR and green up to room temperature. At least two different luminescent Er centres were observed.

[1] Departamento de Física, Universidade de Aveiro

Advanced magnetic systems for devices

N.P. Barradas, N. Franco, E. Alves, M.A. Reis, R.C.V. Mateus, S. Cardoso[1], P.P. Freitas[1]

ITN has a long-standing collaboration with the INESC magnetic systems group led by Prof. Paulo de Freitas. The role of ITN is to provide structural characterisation of the highly complex advanced magnetic systems produced at INESC. This is a highly interactive collaboration that has proved to be very successful.
This year the work was concentrated in the compositional and structural characterisation of spin tunnel junctions based on MgO barriers and CoFeB magnetic layers. Their properties depend critically on the quality of the insulating barrier, on the B concentration in the magnetic layers, and on the crystalline structure of the layers. Different annealing treatments were employed in order to control these properties. Several complementary characterisation techniques were used at ITN. With RBS the concentration of the heavier elements, as well as some information on the lighter elements, was obtained. Interface roughness and interdiffusion was also studied. PIXE (and, for the first time in these systems, PIGE) was increasingly used to determine the B concentration. XRD and XRR were used to study the crystalline structure of the different layers. Five papers were published in 2005 in international journals.

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Thermophotovoltaic materials based on GaSb

V. Corregidor, N.P. Barradas, E. Alves, L.C. Alves, M.A. Reis, P.C. Chaves, N. Franco, and the TPVCell RTN[1]

Thermophotovoltaic (TPV) cells convert thermal infrared radiation into electricity. Operating temperatures are in the 1000-1500 ºC range, which implies an optimum TPV cell with a band gap between 0.4 and 0.7 eV. Ternary and quaternary III-V semiconductors based on GaSb, like GaAsSb, GaInSb, InGaAsSb, allow one to control the bandgap by changing the In and As concentration. Another important aspect is the ability to control the lattice parameter in quaternary materials, in order to lattice match epitaxial layers to the substrate at the desired bandgap. On the other hand, high quality large bulk quaternary crystals have not yet been produced.
We used RBS and PIXE to determine the composition and thickness of GaInAsSb thin films grown by MOVPE on GaSb. A correlation between the growth conditions and the composition of the layers was found, which was used to optimise the growth process. Complementary XRD experiments were done. Also, GaSb, GaInSb and GaInAsSb crystals grown by Vertical Bridgman and Feeding Techniques, and with an alternating magnetic field, were studied by microbeam/PIXE and XRD. The homogeneity of the In and As distribution was determined, and the quality of the crystals was assessed. Five papers were published in 2005 in international journals.

[1] European Union Research Training Network on Thermophotovoltaic Cells, 1 February 2002 - 31 July 2005, included 9 Institutions.

Advanced data analysis for IBA

N.P. Barradas, C. Jeynes[1], C. Pascual-Izarra[2], N. R. Nené, A. Vieira[3]

Ion Beam Analysis (IBA) is a cluster of techniques dedicated to the analysis of materials. Our goal is, on the one hand, to improve the accuracy of the data analysis by developing advanced physical models and introducing them in computer codes available to the community, and on the other hand to automate the data analysis.
We developed a new model to calculate accurately the signal of sharp resonances, which is essential for instance in resonant depth profiling, but also whenever a resonance occurs deep in the sample. A new model to calculate the signal of inclusions, voids, and quantum dots, was developed, opening a whole new range of possibilities for the application of RBS. The models to calculate the influence of double and multiple scattering, and sample roughness, were also improved. The work on automation was centred on developing artificial neural networks for extremely complex systems. Finally, Bayesian inference with the Markov chain Monte Carlo technique was used to determine the stopping power of ions in matter. Five papers were published in 2005 in international journals.

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Characterisation of advanced materials for Nuclear Fusion reactors

E. Alves, L.C. Alves, A. Paúl [1], N. Franco, M. R. da Silva [2], J. A. Odriozola [1]

The study of advanced materials to be employed in the ITER and DEMO nuclear fusion reactors was continued, in particular for the case of titanium beryllides and ODS-RAFM (Oxide Dispersion Strengthened – Reduced Activation Ferritic Martensitic) steel samples. The beryllium-titanium compounds under study had a nominal composition of Be-5at%Ti and Be-7at%Ti. The structural stability of titanium beryllides and its oxidation behaviour under air annealing was investigated. High resolution x-ray diffraction, nuclear microbeam and SEM techniques were used to follow the evolution of the composition and crystalline phases as well as the microstructure. Based on the EUROFER 97 composition reinforced with Y_2O_3, two types of ODS steel samples were studied. Microstructure characterization experiments of these steels were performed in the initial normalized and tempered condition and after long term annealing (700ºC during 5000h in ambient atmosphere) using nuclear microprobe and SEM techniques. The different results obtained for the extension of the oxidized layer point out for a better understanding and a refinement of the manufacturing procedure.

[1] Instituto de Ciencia de Materiales de Sevilla, Spain;
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Development and applications of ionoluminescence to study optical active defects and impurities in materials

L.C. Alves, C. Marques, R.C. da Silva, E. Alves

An Ionoluminescence facility was installed at the nuclear microprobe. The set-up consists of a Jobyn-Yvon TRIAX190 spectrograph and a Peltier-cooled multi-array CCD detector for selection and detection of electro-magnetic radiation in the range of 300-1000 nm, coupled to a specially made optical device for light collection and optical fibres for transmission to the spectrograph. Light emitted during ion irradiation can give information on the molecular structure of compounds, band gap transitions on insulators and semiconductors, crystal defects and the presence of some type of impurities, while maintaining, at the same time, all the other capabilities of ion beam analytical techniques. The technique is being applied to the characterization of sapphire implanted with Mn or Eu and to the study of surface corrosion processes of glass. It is also expected to be used in the study of zonation in minerals and then contribute to the knowledge of the processes involved in ore genesis.

[1] In collaboration and with financial support from Centro de Física Nuclear da Universidade de Lisboa (CFNUL).

Formation of Nanoclusters by Thermal Oxidation of SiGe and Deposition of Discontinuous SiGe Layers

A. Kling, A. Rodríguez[1], T. Rodríguez[1], J. Sangrador[1], M.I. Ortiz[1], C. Prieto[2], M. Avella[2], J. Jimenez[2], C. Ballesteros[3], J. C. Soares[4]

Ge, Si and SiGe nanoparticles embedded in a SiO_2 matrix are used for nanomemories and optoelectronic applications. Promising approaches for their fabrication are the thermal oxidation of SiGe layers and the direct deposition of discontinuous SiGe layers sandwiched by SiO_2 using conventional low pressure chemical vapour deposition (LPCVD). In the course of this project (Acção Integrada AI-E-24/03) both approaches were investigated. The processes involved in the oxidation of SiGe layers of various thickness and compositions in dry and steam atmosphere were studied by Raman spectroscopy, infrared absorption spectroscopy, cathodoluminescence, TEM and grazing incidence RBS. Important information on the segregation of Ge and the subsequent formation of nanoparticles as well as their dependence on different processing parameters was obtained. During the studies of discontinuous SiGe layers with nominal thickness below 1 nm a model for estimating size and density of nanoparticles using RBS measurements under grazing incidence has been developed. This will help to reduce in future research the number of time-consuming TEM investigations.

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[2] Departamento de Física de la Materia Condensada, ETSI Industriales, Universidad de Valladolid, Spain
[3] Departamento de Física, E.P.S., Universidad Carlos III de Madrid
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Biomedical Studies

Teresa Pinheiro

The research activities within the Biomedical Studies group make use of focused ion beams techniques as well as molecular biology and biochemistry techniques gathering know-how and expertise on a wide range of disciplines from Biochemistry and Biology to Medicine and Physics. The most relevant applications are relative to the study of human pathologies, by assessing elemental distributions in tissues together with clinic, biochemical and genetic indicators. The work performed is carried out exclusively under research contracts that associate several national and international research centres.

The multidisciplinary characteristic of the joint teams also permit to attract young scientists to carry out their B.Sc., M.Sc., and Ph.D. thesis, which programmes of study are often within the activities of financed projects.

Apart from research activities, technical services are provided to private institutions, mainly on the charac-terisation of raw materials for the pharmaceutical industry.

Presently the instrumental capabilities for elemental and morphology determination using ion beams are becoming fully explored and rapidly overwhelmed by new instrumentation developed in the past decade. Thus, some efforts are being done to diversify the analytical possibilities, such as to explore the combination of nuclear microscopy with other microscopy techniques and to determine molecular probes to assess cell/tissue response. New research projects for the forthcoming triennium and the recently approved FCT projects of the programme for infrastructure modernisation, in particular those that will enable the acquisition of modern tools on the analysis of chemical elements and their species will open novel possibilities to broaden research activities on current issues.

The main achievements of the research developed during 2005 are summarised in the following pages.

Research Team

Researchers (*)

T. PINHEIRO, Aux., Group Leader
L.C. ALVES, Aux. (25%)

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Technical Personnel

R. PINHEIRO

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(*) Also members of CFNUL.

Inflammation and redox status in human diseases

P. Napoleão, A. Veríssimo, M.C. Santos[1], A.M. Viegas-Crespo[2],A. Bugalho de Almeida[3], P. Monteiro[3] A. Barreiros[4], L. Veiga[5], T. Pinheiro

The human pathologies highly prevalent in the western population such as atherosclerosis, with a particular emphasis on coronary artery disease (CAD), and chronic obstructive pulmonary disease (COPD), have been the prime areas of research in the past years. How morphologic, metabolic, inflammatory and redox markers can interact to initiate and propagate disease are the common ground of the research activities.

Atherosclerosis, the main cause of CAD, is an inflammatory disease in which immune mechanisms interact with metabolic risk factors to initiate, propagate, and activate lesions in the arterial tree.

The developed research on atherosclerosis under the Project POCTI /ESP/41008/2001-2005, evolved to the study of CAD, under a Ph.D. thesis programme (SFRH/BD/18822/2004) with the collaboration of the Department of Cardiology of Hospital Sta. Marta (Lisbon). Some of the morphologic, metabolic and inflammatory indicators studied, so far, were narrowly interpreted and others included or combined. Presently, global health status is assessed for all patients and healthy cohorts (morphologic data, and systemic indicators, as lipid profile, haemogram, metabolism of Fe, activity of transferases, C-reactive protein, albumin, among others) enabling to progressively establish and enlarge data basis. Pro-inflammatory cytokines (TNF-a, and interleukins), anti-inflammatory interleukins, soluble cytokine receptors and adhesion molecules (e.g. P-selectin), and indicators of metabolism and redox balance, as nitric oxid (NO), LDL oxidation (ox-LDL) and paroxonase activity, respectively, are parameters included in the study.

The different markers are being assessed longitudinally, in patients with CAD, from acute coronary failure along recovery. The variations observed for some of them are illustrated in Fig.1-a,b.

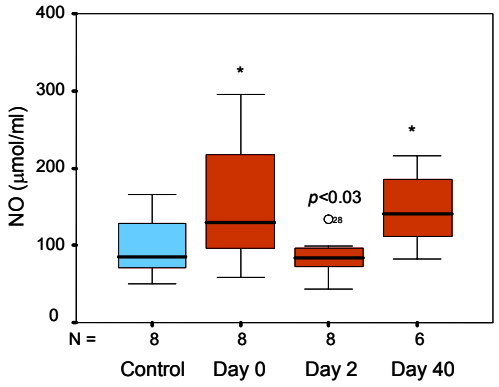

Fig. 1a – NO concentration for controls and CAD patients. Significant differences to controls (*) and within CAD (p-value).

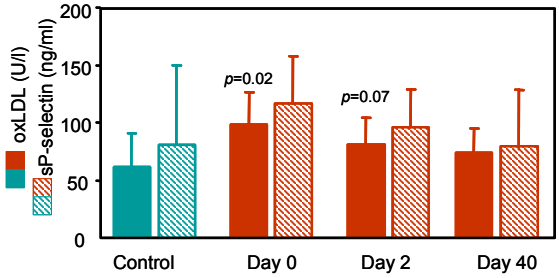

Fig. 1b – Soluble P-seletin and ox-LDL concentrations for controls and CAD patients. Significant differences to controls (p-value).

Chronic Obstructive Pulmonary Disease (COPD) is a highly prevalent disease (affecting ca. 5% of the Portuguese population) associated with airway inflammation. The relationship between functional parameters, and indicators of redox balance and inflammation were studied (Project FCG/SDH.IC.I. 01.22/2001-2005). Changes in inflammatory and redox markers both locally (sputum) and systemic were found for stable and exacerbated patients with COPD. These changes could not be associated to the smoking history and/or habits of the patients, although some of them can be associated to the severity of the disease as is the case for interleukin 8, eosinophilic cationic protein, plasma contents of Fe, and Se, and activities of specific enzymes of the redox balance. The parameters that better evidenced COPD changes show combined variability, as illustrated in Fig. 2.

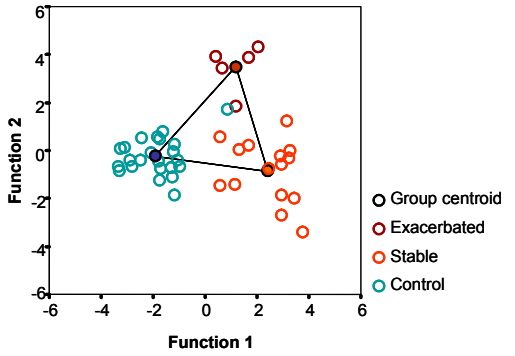

Fig. 2 – Discriminant analysis for the COPD data set established, separating the three studied groups. Retained parameters having significant correlation for sputum (S) and blood indicated in the graph.

[1] Centro de Química e Bioquímica, FC-UL
[2] Centro de Biologia Ambiental, FC-UL
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Assessing iron overload through skin in human metabolic disorders

T. Pinheiro, L.C. Alves, I. Guinote, R. Silva[1], R. Fleming [2], A. Barreiros [3]*

Hereditary or secondary hemochromatosis induces iron overload facilitating the occurrence of a variety of diseases, including cirrhosis, congestive heart failure, diabetes, and hepatocellular carcinoma. Skin is an accessible organ, affected by this disease and can be used to monitor body iron status. Iron metabolism indicators, such as serum ferritin concentration, total iron binding capacity and transferrin saturation, iron concentration in serum, plasma, and skin, and the determination of iron deposition in liver were assessed in nine patients with hereditary hemochromatosis (hetero or homozygoty for at least one HFE gene mutation – C282Y or H63D) along the therapeutic programme. Skin and serological evaluation was made before and after the initial phase of therapeutic (weekly phlebotomies) and six months after stopping the initial phase of the phlebotomy programme. Liver iron deposits were determined at least before and after therapy. A strong relationship between iron concentrations in skin and plasma iron and serum ferritin contents was found ($p < 0.02$). Iron deposition increase in liver, as assessed by Nuclear Magnetic Resonance, was related to ferritin concentration and transferring saturation rise in serum ($r^2 > 0.9$; $p < 0.001$) and at a less extend to increased iron concentrations in skin ($r^2 = 0.65$; $p<0.1$). Also the serum hepcidin content a peptide excreted by liver that is believed to regulate intestinal Fe absorption is being determined.

The relationship of the parameters measured for iron metabolism and organ deposition may help to a better understanding of iron pools mobilisation. In particular skin due to its accessibility may constitute an alternative marker to the disease progression and therapy efficacy. The study is supported by the projects SPDV /2004-2006 and IAEA RC 302-F1.20.19-POR-13262 2005-2007.

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* IEFP fellow at ITN

Skin Permeability to Nanoparticles

T. Pinheiro, L.C. Alves, A. Veríssimo, M. Amin+, R. Silva[1], J.N. Silva[1], P. Filipe[1], P. Moretto[2], J. Pallon[3], T. Butz[4]*

Nanoparticles of TiO_2 and ZnO are widely used in commercial sunscreens by their capacity to scatter UV wavelengths of sunlight. Skin exposure to commercial products containing nanoparticles of Ti, Zn, and Si oxides, among others and their trans-epidermal diffusion has been studied using nuclear microscopy techniques. One of the objectives of the work is to assess the percutaneous penetration depth of Ti oxides. Therefore, methodologies were adjusted to enable the validation of elemental distribution maps or profiles with high-resolution images originated in transmission mode (STIM, Scanning Transmission Ion Microscopy). The work is carried out under a European consortium EC/QLK4-CT-2002-02678.

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[4] University of Leipzig, Leipzig, Germany; * ITN fellowship, + M.Sc. student UM, Braga.

Bioavailability of Fe, Cu and Zn in small mammals in a pyrite mining area, South Portugal

T. Pinheiro, M.A. Barreiros [1], C. Ralheta [1], C. C. Marques [2], S. L. Gabriel [2], M. L. Mathias [2]

Mining areas are ecologically significant sources of metal contamination. Chemical analysis of soil and water can provide useful information on environmental contamination, but cannot easily assess the bioavailability and toxicity of metals in living organisms. Small mammals have been shown to be relevant in habitat contamination monitoring. The Algerian mouse, *Mus spretus,* is a widespread species across its range and has been occasionally used in some ecotoxicological studies. The biological availability of metals in mice inhabiting contaminated areas can be assessed by comparing the concentration of metals in the environment (e.g. surface water) with the corresponding body burdens of the exposed animals. This work is part of an ecotoxicological survey (project POCTI/BFE/3991/2001-2005) carried out in a mining area, included in the Iberian Pyrite belt, South Portugal. A reference area with similar environment conditions (climate and vegetation) was chosen based on the absence of known sources of contaminants. The metals present in water were determined using Total Reflection X-Ray Fluorescence and the elemental contents in liver samples were quantified using both Particle Induced X-Ray Emission and Total Reflection X-Ray Fluorescence techniques. In the mining area, the contamination of surface water with Fe, Cu and Zn is perceptible. However, only Fe accumulates in the liver of exposed animals when compared with those from the reference areas. Also, an increase in Se concentration was observed suggesting changes in the health condition of the exposed animals.

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Elemental Characterization and Speciation
CEEFI

Miguel A. Reis

The Elemental Characterization and Speciation Group of the LFI (CEEFI) was born in 2003 in the sequence of a small reorganization of activities using the 2.5 MV Van de Graaff accelerator of ITN, namely in what concerns activities previously in the framework of the Atmospheric Elemental Dispersion (DEA) unit.

CEEFI carries out work of research, development and application of ion beam based nuclear analytical techniques for the characterization of samples elemental composition, aiming also at speciation methodologies. So far, the main focus is put on particle induced x-ray emission (PIXE) and airborne material. Atmospheric environment related samples like airborne particulate matter and/or biomonitoring samples are different faces of this focus. Widening of this focus is presently being undertaken in order to cover a broader but more concise focus on small mass samples as particulate like and/or thin film samples.

In complementary lines of work, the group assumes that it is important not to depend exclusively on collaborations neither for sampling nor for data handling processes. Therefore, R&D is carried out on airborne particles sampling and on data handling methods, both for spectra handling and for aerosol and biomonitor multielemental data analysis.

Taking into account that PIXE is already a matured analytical technique, services are provided to both the community in general and the scientific community in particular. In this last case, the analysis of samples other than environmental is carried out, and case studies do sometimes lead to spin offs associated to details or specific developments of the PIXE technique.

Within the organics of the Ion Beam Laboratory (LFI), CEEFI is responsible for the maintenance and improvement of the PIXE line, assuring that (at least) there are no losses on the installed capacity.
In 2005, the groups' activity was focused on preparing the launch of a large re-equipment project approved in 2004, namely the: Laboratory for Characterization and Speciation of Aerosols (LCEA). These included training of young members, testing the robustness of airborne particles sampling prototypes developed at ITN, and improvements on the existing data handling software. Still, during 2005, the major funding for this project become available only in the end of the year, therefore only the first steps of the projects could be carried out.

Research Team

Researchers (*)

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Students

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S. ALEIXO, Undergraduate student

Technical Personnel

R. PINHEIRO

(*) Also member of CFNUL

Characterization and Speciation of Aerosols

M.A. Reis, P.C. Chaves, A. Quaresma, R. Pinheiro

Objectives

The characterization and speciation of aerosols, is the basis and central issue of the CEEFI group work, since it is based on this data that uptake and/or impact models are tentatively established. Each of the specific activities of the group therefore converges towards this aim, or emerges from it. During 2005, the main activity undertaken was the operation of an airborne particle sampling unit at ITN campus, and the advanced formation and renewal of members of the CEEFI team, aiming at the launching of the Laboratory for the Characterization and Speciation of Aerosols (LCEA) during 2006. LCEA will be a major demonstration unit infrastructure intended to characterize as best as possible the aerosol present at the ITN Campus, and as well as airborne particulate matter sampled in a few locations that will configure a small network spread across the country.

Results

During 2005 the monitoring protocol used was identical to that used during 2004, namely an intermittent (6 minutes on, 18 minutes off) all days sampling with filters being replaced every week. In this way an almost continuous monitoring is achieved while preserving the number of samples within reasonable limits. In parallel to this, a database structure, which includes samples historic record, was created. Presently this database is under thorough debugging of both structure and data. Publication of this database is scheduled for mid 2006.

In Fig. 1 the time series of week averages of chlorine in airborne particles determined during 2004 is presented. The comparison to the results from 2005 show that in both years events showing very high Cl concentrations in fine particles were identified essentially in the same periods of the year. Further data gathered from these samples leads to a hypothesis of a problematic situation originated from a combination of anthropogenic emissions (pollution) clear sky and strong marine influence. Still no information is yet available on the chemical species holding this chlorine although the NaCl possibility can be practically excluded based on results from XRD. Further investigation is nevertheless necessary to trace this PM2.5 chlorine origin. The results from 2005 definitely exclude the hypothesis of single occurrence that was posed when only the 2004 data was available. The unexpected nature of these results clearly shows the importance of multi-element continuous monitoring of airborne particles composition

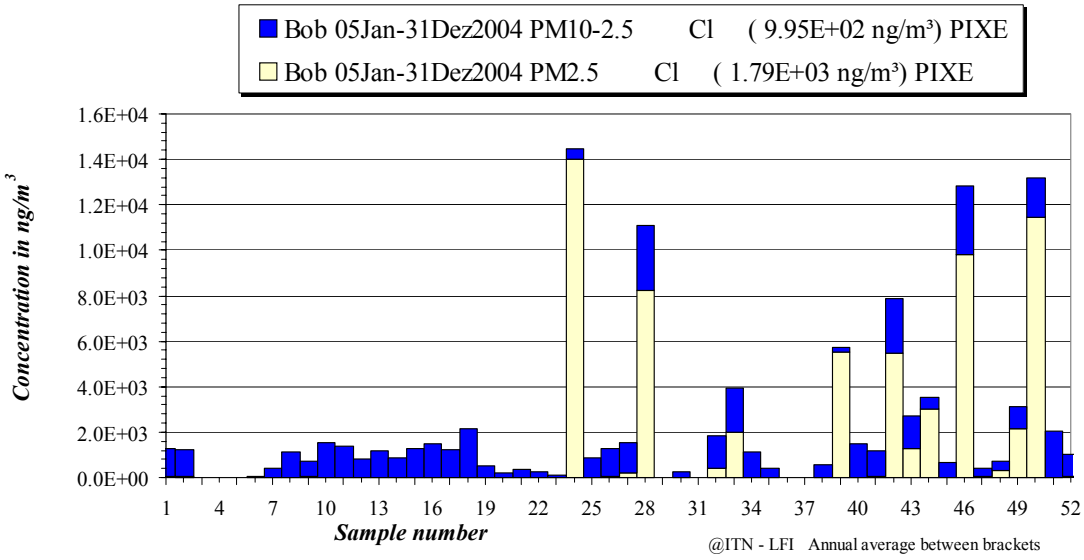

Fig. 1: Airborne chlorine week average concentration in PM10 specifying the PM2.5 component, determine at ITN during 2004.

Materials Characterization with Radioactive Nuclear Techniques

João Guilherme Martins Correia

A **laboratory infrastructure** on materials characterization is maintained and developed at ISOLDE-CERN by the Nuclear Solid State Physics group of ITN and CFNUL. ISOLDE is a unique facility in the world where more than 750 isotopes and 75 elements are produced and delivered as ion beams of high elemental and isotopic purity. In this context nuclear techniques such as **Emission Channeling (EC)** and **Perturbed Angular Correlations (PAC)** provide complementary information to the materials analysis capabilities available at the ITN home institute. The ITN-CFNUL infrastructure and related projects are refereed and reevaluated each year within the scope of FCT-supported CERN projects. The scientific work is currently centered in three research subjects, which have been approved with beam time at ISOLDE by the ISOLDE Scientific Committee:

a) IS368 "Lattice Location of Transition Metals and Rare Earths in Semiconductors". Within this subject, the lattice sites of impurities in technologically relevant semiconductors (e.g. Si, Ge ZnO, GaN) and oxides (e.g. $SrTiO_3$, $BaTiO_3$) are studied by means of the emission channeling technique.

b) IS360 "Studies of High-Tc Superconductors doped with radioactive isotopes". The PAC technique is used to study the atomic ordering of fluorine and oxygen dopants at the Hg planes of the first three members of the $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$, high-Tc family of superconductors. The aim is to understand if dopant ordering and consequent lattice deformations are related or unrelated with charge ordering stripe formation at the superconducting planes.

c) IS390 "Studies of colossal magnetoresistive oxides with radioactive isotopes". PAC is used to probe local lattice deformations and relaxation of the $Mn^{3+}O_6$ octahedra on manganites as a function of doping and temperature. In this way phase coexistence and polaron dynamics are studied, which are local phenomena that are correlated with charge transport mechanisms in giant magnetoresitive materials.

The group is also involved in technical research and development of position-sensitive Si pad detectors. The aim is to implement fast, self-triggered detectors which will allow performing EC experiments on-line with short lived isotopes, which cannot be accomplished with the present set of detectors. The first of the new detectors is scheduled to run in 2006.

Since the obtained information (i.e. the precise lattice location and rms displacements of impurities in crystalline solids, or impurity interactions with point defects or with local lattice deformations) is not accessible by other techniques, radioactive methods also have the potential for being applied to different subjects or new materials. It is intended that in the near future new EC and PAC experiments will provide high precision insight on low temperature phenomena such as element relaxation in semiconductors and superconductors, or on charge diffusion processes in insulators.

At CFNUL we support and form young engineers working in nuclear electronics, with the aim of developing and implementing new detectors with LYSO scintillators, for improved energy resolution in complicated PAC cascades.

Of interdisciplinary nature, these activities integrate and initiate young students, from different backgrounds and universities, in applied nuclear physics. With shared work between the different environments of ITN, CFNUL and ISOLDE – CERN, there participate students and senior researchers from the universities of Lisbon, Aveiro, Porto, Braga, as well as from Leuven, and Bonn. Actually, five Ph.D., one M.Sc. and three diploma students accomplish their work within this infrastructure and scientific proposals

Research Team

Researchers

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E. ALVES, Aux. (10%)

U. WAHL, Pos-Doc. (30%)

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A.L. LOPES, Ph.D. student, FCT grant
S. DECOSTER, Ph.D. student, IKS-Leuven grant
B. DE VRIES, Ph.D. student, IKS-Leuven grant
T. MENDONCA, Graduate student, POCTI grant
S. COSTA, Graduate student, POCTI, grant

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Emission channeling lattice location studies

U. Wahl, J.G. Correia, E. Rita, A.C. Marques, E. Alves, B. De Vries[1], S. Decoster[1], A. Vantomme[1], J.C. Soares[2], and the ISOLDE collaboration[3]

Objectives

The aim of this work is to study the lattice location of dopants and impurities in technologically relevant semiconductors and oxides by means of emission channelling (EC) from radioactive isotopes. The experiments are carried out using the ITN/CFNUL infrastructure installed at CERN's ISOLDE facility.

Results

1. Arsenic as a Zn-site impurity in ZnO

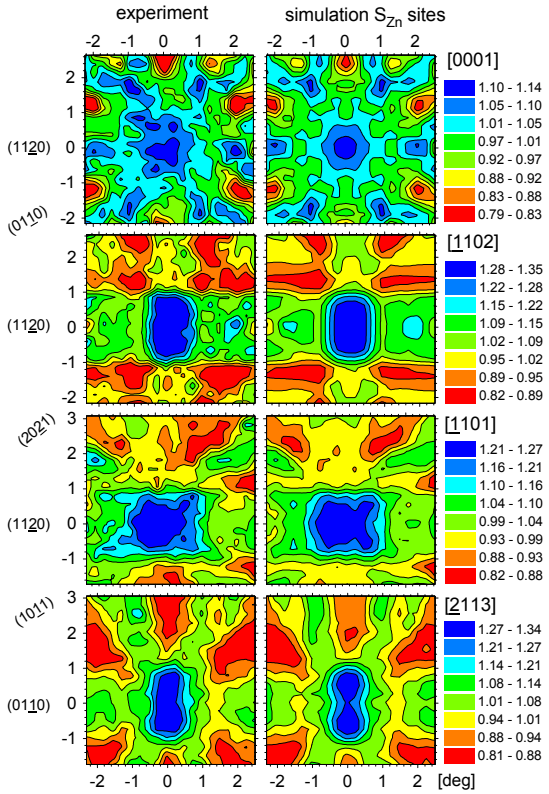

Fig. 1: Experimental EC patterns from ^{73}As in ZnO (left) and simulations for As on Zn sites (right).

Arsenic has been reported in the literature as one of the few p-type dopants in the technologically promising II-VI semiconductor ZnO. However, there is an ongoing debate whether the p-type character is due to As simply replacing O atoms or to the formation of more complicated defect complexes, possibly involving As on Zn sites. We have determined the lattice location of implanted As in ZnO by means of conversion electron emission channelling from radioactive ^{73}As. In contrast to what one might expect from its nature as a group V element, we find that As does not occupy substitutional O sites but in its large majority substitutional Zn sites. Arsenic in ZnO (and probably also in GaN) is thus an interesting example for an impurity in a semiconductor where the major impurity lattice site is determined by atomic size and electro-negativity rather than its position in the periodic system.

2. Lattice sites of implanted Fe in Si

Fe represents, together with other transition metals such as Cu, Ni or Co, one of the most dangerous contaminants in Si processing technology. However, little has been known on possible lattice sites of Fe in Si. Using β^- emission channelling from the radioactive isotope ^{59}Fe implanted into Si single crystals at fluences from 1.4×10^{12} cm^{-2} to 1×10^{14} cm^{-2}, we identified Fe on three distinct sites: ideal substitutional, displaced substitutional and displaced tetrahedral interstitial. Whereas displaced substitutional Fe was dominating for annealing temperatures below 500°C, annealing between 500-700°C caused the majority of Fe to occupy displaced tetrahedral interstitial sites. Ideal substitutional positions were increasingly populated following annealing at 800°C and above.

3. Lattice location of implants in $SrTiO_3$

$SrTiO_3$ is a semiconducting, perovskite-type oxide with a band gap of 3.2 eV and a high bulk dielectric constant. Its optical, magnetic or electrical properties can be modified by doping, allowing for some possible applications in microelectronics. Since implantation damage in $SrTiO_3$ is removed around 400°C, ion implantation has the potential to represent an attractive approach for doping, however, little has been known whether implants are incorporated on proper lattice sites. In that respect and in order to further investigate the annealing behaviour of implanted $SrTiO_3$, we are currently carrying out lattice location studies of a number of implanted impurities such as Cu, Ag, Fe and Sr. First results indicate that the group Ib impurities Cu and Ag mainly substitute for Sr atoms while Fe prefers Ti sites.

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IS360 experiment – Atomic ordering of fluorine dopant in $HgBa_2CuO_{4+\delta}$ and of oxygen in $HgBa_2CaCu_2O_{6+\delta}$ high-Tc superconductors

T. Mendonça, J.G. Correia, H. Haas, S. Costa, A.M.L. Lopes[1], J.P. Araújo[2], A. Pereira[2], V. Amaral[1] and ISC[3]

Lattice sites and collective ordering of fluorine atoms in oxygen-reduced samples of $HgBa_2CuO_4$, Hg1201, and of oxygen doped samples of $HgBa_2CaCu_2O_{6+d}$, Hg1212, were investigated with the perturbed angular correlation technique by measuring the electric field gradients induced at ^{199m}Hg nuclei. For the Hg1201:F doped samples the experimental data were interpreted with the help of ab-initio calculations of charge distributions for different fluorine configurations in $Hg_mBa_{2m}Cu_mO4_mF_n$, supercells. Internal parameters were allowed to relax, to cancel residual atomic forces due to the dopant. The experimental results show clearly that fluorine occupies only the center of the mercury mesh. For a fluorine content $\delta F > \sim 0.35$ best agreement with theoretical data is obtained under the assumption that fluorine shows a tendency toward ordering along interstitial rows parallel to a, b. No strong ordering of the transferred charge at the copper planes is present in the computed charge density, even when the fluorine atoms order at high concentrations. Therefore, it is concluded that charge stripes observed at the superconducting Cu planes do not seem correlated to the dopant atomistic behavior. For the oxygen doped Hg1212 samples, a new sol-gel method of preparing the precursors by replacing the acrylamide transport agent by urea was implemented with success. After high pressure mercurization the right Hg1212 phase was obtained with high purity and the PAC experiments were done under oxygen pressure. Still under analysis, these results hint the dopant reordering as a function of temperature and concentration – work to be accomplished in 2006.

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IS390 experiment – Studies of free percolative phase transition on ferromagnetic insulator manganites

A.M.L. Lopes[1], J.P. Araújo[2], J.J. Ramasco[2], E. Rita, V.S. Amaral[1], J.G. Correia, R. Suryanarayanan[3] and ISC[4]

We report atomic scale studies of the ferromagnetic insulator manganite $LaMnO_{3.12}$ using PAC spectroscopy. Data analysis reveals a nanoscopic transition from an undistorted to a Jahn-Teller- distorted local environment upon cooling. The percolation thresholds of the two local environments enclose a macroscopic structural transition (Rhombohedric-Orthorhombic). Two distinct regimes of JT-distortions were found: a high temperature regime where uncorrelated polaron clusters with severe distortions of the $Mn^{3+}O_6$ octahedra survive up to T ~ 800 K and a low temperature regime where correlated regions have a weaker JT distorted symmetry. Such work is being extended to several other doping stoichiometry and $^{16}O/^{18}O$ isotopic ratios.

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R&D development – new self-triggered Si pad detectors for position sensitive electron detection

A.C. Marques[1], U. Wahl, J.G. Correia, P. Weilhammer[2], E. Chesi[2], A. Rudge[2]

This development is made in collaboration with CERN's Compton camera project on new positron emission tomography (PET) devices http://xray.web.cern.ch/xray/publications/Lyon2000PaperCERNPreprint.pdf, whose technology and detectors also fulfill the requirements for electron emission channeling experiments. In 2005 a 1 mm thick 22×22 Si pad detector was mounted on a newly designed printed circuit board equipped with fast VATAGP3 preamplifier chips. The tests of the VME readout methodology and the readout chain in "sparse" (single channel readout) and "serial" (full readout) modes are now completed. The available data acquisition software for the Compton camera project was modified to better serve the emission channeling purposes for on-line/off-line experiments. Several hardware tests were done with different X-ray sources to study gain linearity, energy resolution (~1.5 keV FWHM at ~17 keV) and to optimize the low energy trigger threshold. The technical design of the detector housing and of a new implantation chamber has been accomplished and will be executed early 2006.

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Nuclear Reactions

Adelaide Pedro de Jesus

This group has been involved in the study of proton-induced nuclear reactions with the objectives to obtain cross sections of nuclear reactions relevant to nuclear astrophysics and to extend analytical capabilities to light elements.

So far, the experimental work has relied upon ITN – Ion Beam Laboratory based on a 2.5 MV Van de Graaff accelerator. This facility has allowed the development of an accurate method to measure in an absolute way cross sections of relevant nuclear reactions. Also for the applied point of view an effort has been done to complement the already installed PIXE facility by developing a set-up of PIGE analysis for light elements.

In order to proceed with experimental work related to astrophysically relevant nuclear reactions, the group has joined LUNA (Laboratory for Underground Nuclear Astrophysics) collaboration and also established collaboration with Prof. Claus Rolfs group of Bochum University. Work under LUNA collaboration was centred on the study of the reaction ^{14}N (p,γ) ^{15}O and in Bochum the work was related to the study of electron shielding effects on nuclear reaction cross sections and also to the study of the reaction $^{7}Li(p,\alpha)^{4}He$, at very low energies. Target preparation and stoicheiometry analysis by ERD, RBS, PIGE and NRA, has been done at ITN. Also the experimental study of ^{7}Li (p,α) ^{4}He at energies above 100 keV is proceeding in ITN.

In the short term the work to develop a calibrated PIGE set-up will be concluded, opening new perspectives in applied work for Environment, Materials and Health Sciences and Geology. The acquisition of a new accelerator will bring new perspectives of studying ITN astrophysical relevant nuclear reactions, opening also a broad field of implementation of analytical techniques.

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Experimental Study of Nuclear Reactions for Astrophysics

J. Cruz[1,2], A.P. Jesus[1,2], Hélio Luís, Micaela Fonseca, J.P. Ribeiro[2,3]

Objectives

A precise knowledge of nuclear reactions cross sections (or S-factor) of light elements is crucial for the understanding of the evolution of the very early universe.

Since these reactions occur in stars at very low energies (Gamow peak), with extremely low cross sections decreasing exponentially with energy, efforts to measure it at theses energies requires pure targets, low background environments and very stable accelerator machines. The going-on work program is related to:

1. Measurement at ITN of cross sections and angular distributions of the reaction ^{7}Li (p,α) ^{4}He.
2. Experimental work on reaction cross-sections at relevant energies (around the solar Gamow peak) under LUNA (Laboratory for Underground Nuclear Astrophysics) collaboration, namely the reaction ^{14}N (p,γ) ^{15}O.

Results

1. Lithium is one of the most interesting and puzzling elements in the field of nucleosynthesis. Its most abundant isotope, ^{7}Li, has the rather unique status of requiring three entirely different nucleosynthetic processes, which are not completely understood.

   The reaction ^{7}Li(p,α)^{4}He is the major reactions of Li destruction, having thus a crucial contribution to Li abundances. Even though there are several different cross sections measurements for this reaction, they lead to different astrophysical S-factors at relevant energies.

   At ITN, the experimental set-up for nuclear reactions measurements has been modified and optimized to study this reaction; also at very low energies measurements were done in Bochum. Fig. 1 pertains to results of the astrophysical factor obtained in Bochum, showing at low energies the electron shielding effect.

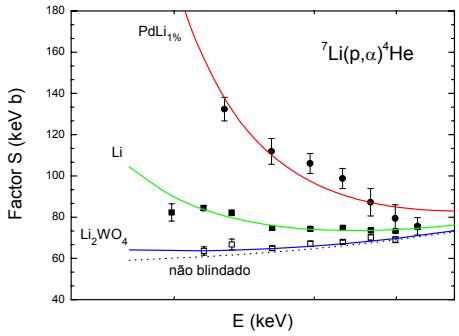

Fig. 1 - Astrophysical factor and screening effect of the ^{7}Li (p,α) ^{4}He reaction measured with different Li targets.

2. At Gran Sasso work on the ^{14}N (p,γ) ^{15}O reaction, was completed. Measurements related to a gas target setup have allowed to attain lower energies than before (with the solid target) leading to a more accurate value of the S astrophysical factor for total capture.

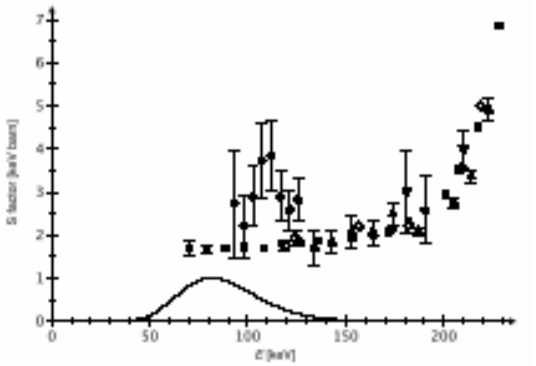

Fig. 2 - Astrophysical S-factor for the ^{14}N (p,α) ^{15}O reaction from the present work (filled squares) and from previous studies. Error bars (1σ statistical uncertainty) are only shown where they are larger than the symbols used. The Gamow peak for $T^{6} = 80$ is also shown**.**

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Calibration of a PIGE Set-up

Bruno Vicente[1,2], R. Mateus[2], Micaela Fonseca[1,2], A. P. Jesus[1,2], Hélio Luis[1,2], J. P. Ribeiro[2,3]

The aim of this work was the extension to further light elements of previous work to install an analytical set-up for light element analysis, based on the detection of the gamma radiation induced by low energy protons, PIGE, in order to complement the already installed PIXE analytical facility.

This technique will open new perspectives of applied work in environment and health problems.

A precise method, based on a code developed in-house that integrates the nuclear reaction excitation function along the depth of the sample, was implemented for thick and intermediate samples. For that purpose some reaction excitation functions were measured in the same analytical conditions. The energy steps needed to define accurately the excitation function were used as energy intervals for the integration procedure.
After the work done for F, Li, B and Na, the excitation function for ^{27}Al (p,p´γ) ^{27}Al, were obtained to introduce as input. Thick target gamma yields for several samples containing Al will be calculated and compared with yields obtained experimentally.

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Condensed Matter Physics

Frederico Gama Carvalho

The Group's main field of research is the development and characterisation of materials with new or improved properties. To this end, radiation is used as a tool to investigate the structure and to induce structural modifications in special samples. Special polymeric materials are currently investigated in collaboration with groups from the Universities of Aveiro and Coimbra, the University of Sophia, Bulgaria, Laboratoire Léon Brillouin (CEA-CNRS-Saclay), KFKI, Budapest, and the Budapest Neutron Centre. During 2005 the main effort was put into the preparation and characterisation of hybrid materials with new properties by radiation induced polymer cross-linking.

The Group is also active in the area of hardware and software instrument development, with emphasis in the design, construction, and testing of systems and components for neutron beam work.

Collaboration with other research groups and a policy of open access for external users to facilities operated by the Group including students are placed high in the ranking of priorities. Two students are presently working for a MSc degree.

The Group's work is supported by funds from FCT, IAEA, ITN and income from services.

Neutron beam facilities. A Two-Axis Neutron Diffractometer (DIDE), and a Small Angle Neutron Scattering Instrument (EPA) are currently under installation in two of the Portuguese RPI research reactor beam tubes. A rotating chopper Time-of-Flight Diffractometer, ETV, is operational. Routine operation of DIDE and EPA is expected to contribute significantly to increase the reactor utilisation and give an additional impetus to the continued operation of the reactor. The TOF Diffractometer is a dedicated instrument for student training. The present RPI reactor flux is adequate for measuring highly dispersive classes of samples and for preliminary measurements preceding data collection at higher flux neutron sources. The reactor also allows in-beam testing of devices such as detectors, collimators and neutron optical components. Upgrading the reactor facility by increasing the power from 1 MW to 5 MW and eventually installing a cold neutron source would open new perspectives for neutron scattering work and the reactor utilisation in general.

Development of components for neutron beam work
Development of the Converging Multichannel Collimator (CMC) based on an original concept was temporarily interrupted in 2005 due to the shortage of manpower especially technicians. The design of a prototype having been completed in 2004, it is intended to proceed in 2006 with the construction and testing of the device.

In-pile components for the Greek research reactor GRR-1, in Athens, were designed, fabricated and already partly installed in December 2005. Fabrication was subcontracted by ITN to ARSOPI, Vale de Cambra, Portugal. The equipment included five aluminium irradiation tubes, two shielding units and two in-pile collimators incorporating beam shutters. The supply of this equipment was contracted with IAEA, Vienna, and the Demokritos Greek Nuclear Research Centre. The in-pile collimators and shutters are to be part of new neutron scattering beam lines.

Design of a new detector assembly for the Two-Axis Neutron Diffractometer DIDE was completed. The assembly with 8 linear position-sensitive ^{3}He counters is projected to replace the old “banana” detector with improved count-rate and equivalent angular resolution. Component acquisition awaits a funding decision.

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Preparation of Silica Based Hybrid Materials by γ Irradiation

F.M.A. Margaça, S.R. Gomes, A.N. Falcão, M. Carrapiço, L.M. Ferreira, F.G. Carvalho and I.M.M. Salvado[1]

Objectives

The purpose of the work is to investigate the influence of the various parameters involved in the preparation process of hybrid materials by irradiation using the ITN ^{60}Co source. This new preparation method avoids the use of solvents and catalysts, required by the sol-gel process, yet undesirable in biomaterial processing.

Results

Silica-based hybrid materials have been prepared by γ irradiation of the precursors polydimethilsiloxane, PDMS, tetraethylortosilicate, TEOS, and zirconium propoxide, PrZr. All samples are macroscopically homogeneous and transparent. Their drying was carried out in air, at room temperature.

The dried mass, normalized to the initial mass, M_{dried}, varies with drying time and with the composition. The pure PDMS sample shows no mass variation. The mass of any sample containing alkoxides decreases with drying time. Fig. 2 shows data plotted in a normalized way by taking the ratio:

$$r = \frac{M_{dried} - M_{PDMS}}{M_{ALK}} \quad \text{with} \quad r \in \Re$$

where M_{PDMS} and M_{ALK} are, respectively, the mass of PDMS and alkoxide used in the sample preparation.

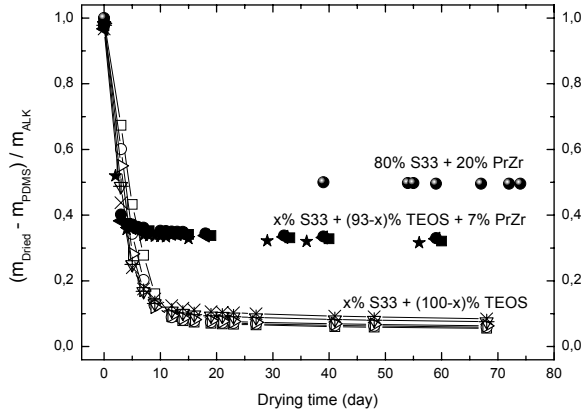

Fig. 2. Normalized dried mass for different content of PrZr and ratios ALK/PDMS = ¼, ½, 1, 2 and 4.

Since the metallic alkoxides are linked to the polymer chains and/or to each other, they lose part of their radicals during the reaction. This process leads to a certain mass loss. For instance, the PrZr molecule $Zr(OC_3H_7)_4$ will loose some carbons and/or hydrogens to link to some other species and in the limit it might become ZrO_2. In terms of molecular weight this means a decrease from 327,57 to 123,22 g/mol. A similar reasoning for TEOS, provides a maximum reduction from the molecular weight variation, when the TEOS molecule $Si(OC_2H_5)_4$ of M_w = 208,3 g/mol becomes SiO_2 for which M_w = 60,09 g/mol. Assuming that, during irradiation and drying, the polymer loses no mass and the alkoxides lose their radicals above, the dried mass, M, could be written as:

$$M = M_{PDMS} + \frac{M_w(SiO_2)}{M_w(TEOS)} \times M_{TEOS} + \frac{M_w(ZrO_2)}{M_w(\mathrm{Pr}\,Zr)} \times M_{\mathrm{Pr}\,Zr}$$

Fig. 3 shows the measured and the fitted values M.

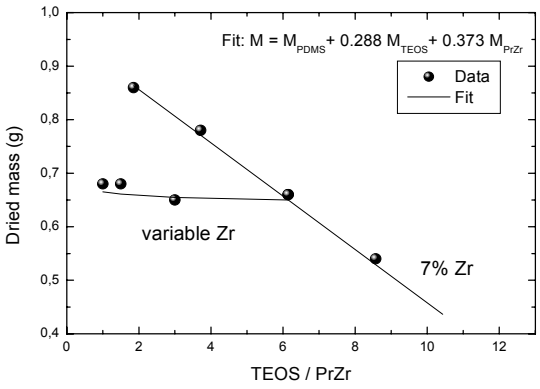

Fig. 3. Data and fit for the dried mass for hybrids prepared with PrZr, TEOS and PDMS.

There is good agreement between the fitting and the experimental data for different alkoxide contents. This evidences the presence of inorganic oxide regions, composed of silica and zirconia. The inorganic oxide mass is ca. 30% of that of the alkoxide. However, when one of the alkoxides is absent there is no formation of an inorganic oxide network, there being only a few individual derived molecules of the other alkoxide linked to the polymer. Both, the dose rate and the polymer molecular weight, were found to have no significant impact in the prepared material. Further investigation, as to the thermal behaviour and the microscopic structure, is in progress.

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New LDPE Copolymeric Films with Enhanced Hydrophilic Properties Prepared by Gamma Irradiation
L.M. Ferreira, A.N. Falcão, M.H. Gil[1]

Graft copolymerisation induced by gamma radiation, from a ^{60}Co source, has being used for the grafting of 2-hydroxyethyl methacrylate (HEMA) branches onto low-density polyethylene (LDPE) films, in order to improve its hydrophilic properties and adequate the material for bio applications.
Sample preparation protocols were selected from previous kinetic studies in order to obtain films with high grafting yields. The obtained PE-g-HEMA copolymeric films were characterized by thermal analysis techniques (DSC and TGA), and by Fourier transform infrared spectroscopy (FTIR).
The results obtained point out that, upon irradiation, there is some loss of cristalinity of the copolymer backbone, but also that the samples keep a good thermal stability. Evaluation of sample water uptake has shown hydration levels up to 95% with a hydration/dehydration average ratio of 1:5, their use as a bio material thus looking promising.
Further work involves haemolysis and oxygen permeability studies of the prepared films as well as the application of the developed technique to other polyethylene based supports, i.e., flexible linear low-density polyethylene (LDPE) tubes.

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Neutron Spectrometers at the Portuguese Research Reactor
A.N. Falcão, F.M.A. Margaça, J.S. Neves, C.M.M. Cruz, M. Carrapiço, D.M.P.S. Silva, F.G. Carvalho

Design work of a new detector assembly for the 2-Axis Neutron Diffractometer DIDE was completed. The new assembly incorporating a set of linear ^{3}He counters is projected to replace the old "banana" detector with improved count-rate and equivalent angular resolution. Implementation of the project awaits a funding decision.
Assembly of the out-of-pile components of the SANS instrument was completed and followed by an extensive series of tests that included beam alignment, improvement of the shielding setup and the measurement of signal-to-noise ratios under different shielding configurations and instrument operating conditions. The tests have shown the necessity of using a cooled beryllium filter preferably before the shutter or immediately after the mechanical velocity selector. First results on the response of the position sensitive detector count-rate to variations of the anode voltage indicate that a further reduction of noise from neutrons of energies above the cadmium cutoff can be obtained by a convenient choice of the high voltage applied.

Design of beam-line components for installation at the Greek research reactor GRR-1
A.N. Falcão, M. Carrapiço, I.F. Gonçalves

In-pile components were designed for the Greek nuclear research reactor GRR-1 installed at the National Research Center for Scientific Research Demokritos. The equipment included five aluminium irradiation tubes, two shielding units and two in-pile collimators incorporating beam shutters. The irradiation tubes and shielding units were ordered to replace existing equipment, whereas the in-pile collimators and shutters are to be part of new neutron scattering beam lines. Design of the new irradiation tubes and shielding units was preceded by careful measurement of the equipment requiring replacement, performed in a delicate operation under high radiation environment. The tubes were measured in different positions, obtained by rotating them around their axis in steps of 30º, using a long ruler and two strategically placed photographic cameras operated by remote control. The final reference dimensions used in the design were calculated using a fitting routine and the data collected with the cameras. The design of the shielding units and that of the in-pile collimators was aided by the Monte-Carlo MCNP code, using semi-empiric approaches of the neutron and gamma ray energy distributions. Construction of the equipment was carried out at the Portuguese company ARSOPI, Indústrias Metalúrgicas Arlindo S. Pinho, Lda, under ITN supervision. Final installation of three irradiation tubes and of the in-pile collimators and shutters was successfully done in December. Installation of the remaining equipment is scheduled to February 2006.

Radiation Technologies: Processes and Products

M. Luísa Botelho

The **Radiation Technologies: Processes and Products** activities focus on the research, development and demonstration of the interaction of ionising radiation with matter for further application in Industry or other entities. Since 1989 these activities have been closely related to the gamma radiation facility (UTR), whose main applications are the sterilization of medical devices and pharmaceuticals and the decontamination of other products. These activities have been leading to an incremental interest by Industrials that have in turn led to a joint venture in 2003 for the management of UTR by CHIP, with scientific and technical support provided by ITN researchers.

Nowadays, the group has a consultant role on sterilization and decontamination procedures, whenever it is solicited by the authorities or private industries. The group also develops work with the National and International normalization, standardization and certification bodies (IPQ, CEN and ISO).

In order to develop new radiation technology applications, the upgrading and renewal of facilities are being carry out. This project implies ionizing radiation equipment (e.g.: accelerator and gamma experimental facilities), a multidisciplinary laboratory with controlled environment and application of an automation/robotic systems in the facilities. These facilities have the main purpose to be open to researchers of National and International Institutions and Industry for developing radiation technologies and/or need of environmental control areas (clean areas) for their work (under REEQ/BIO/996).

The Group main R&D activities are focused on new technologies for further application of the ionising radiation on Food, Pharmaceutical, Wastewater treatment and other areas.

In order to improve our understanding of the Radiation Procedures, the influence of dose rate and the type of radiation (γ and e-beam) in/on products are being studied using Analytical Methods of Microbiology, Chemistry and Physics.

Other purpose of the microbiological work is to develop and implement validation technologies for inactivation procedures for microorganisms, mainly by ionizing radiation (e.g.: γ and e-beam).

These technologies are based on microbiological studies on the bioburden in/on the products, and aim to improve quality in this field. Molecular Biology techniques are also being developed to detect potential pathogenic microorganisms on environmental samples.

Hazard analysis and the control of critical points in the production lines of the studied products are part of the validation studies, carried out for the Pharmaceutical and Food Industries. Environmental control in surgical operation theatres at hospitals is also carried out.

The training and the know-how diffusion are one of the main issues of this Group, so National and International students are developing work within our projects in order to obtain academic degrees (Graduation, M.Sc., Ph.D.)

The financial support of work and students salaries are based on two IAEA projects, one AdI/FCT project, one LPM/MDN PIDDAC project, one re-equipment FCT project, industrial contribution, two IEFP/FSE grant and one FCT Ph.D. grant.

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Effluents

M.L.Botelho, R. Melo, J. Branco, S. Cabo Verde, L. Alves, I. Sousa

Objectives

To implement wastewater and sludge treatment by ionizing radiation in Portugal, R&D work is being developed. This study presents a summary of results that continue to sustain the application of ionizing radiation as complement to biological (2ry phase) and disinfection (3ry phase) on wastewater treatment.

Results

Sets of wastewater, randomly sampled, were analysed by chemical and biological methods after irradiation, at 0.9 kGy.h^{-1}dose rate, with several doses. Results were compared with non irradiated samples.
Instrumental Neutron Activation Analysis and Ionic chromatography (IC) were used to characterize the sludge extractable fraction (soluble) and his potential nutrients.
As shown at Table 1, heavy metal values are below legal limits, for irradiated sludge at low dose rate.

Table 1 - Elemental analysis (INAA) for irradiated (7kGy) and non irradiated sludge (LVE, legal values according to the Portuguese Legislation.

	Concentration (ppm)			
	Cd	Cr	Cu	Zn
Irradiated	5.9±1.2	49.7±1.2	0	579.2±18.8
LVE	20	1000	1000	2500

IC results showed that major sludge solution ion species are Na^+, NH_4^+, Ca^{2+}, SO_4^{2-} and Cl^-. Other important species are K^+ and PO_4^{3-}. Therefore, the leachable components (solution fraction) seem to be rich on the major macronutrients for plants.

To stress the sludge potential as fertilizer, preliminary tests were conducted with clover and maize to evaluate the phytotoxicity of the sludge. The seeds of clover in the water (blank test) germinated at the end of the first day (24 hours) whereas in the sludge treatments the germination only started on the second day. As for the maize, the seeds germination only started one week after the beginning of the experiment. The results obtained in the treatment with the non irradiated and irradiated sludge showed that, till the fourth day after the beginning of the germination, the best results are those with the

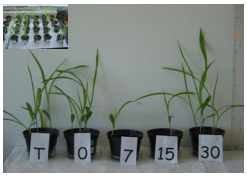

Fig. 1 - Phytotoxicity test using seeds of maize with sludge treatment at 0 kGy up to 30 kGy.

treatment with irradiated sludge at 30 kGy. The pot trial observations are in accordance with these results, as shown in Figure 1.
Microbiological studies showed that microbial populations were heterogeneous with respect to γ radiation resistance. The least resistant organisms appear to dominate the samples, since inactivation was of 99,999 % at 11 kGy, showing an exponential curve with the most resistant organisms present at a tail end at 30 kGy. The predominant bacteria that survived irradiation were gram positive cocci. Comparative kinetic studies were done to compare the growth rate of two isolated strains into wastewater previously irradiated, non irradiated and a standard substrata (TSB) (Fig. 2).

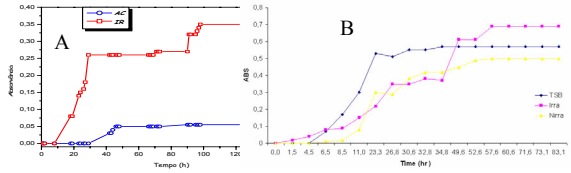

Fig. 2 - Bacterial growth in: A) irradiated and non irradiated effluent and B) irradiated, non irradiated effluent and in TSB.

The results of the irradiated effluent exhibited lower or none lag phase and a lopsided exponential phase whereas the non irradiated effluent displayed a long lag phase and a short exponential phase. The inoculated strain in TSB showed a typical growth curve with a well defined lag, exponential and stationary phase. The biomasses attain higher concentration in the irradiated effluent than in the others subtracts. Therefore, results showed that microbiota microorganisms degrade better the wastewater after irradiation that could be due to a molecular scissor effect, namely at low dose rate.
In conclusion, results point out: 1) according to heavy metal legislation it could be possible to use the treated sludge as fertilizer; 2) can be postulate that sludge has no phytotoxicity effect; 3) γ radiation could lead to the selection of microorganisms that could be useful for bioremediation; 4) sludge irradiation could lead also to fast plant growth.
The overall results, including economical ones, pushed to the benefit of this technology.

Food Irradiation

S. Cabo Verde, M. L. Botelho, M. J. Trigo[1] R.Tenreiro[2], S. Martins[3], P. Luís[3], P. Pinto[3], G. Lima[3], A. Santana[3]

This area aims the application of irradiation as a food safety tool. The "Sanitation of chicken eggs by ionizing radiation" (FCT/BD/2942/2000) project aims the development of the application of irradiation technology to shell eggs and egg-products, in order to get a product free from pathogenic microorganisms, without major effects in nutritional and functional egg properties. Egg-products samples were irradiated in a Co-60 facility, at sub-lethal doses (0.2 to 5 kGy) with a dose rate of 1 up to 4.7 kGy/h. The D_{min} of radicidation and D_{values} were determined for total natural contaminants in egg-products; Comparing thermal and γ-irradiation treatment (≥ 1 kGy), the latter shows higher efficiency than pasteurization in the treatment of the liquid yolk. Egg-products irradiated at doses up to 2 kGy show no detectable alterations on the composition of phospholipids, and a decrease in the viscosity and peroxide index similar to that obtained after egg pasteurization. The sponge cakes and mayonnaises prepared with irradiated egg-products were globally classified as good by a non trained sensorial analysis panel. To guarantee organoleptic acceptable and safe egg-products, a radicidation dose of 1.5 kGy is proposed. To identify possible critical control points in the egg production line, it was applied molecular biology typing methods to egg and its environmental strains to assess their genetic similarity and confirm contamination links. The results obtained support the hypothesis that the feed should be assumed as a Critical Control Point. The Project for improvement of quality and safety of minimally processed fruits and vegetables by gamma radiation (IAEA/POR/11682/RDF) is in its final stage. No important differences were found on the overall sensorial and the physico-chemical properties after irradiation up to 1 kGy, although a decrease of natural microbiota was noticed (>2 log) which leads to an extension of the shelf-life of the analysed fruits and vegetables of at least 3 days.

1 National Agronomic Station, Oeiras, Portugal.
2 Molecular Biology and Genetic Center, Institute of Applied Science and Technology, Faculty of Sciences, University Lisbon, Portugal.
3 Santarém Superior Agrarian School, Santarém, Portugal.

Environmental Control

S. Cabo Verde, M. L. Botelho, S. Cajão, P. Martinho, J. Santos, S. Xisto[1], P. Mazarelo[1],

The project on environmental control of surgical rooms at the Army Hospital is being developed. This study focuses on the development and improvement of alternative techniques to control the environment in surgical rooms in Hospitals. The efficiency of the cleaning protocol was evaluated through the determination of the bioburden, before and after the cleaning action in one surgical room, by means of air sampling (biocolector MAS100), floor and equipment surface swabs, and aliquots of the cleaning solutions. The results obtained point out to a 91% reduction on the floor bioburden after the cleaning action. The cleaning procedure shows not to be so effective on the equipment surfaces and in the air. These results indicate that some corrective actions should be established in the hospital cleaning procedure, namely new disinfectants, in order to improve the air born conditions and eliminate potential nosocomial microorganisms. The air bioburden was also determined before, during and after orthopaedics' surgeries using the biocolector MAS100. The results obtained were compared with previous (2004) bioburden values; a reduction was observed in the number of the microorganisms isolated in the different phases of air collection along two years of studies. The obtained hospital data point to the usefulness of the implemented HACCP study to assess infection risk and nosocomial antibiotic and disinfectant resistant strains. The studies are in progress in order to continue the actions to reduce the risk of infection.

1 Militar Laboratory of Chemical and Pharmaceutical Products, Portuguese Army, Lisbon, Portugal.

Facilities Upgrade for Radiation Technologies Applications

M. L. Botelho, A. Belchior, F. Pereira, S. Cabo Verde, R Melo, L. Alves, H. Marcos

In this field, the project "Upgrading of Radiation Technology unit" FCT CONC-REEQ/996/2001[1] was signed at the end of 2005. Since June 2005 work has progressed, namely 1) Meetings were held with collaborators and potential items deliverers 2) -Controlled lab area-a data base for all equipment specifications is being developed; and 3)-Ionizing radiation equipment – dosimeter systems are under study (e.g.: MNCP, Chemicals).

1 Vide Group Projects.

Nuclear Instruments and Methods

João B. Manteigas

The strategy of the group involves activities in the following lines:

1. Modelling of radiation fields, calculation of neutron physic parameters, measurement of neutron cross-sections;
2. Development of software for control;
3. Design of electronic instrumentation for nuclear applications;
4. Instrumentation and technical assistance.

Modelling of radiation fields, calculation of neutron physic parameters

The MCNP code is being used to calculate the pertubation of the neutron thermal flux by a sample in the presence of a moderator.
Monte Carlo calculations have been carried out in the field of the project POCI/FP/63433/2005 "Participação do ITN na Experiência n_TOF (PS213) no CERN (Quarto ano)" and EUROTRANS Project (IP EUROTRANS, 516520).

Measurement of neutron cross-sections

The analysis of the data for cross-section measurement, taken in the TOF spectrometer installed at the CERN, was carried out.

Development of software for control

- Control of EPA detector movements;
- Control of analytical balance.

Design of electronic instrumentation

Some electronic devices have been designed and produced for energy measurements at the DPRSN Sector and for the EPA motor control at the RPI Sector.

Instrumentation and Technical Assistance

The main objectives are the development of equipment for internal groups, fabrication of equipment for specific applications and assistance to industrial companies and scientific institutions as well as technical consulting.
The technical assistance takes mainly the forms of specialised consultant engineering advice, installation of nuclear gauges, including calibration maintenance and repair and recharging of gauges with imported radioactive sources.

Co-operation with other institutions

The Group is involved in the following collaborations:

1. n_TOF collaboration, a consortium of 40 laboratories in Europe and USA;
2. Accelerator Driven System (PDS-XADS – FIS5-2001-00089;
3. Sociedade Ponto Verde
4. Institute of Fluid-Flow Machinery, Poland.

EUROTRANS project, an integrated project with 48 institutes and universities in Europe.

Research Team

Researchers

J. MANTEIGAS, Aux., Group Leader
C. CRUZ, Aux.
I.F. GONÇALVES, Aux.
J. NEVES, Aux.
N. PINHÃO, Aux. (20%)
F.G. CARVALHO, Coord. (15%)

Students

L.C. MARQUES, Ph.D. Student
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A.C. TRIGO, BIC/FCT
C. SANTOS, MSc. student, FCT/UNL

Technical Personnel

T. JESUS
N. INÁCIO
M. CABAÇA

Technical Assistance in the Field of Engineering Applications of Radiation and Radioisotopes

J.B. Manteigas, J. Neves, C. Cruz, F.G. Carvalho

Objectives

The main objectives are the development of equipment for internal groups, fabrication of equipment for specific applications and assistance to industrial companies and scientific institutions as well as technical consulting.

Results

A summary of the more relevant work carried out is:

(i) Technical and scientific participation in the n-TOF (PS213) experiment at CERN.

(ii) Optimisation of the instrument movements control software. Development of software for analysis control. User's manual for an analytical balance.

(iii) Technical support (maintenance and set up operations) for the Small Angle Neutron Scattering instrument and EPA installed at the RPI.

(iv) Development and maintenance of electronic equipment to RPI, Physics, Chemical, UTR and DPRSN Sectors.

Summary of the more relevant services rendered in 2005

Activity	Quantity	Client	Price (Eur)
Supply of radioactive sources and source containers	**4**	CIMPOR/Alhandra	9222,50
Technical assistance to RAD X 100	**4**	Marinha/Arsenal do Alfeite	85,00
Technical assistance to **-** Source Containers	**6** **5**	PORTUCEL/Cacia Siderurgia Nacional	1800,00 500,00
Measuring and control of source activities	**12**	PORTUCEL/Cacia	1620,00
Laboratory equipment for the determination of radioactive element traces by electro-deposition	**1**	NATS/Kuwait	1600,13
Fellowship training	**1**	Centro de Emprego de Moscavide	1410,12
Prices including TAX (VAT)		**Total Amount (EUR):**	**16 237,75 €**

Participation of ITN in the n-TOF experiment (PS213) at CERN (third and fourth years)

P. Vaz, I.F. Gonçalves, C. Cruz, J. Neves, A. Albornoz-.Trillo, C. Carrapiço, L. Marques, C. Santos, R. Crespo, L. Ferreira, L. Távora[1]

The n-TOF Collaboration, a consortium of 40 laboratories in Europe and U.S.A., has proposed an ambitious programme to perform high accuracy measurements of neutron cross-sections in the range from 1 eV to 250 MeV. An experimental programme (PS213) is being carried out since 2001 at the neutron time of flight (TOF) facility at CERN, using the CERN/PS accelerator complex. A single proton pulse of $7 \cdot 10^{12}$ protons of 20 GeV impinges on a lead target every 2.4 seconds. After collimation, a neutron flux of the order of 10^5 neutrons/cm^2/pulse is available for cross section measurements in the detectors station located 185 m downstream the target area.

These cross-section measurements are required in many emerging applications that require the use of high-intensity and medium-energy (in the hundreds of MeV) proton beams impinging on a thick target of an heavy element. These applications range from the design of innovative Accelerator Driven Systems (ADS) for incineration of nuclear waste and energy production, radioisotope production for medical and industrial applications and to many other subjects in Astrophysics, Nuclear Physics and Nuclear Technology. New or improved measurements of neutron cross-sections will also be very valuable for Radiation Shielding, Dosimetry and Monte Carlo Radiation Transport calculations.

This project deals with the following issues: i) radiation transport calculations using state-of-the-art Monte Carlo programs, ii) radiation detection and measurement techniques iii) particle detectors and associated electronics iv) high-precision measurements of neutron cross sections and v) physics analysis and nuclear data evaluation

During 2005, ITN researchers in cooperation with researchers from CIEMAT/Madrid and INFN/Bari:

- Participated in the analysis of the resonance parameters for the ^{237}Np, ^{240}Am, ^{243}Cm isotopes
- Continued the analysis of the data for the ^{94}Zr isotope, initiated during 2004
- Participated in the checks of the time stability of the behaviour of the the TAC calorimeter and the Silicon monitors and assessed the quality of the data taken during 2004

1 – Centro de Instrumentação / U. Coimbra