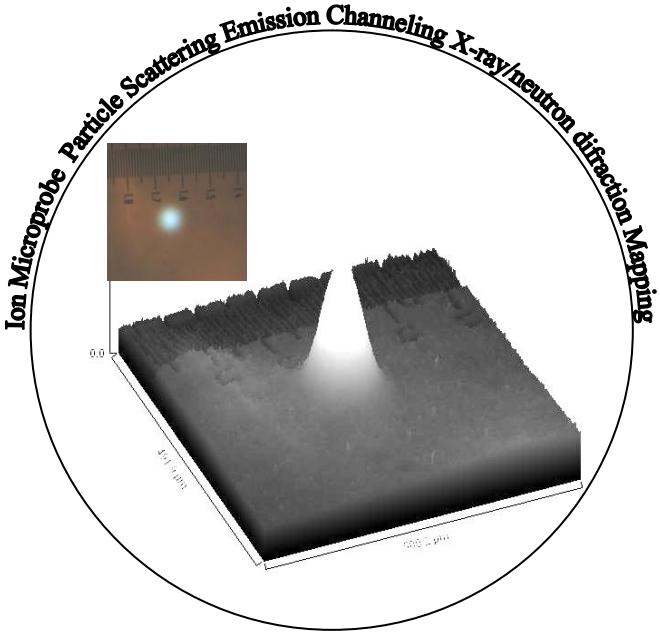
Physics Sector



Physics

Eduardo Alves

In 2007 the research groups in the Physics Sector ran applied and fundamental science projects in Materials, Environment and Health Sciences. Along with the scientific achievements a major commitment continued on enrolling graduated students in research activities, leading to M.Sc. and Ph.D. theses. The researchers further reinforced the network of collaborations with Institutions and Universities worldwide, continuing the policy of making the installed facilities available to external users. These strategic interactions are fundamental to keep the high output and scientific level of the research work. The following laboratories are hosted in the Physics department:

1 – Ion Beams Laboratory (IBL) has a 2.5 MV Van de Graaff Accelerator with an ion microprobe end-station, a 3 MV tandem accelerator with a micro-AMS system, and a 210 keV high fluence ion implanter. This infrastructure is open to external users and the experimental studies cover the fields of Materials Science, Environment, Health, Biomedical, Atomic and Nuclear Physics (cross-sections measurements). The research highlights will appear in the next pages under the headings *Advanced Materials Research Group, Elemental Characterization and Speciation Group, Group of Biomedical Studies*, and *Nuclear Reactions Group.*

2 – High Temperature Materials Laboratory (MA^3T) with a high-resolution, high-temperature (*Hotbird*) diffractometer and one high resolution diffractometer for low dimensional structures studies. The *Hotbird* with its high specificity and enhanced capabilities is used to solve difficult problems in advanced materials, *e.g.* materials for the electronics industry, high temperature alloys for fusion applications, superconductors, *etc*. The research activity in the laboratory is merged with the Advanced Materials Research Group.

3 – Neutron Spectrometers Laboratory at the ITN nuclear research reactor RPI, comprises one 2-axis diffractometer (DIDE), the SANS instrument (EPA), and a TOF spectrometer for educational purposes (ETV). As the RPI core has been converted from HEU to LEU, it is predicted this change will have an impact in both the total thermal neutron flux and on the signal to noise ratio at these instruments. Work to determine how far they are affected is underway. Research on new polymeric and hybrids materials is in progress, in collaboration with groups in Aveiro, Saclay and Budapest. The activities will be presented under *Condensed Matter Physics.*

4 – Ionising Radiation Laboratory is fitted with a Co-60 unit (UTR) with a semi-industrial dimension that 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 have been carried out by the *Radiation Technologies: Processes and Products Group*. The project implies new ionizing radiation equipment (e.g.: electron accelerator and gamma experimental facilities), a multidisciplinary laboratory with controlled environment, and use of automation-robotic systems in the facilities. The main R&D activities will appear under *Radiation Technologies: Processes and Products Group.*

5 – Nuclear Instruments and Methods Laboratory activities are focussed in modelling radiation fields, calculating neutron physics parameters, measuring neutron cross-sections and application of electric discharges in analytical methods and environmental problems. The design of instrumentation for nuclear applications, and providing of specialized technical assistance in nuclear instrumentation is also part of the activities carried out. These will be presented under the title *Nuclear Instruments and Methods.*

Physics Staff

Researchers

E. ALVES, Princ.
F. MARGAÇA, Princ.
J.G. CORREIA, Princ.
R.C. da SILVA, Princ.
U. WAHL, Princ.
C. CRUZ, Aux.
I. GONÇALVES, Aux.
J. MANTEIGAS, Aux.
J. NEVES, Aux.
L.C. ALVES, Aux.
M.L. BOTELHO, Aux.
M.T. PINHEIRO, Aux.
M.A. REIS, Aux.
N.R. PINHÃO, Aux.
L.M. FERREIRA, Assistant

Technical personnel

J. ROCHA
M. CABAÇA
M.F. BAPTISTA
N. INÁCIO
P. PEREIRA
R. PINHEIRO
T. JESUS

Administration and Informatics

A. FARIA
H. MARCOS
M.T. COSTA

Advanced Materials Research

Eduardo Alves

The Advanced Materials Research Group (GIMA) is responsible for running the Ion Beams Laboratory (IBL). The laboratory is equipped with a 2.5 MV Van de Graaff accelerator featuring an ion microprobe with an external beam facility, a 3 MV tandem accelerator with an Accelerator Mass Spectrometry (AMS) line, and a 210 kV high fluence Ion Implanter.

The work carried out during the last decades allowed the group to achieve a large expertise in the fields of applications of ion beams to characterization and processing of materials. The recent activities of the group have been focused on the study of advanced materials with high technological impact. Several national and international collaborations allowed a continuous exchange of expertise and mobility of researchers, a key condition to keep the scientific activity of the group at the forefront of research in its field.

The research activities of the group were essentially centred in two kinds of materials: wide band gap semi-conductors, and nanostructures and insulators. Wide bandgap semiconductors are the base of optoelectronic devices operating in the visible wavelength range of the electromagnetic spectrum and are under intense research worldwide. Our work was focused on the optimization of the implantation conditions of magnetic and optically active dopants. Other relevant research work is being carried out in quantum well structures and quantum dots. An intense study of the structural properties of GaN/InGaN structures is under way in collaboration with the Universities of Aveiro and Strathclyde. Structural and optical studies of Ge and GaN quantum dots are also being studied in collaboration with the Universities of Aveiro and Grenoble.

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, tunnel junctions, and oxynitride coatings, in collaboration with INESC and University of Minho.

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 titanium beryllides, the characterisation of the new Eurofer (ODS) steel and the study of surface erosion and fuel retention of W under ITER conditions.

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

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

The scientific activity of the group in 2007 was materialized in:

Publications (peer reviewed journals): 38
Conference and workshop contributions: 5 invited, 16 oral and 19 posters.
Running projects: 24

Researchers(*)

E. ALVES, Princ. (Group leader)
R.C. DA SILVA, Princ.
U. WAHL, Princ.
L.C. ALVES, Aux. (75%)
N. BARRADAS, Aux. (10%)
A.R. RAMOS, Aux. (10%)
A. KLING, Aux. (5%)
K. LORENTZ, Post-Doc. fellow, FCT

Students

A. FONSECA, Ph.D. student, Project grant**
A. RODRIGUES, Project grant
C.P. MARQUES, Ph.D. student, FCT grant
J. VAZ PINTO, Ph.D. student, FCT grant
M. VILARIGUES, Ph. D. student***
N. FRANCO, Ph.D. student, FCT grant**
S. MAGALHÃES, Project grant**

Technical Personnel

J. ROCHA
M.F. BAPTISTA
P. PEREIRA

Collaborators

L. REDONDO
M.R DA SILVA
S. PEREIRA

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

RBS analysis of InGaN/GaN quantum wells for hybrid structures with efficient Förster coupling

N.P. Barradas, E. Alves, S. Pereira[1], I. M. Watson[2]

Objectives

There is strong current interest in Förster resonant energy transfer (FRET) from a semiconductor quantum well (QW) to an overlayer of another luminescent material. The FRET process becomes efficient when the two materials are placed at interaction distance of a few nanometres. The additional requirement of large spectral overlap between the energy donor and acceptor can be satisfied by combinations of InGaN/GaN QWs (as donors) and overlayers of either light-emitting polymers or nanocrystalline semiconductor quantum dots (as acceptors), both of which can be tailored to have high absorption in the QW emission region.

Here we study a set of custom grown InGaN/GaN single QW samples, in which the GaN cap layer thickness was varied to modulate the FRET rate in hybrid structures. We used high-resolution grazing-angle RBS experiments to determine the GaN cap layer thickness, varied from 2 to 12 nm, which controlled the interaction distance between the QW and the coupled luminescent medium in hybrid structures. The measured thickness values were used to confirm the dominance of sheet-to-sheet dipole-dipole interactions in QW-polymer hybrid structures.

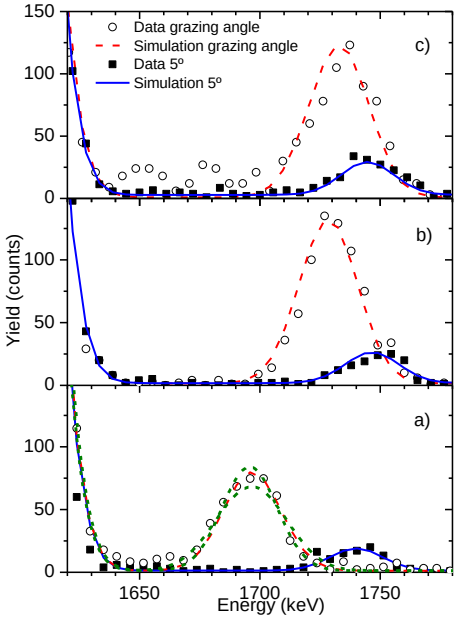


Fig 1. RBS spectra for samples a) A, b) B and c) C. Simulations for the derived parameters are shown. For sample A, simulations x = 0.02 and x = 1 are also shown.

Results

Fig. 1 shows the near-normal and grazing angle spectra for each sample. From the shift in the In peak it is possible to determine the GaN cap layer thckness, which determines the FRET efficiency. The main difficulty is that the problem is ambiguous, as many different solutions lead to acceptable fits. An involved manual analysis can resolve the ambiguity as shown in Fig. 2: the only In QW concentration y consistent with all data is x = 0.07(1) and $t_{GaN,exp}/t_{GaN,nominal}$ = 0.79(5). Using these values we can determine the cap thickness for each layer.

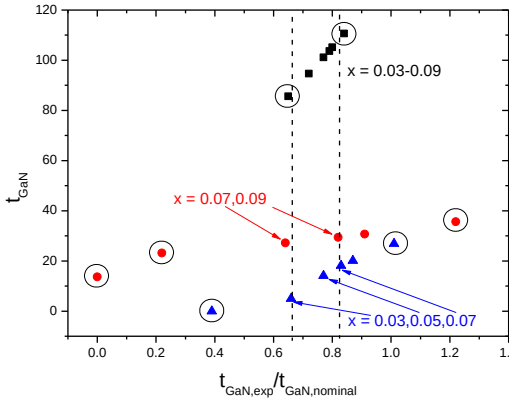


Fig 2. Possible solutions for each sample. The only consistent set implies x = 0.07(1), and GaN cap layer thickness of samples A, B and C:
11.8(8) nm, 3.2(5) nm, 1.9(5) nm.

The results were used to explain quantitatively the FRET process.

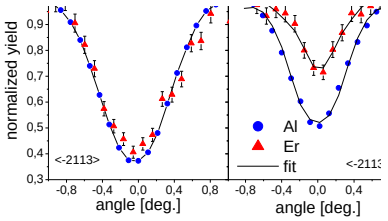
[1] CICECO, Universidade de Aveiro
[2] Institute of Photonics, University of Strathclyde, 106 Rottenrow, G4 0NW, Glasgow, UK

Lattice site location, damage and optical characterization of Eu implanted $Al_XGa_{(1-X)}N$ layers

K. Lorenz, E. Alves, T. Monteiro[1], M. Peres[1], A. J. Neves[1], K. Wang[2], R.W. Martin[2], K. P. O'Donnell[2]

Eu doped GaN has been extensively studied due to the sharp emission in the red spectral region interesting for applications in electroluminescent devices and lasers. The semiconductor band gap can be tuned when using the ternary alloy $Al_xGa_{(1-x)}N$ with different Al/Ga ratios. This can change the excitation mechanisms of the rare earth ions and the efficiency of light emission processes can be optimized by choosing the appropriate $Al_xGa_{(1-x)}N$ host.

$Al_xGa_{(1-x)}N$ films with AlN contents from 0% to 100 % were implanted with Eu ions. The implantation damage and the lattice sites were studied by Rutherford Backscattering and Channelling spectrometry. Al-containing alloys are more resistant to implantation damage than GaN. The Eu ions are incorporated on lattice sites slightly displaced from the substitutional cation-site along defined directions (see figure).



The displacement increases with increasing AlN fraction probably because of the decreasing lattice parameter leaving less free space to accommodate the large RE ion as well as defects. Experiments performed with different implantation geometries indicate that the displacement is due to the interaction with defects caused by the implantation. Photoluminescence (PL) spectra show Eu related luminescence lines in the red spectral region for all samples after annealing. The PL intensity strongly depends on the composition with best results for ~30% AlN content. Excitation spectra show the AlGaN band gap and two excitation bands below gap: X_1 peaks at 3.26 eV in GaN and up-shifts linearly by 0.28 eV as x increases to 1. For $x > 0.6$, a second band, X_2, emerges, showing a similar energy shift. We identify $X_{1,2}$ as core-exciton-like complexes of Eu emitting centers.

[1] Departamento de Física, Universidade de Aveiro, 3810-193 Aveiro, Portugal
[2] Department of Physics and Applied Physics, University of Strathclyde, Glasgow, G4 0NG, Scotland, UK

Structural and optical characterization of AlInN ternary alloys

K. Lorenz, N. Franco, E. Alves, S. Pereira[1], I. M. Watson[2], K. Wang[3], R.W. Martin[3], K. P. O'Donnell[3]

In addition to a band-gap covering a very wide energy range (0.7 eV to 6.2 eV) the ternary semiconductor AlInN has the advantage that it can be lattice-matched to GaN. $Al_{1-x}In_xN$ layers were grown by MOCVD on GaN buffer layers at temperatures between 760 ºC and 840 ºC to give InN contents between 13% and 24%. While for growth temperatures ≥ 800 ºC the AlInN films grow coherently on GaN, with good crystal quality and homogeneous InN concentration, the sample grown at 760 ºC shows an increase of InN content with depth, a relief of strain towards the surface and a deterioration of crystal quality. AFM studies suggest that the relaxation is accompanied by an onset of three-dimensional growth. The pattern of compositional grading is the opposite to that often observed in InGaN/GaN bilayers with relaxed near-surface InGaN, where InN incorporation is inhibited in the compressively-strained interfacial region and increased in the relaxed surface region. In AlInN, compressive strain seems to facilitate the InN incorporation. Our results imply a relaxation mechanism for AlInN in which strain relief takes place mainly via the change of InN content towards the value of lattice matched material (17-18 %). Photoluminescence (PL) measurements show a clear red-shift of the $Al_{1-x}In_xN$ emission peak with increasing InN fraction and comparison of the emission wavelengths with PL excitation data reveal strong Stoke's shifts.

[1]Dep. Física, Universidade de Aveiro, Portugal, [2]Institute of Photonics, SUPA, University of Strathclyde, Glasgow, UK
[3]Department of Physics and Applied Physics, University of Strathclyde, Glasgow, Scotland, UK

A stable $In–V_N$ complex in AlN and GaN: a new hypothesis to explain exciton localisation in nitrides

K. Lorenz, E. Alves, J. Schmitz[1], J. Penner[1], R. Vianden[1]

The fact that especially In-containing III-nitride emitters are relatively insensitive to the large densities of defects (mainly threading dislocations) found in standard $Ga_xIn_{1-x}N$ LEDs and laser diodes, has been the subject of a lively discussion. InN rich nanoclusters, compositional or strain inhomogeneities are possible explanations. Channelling measurements showed that close to 100% of implanted In ions occupy substitutional cation sites in GaN and AlN. However, Perturbed Angular Correlation measurements showed that after annealing only ≈50% of the In probes occupy relatively undisturbed substitutional sites at 293 K while the remaining fraction traps a nearest neighbour point defect. Above 293 K this fraction decreases strongly until all In probes are found in undisturbed substitutional sites. The effect is completely reversible. A model involving an indium–nitrogen vacancy complex is suggested to explain this behaviour. Possibly this complex can act as radiative recombination centre or as seed for phase segregation during growth.

[1] Helmholtz-Institut für Strahlen- und Kernphysik, D-53115 Bonn, Germany

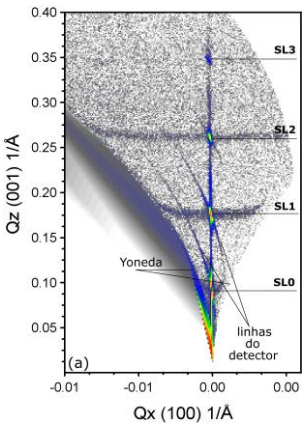
Properties of Ge islands embedded in multilayer and superlattice structures

S. Magalhães, E. Alves, J. P. Leitão[1], A. Nikiforov[2]

Si/Ge low-dimensional structures attract the attention of the scientific community due to their potential to develop new electronic and optoelectronic devices.

In this work we compared Ge quantum dot heterostructures with a planar Ge/Si multilayer. The islands were evidenced using X-ray dispersion techniques, ion beam techniques and photoluminescence. It was found that in the case of the Ge quantum dots samples, the dots created strain phenomena significantly different than the planar homogenous samples, showing the dots presence. The inset figure shows features in a XRR reciprocal space map that are a fingerprint of a correlated vertical structure (the quantum dots). Also, the comparison of the Ge minimum RBS yield from the scans along tilted directions show that, due to the larger Ge lattice constant, the scattering probability increases consistent with the presence of the dots.

The photoluminescence measurements for single layer and multilayers samples indicate the possible presence of islands, located in the range hυ < 0.8 eV. It is well known that the buried Ge layers create strain fields for the subsequent layers which results namely, in the reduction of the critical thickness for the 2D-3D growth transition.



[1] Departamento de Física, Universidade de Aveiro, 3810-193 Aveiro, Portugal
[2] Institute of Semiconductor Physics, 630090, Novosibirsk, Russia

Structural characterization of oxidized NbO_xN_y coatings under air annealing

E. Alves, N. Barradas, J.M. Chappé[1], S. Lanceros-Méndez[1], F. Vaz[1], M. Fenker[2], H. Kappl[2]

In the present work the oxidation resistance behaviour of NbON multilayer films was studied. The depositions were carried out by DC magnetron sputtering with a reactive gas pulsing process. The nitrogen flow was kept constant and the oxygen flow was pulsed. Pulse durations of 10 s produced multilayered coatings with a period of $\lambda = 10$ nm. Three different films with increasing duty cycles have been deposited.

Rutherford Backscattering Spectrometry (RBS) was used to study the chemical composition variations for different annealing temperatures (as-deposited, 400 ºC, 500 ºC and 600 ºC) combined with X-ray diffraction (XRD) to identify the crystalline phases formed. At 400 ºC, for all films a very thin layer starts to form at the surface with enhanced O concentration. The composition of the deeper part of the samples remains unchanged. At 500 ºC, the oxide scale grows, encompassing about half the film thickness. At 600 ºC, the process is finished and a single layer is formed with reduced Nb and increased O concentration. Fourier-Transform Infrared (FTIR) spectroscopy results confirmed the increase of this surface oxidation, while XRD revealed that crystallization of Nb_2O_5 occurs at 600 ºC.

[1] Universidade do Minho, Dept. Física, Campus de Azurém, 4800-058 Guimarães, Portugal
[2] FEM, Dept. POT-MPh, Katharinenstr. 17, D-73525 Schwäbisch Gmünd, Germany

Intrinsic p type ZnO films deposited by R.F. Magnetron sputtering

E. Alves, Jinzhong Wang[1],Elvira Fortunato[1],T. Monteiro[2]

In this work, ZnO films were deposited on c-plane sapphire substrate in Ar gas by R.F. Magnetron sputtering method. Furthermore, the films were annealed at 400 °C in reducing ambient. The properties of the as-grown and annealed films have been characterised by means of X-Ray Diffraction (XRD), Rutherford Backscattering Spectrometry (RBS), Elastic Recoil Detection Analysis (ERDA), Hall measurement and Photoluminescence (PL) spectra, respectively. XRD studies indicate that after annealing, the crystal quality of ZnO films increases and the strain in the films changes. From RBS and ERDA, we can see that although there is no H_2 introduced in the sputtering chamber, H has been found in the as-grown ZnO films. After annealing, the amount of H in the film increases. Compared with the as-grown ZnO films, the ultra exciting intensity obviously decreases and new optical active centres in the blue/violet (~3.0 eV) and red (~1.9 eV) are enhanced in the PL spectrum of the annealed sample. Hall measurements indicated that the as-grown film reveals p-type conductivity. The p-type conductivity improves with annealing, but in a long term (9 days) the conductivity changes from p- to n-type.

[1] Universidade Nova de Lisboa, CENIMAT/I3N
[2] Institute of Semiconductor Physics, 630090, Novosibirsk, Russia

Effect of ITER-relevant material mixing on fuel retention and material characteristics

L.C. Alves, N.P. Barradas, E. Alves, Graham Wright[1]

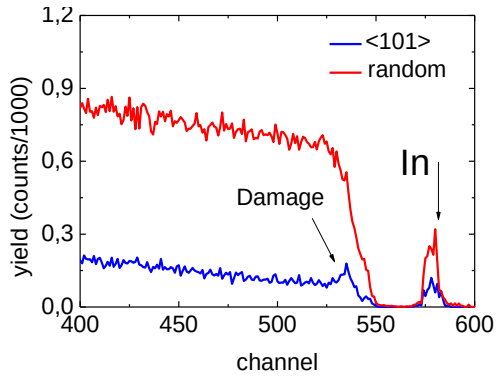
The major goal of the study was the full characterisation of the surface composition and morphology, and fuel retention of W targets exposed to plasma fluxes similar to the ones expected in the ITER divertor (> 10^{23} $m^{-2}s^{-1}$). Tungsten samples were exposed to plasma fluxes in PSI-2 and studied with ion beam techniques and electron microscopy. Fuel retention in the samples and its depth distribution was quantified with Elastic Recoil Detection Analysis (ERDA) and Nuclear Reaction Analyses (NRA).
The W targets exposed in Pilot-PSI were analysed ex-situ with ^{3}He(d,p)α Nuclear Reaction Analysis (NRA) and Thermal Desorption Spectroscopy (TDS). Initial NRA data shows a D depth profile that is peaked at the surface and significant D retention (0.01 at.%) at a depth of ~3 μm after only 40 s (10 discharges) of total plasma exposure time. This demonstrates the trapping of D that has diffused away from the ion implantation zone towards the bulk. The effects of surface polishing/roughness and pre-annealing targets before plasma exposure was investigated through the comparison of D retention as determined by NRA and TDS analysis. The results show that a W target with a surface roughness of <1 μm has nearly 6 times more D retention in the first 3 μm of the surface than an "as received" W target.

[1]FOM-Institute for Plasma Physics Rijnhuizen, Association Euratom-FOM, Netherlands

Ion beam studies of InAs/GaAs self-assembled quantum dots

E. Alves, S. Magalhães, N.P. Barradas, N.V. Baidus[1]*, M.I. Vasilevskiy*[1]*, B.N. Zvonkov*[2]

Self-assembled InAs/GaAs quantum dots (QD's) emit in the telecommunication wavelength range (1.3-1.55 μm) revealing an enormous potential to become the active elements of low threshold lasers and light emitting diodes. However, the luminescence is dramatically quenched at room temperature (and even below) due to the defects in the GaAs matrix which open non-radiative recombination paths.
In this study we combine Rutherford Backscattering Spectrometry/Channelling (RBS-C), High resolution X-ray diffraction (HRXRD) and Photoluminescence (PL) techniques to correlate the structural and optical properties of the InAs/GaAs QD heterostructures. The heterostructures were grown by Atmospheric Pressure Metal Organic Vapour Phase Epitaxy, feature a combined InGaAs/GaAs capping layer and exhibit sizable PL in the vicinity of 1.5 μm. Channelling measurements reveal a good crystalline quality along the main axial directions with minimum yields in the range of 4% to 6% through the entire capping layer. An increase on the dechannelling rate is observed in the region where the InAs quantum dots were buried (see figure). The channelling results also give evidence for the presence of defects preferentially oriented in the (110) planes. Detailed angular scans in a structure with a 25 nm cap allowed the study of the In position with respect to the GaAs matrix and a perfect alignment was found. This proves that the growth interruption and surface treatment using tetrachloromethane during the capping layer deposition, improve the crystal quality of the heterostructure. This helps to overcome the PL quenching at room temperature.



[1] Universidade do Minho, Departamento de Física,4170-057 Braga,Portugal
[2] N. I. Lobachevskii State University, Nihznii Novgorod, Russia

Study of SiGe alloys with diferent germanium concentrations implanted with Mn and As ions

S. Magalhães, V. Batista, N. A. Sobolev[1]*, E. Alves*

In this work we studied the structural properties of SiGe alloys with different Ge molar compositions co-implanted with manganese and arsenic ions. The ions were implanted at room temperature to fluences of 1×10^{15} cm^{-2}, 5×10^{15} cm^{-2} and 1×10^{16} cm^{-2} and energies of 170 keV (Mn) and 200 keV (As) in order to achieve the overlap of the implanted profiles. The alloys were studied with Rutherford Backscattering Spectrometry/Channelling (RBS/C) and X-Ray Diffraction (XRD) techniques. After implantation the implanted region (150 nm) turns into amorphous according with RBS/C. The evolution of the lattice parameter was studied using XRD. The annealing at 550 ºC induces the recrystallization of the amorphous layer for the sample implanted with the lower fluence and the full recovery is complete after annealing at 700 ºC. The samples implanted with higher fluences didn't reveal any noticeable recovery. The evolution of the Mn and As profiles during the annealing at 550 ºC do not reveal significant changes.

[1] Universidade de Aveiro, 3810-193 Aveiro, Portugal

In-situ XRD Studies of thermal stability of pure silica and Ti-MCM-41 materials

N. Franco, E. Alves, C. Galacho[1], P.J.M Carrott[1]

In this work we present a study on the thermal stability of silica and titanium containing ordered mesoporous materials with MCM-41 structure, synthesized at ambient temperature and pressure. Calcined grades were analyzed *in-situ*, in the form of compacted powder, to assess its influence on the order-disorder transition temperature. The temperature was raised up to 1000 ^{o}C under vacuum (~10^{-5} mbar) and flowing N_2 (~10^{-3} mbar). An intense X-ray beam collimated by a Göbel mirror was used to follow *in-situ* the temperature dependence of the unit cell dimension in θ-2θ configuration. During the annealing, in steps of 100 ^{o}C, the unit cell parameter decreases, as well as the diffracted signal leading to its extinction at around 1000 ºC. The results show that under vacuum, this transition is reversible and the diffraction peaks (100), (110) and (200) of the two-dimensional hexagonal lattice appear and are slightly shifted to higher angles after cooling to room temperature. The same result, although not so pronounced, was observed when the measurements were done in flowing nitrogen gas.

[1] Centro de Química de Évora e Departamento de Química, Universidade de Évora, 7000-671 Évora, Portugal

Stability of GaN Films Under Intense MeV He Ion Irradiation

C.P. Marques, E. Alves, O. Ambacher[1], M. Niehus[2], E. Morgado[3], R. Schwarz[3]

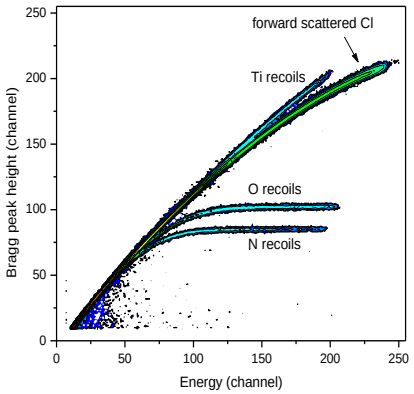
We have exposed MOCVD-grown GaN films to a 1 nA beam of 1.5 MeV $^{4}He^{+}$ particles produced by the Van de Graaff accelerator at ITN. The material quality was tested by measuring dark conductivity and steady-state as well as transient photoconductivity at room temperature, in coplanar layout. Photocurrent spectra taken below the band gap reveal a broad defect density-of-states distribution. After 5 ns irradiation with laser pulses from a frequency-doubled Nd:YAG laser, the induced photocurrent shows a very slow decay over several orders of magnitude. Compared to the decrease of photosensitivity in thin undoped a-Si:H films under He^{4} irradiation – a decrease surprisingly similar to c-Si – we observe that degradation of GaN also sets in at about 10^{12} cm^{-2}, but decreases much more slowly as indicated by the smaller negative exponent in the photocurrent-fluence power law plot. After about 3×10^{15} cm^{-2} the mobility-lifetime-product decreased by half an order of magnitude. This indicates a much higher radiation resistance of GaN when compared to amorphous or crystalline Si.

[1] Technische Universität Ilmenau, Center for Micro- and Nanotechnologies, D-98684 Ilmenau, Germany
[2] Instituto Superior de Engenharia de Lisboa, P-1949-014 Lisboa, Portugal
[3] Instituto Superior Técnico, Physics Department, P-1049-001 Lisboa, Portugal

Surface analysis of oxynitride compounds with ion beams

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

Titanium nitride and oxynitride compounds exhibit interesting properties for applications in fields ranging from protective/decorative coatings to solar panels. The properties of these compounds are related to the oxide/nitride ratio and can be tailored by tuning this ratio. Furthermore the thermal stability is other important issue with regarding potential applications. Thus, accurate composition measurements are fundamental to understand the behaviour of these structures. Ion beam based techniques (IBA) are unique for this purpose. The composition was determined by Rutherford Backscattering Spectrometry (RBS) throughout the entire thickness of the films. To get information on the profile of light elements (O, N) and detect the presence of hydrogen on the films, Heavy Ion Elastic Recoil Detection Analysis (HI-ERDA) was performed (see figure).



The results indicate a nearly constant stoichiometry through the entire analysed depth. 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. The annealing of the samples in the temperature range of 400 °C to 900 °C, in controlled atmosphere and in vacuum, leads to the formation of new phases. When Zr atomic content is higher than 80% the heat treatment in controlled atmosphere reveals the annealing of defects and the formation of m-ZrO_2 and t-ZrO_2. When oxygen content of the films varies from 6% to 14% the GIXRD reveals the development of t-ZrO_2 at 600 ^{o}C or above.

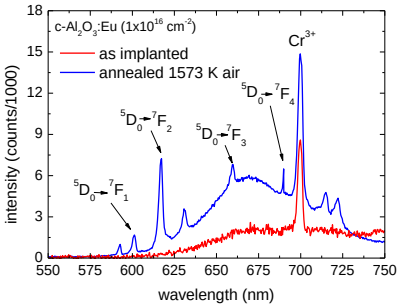
[1] Universidade do Minho, Dept. de Física, Campus de Azurém, 4800-058 Guimarães, Portugal
[2] Forschungszentrum Rossendorf e.V., Postfach 510119, 01314 Dresden, Germany

Ionoluminescence studies of Eu implanted Sapphire

C. Marques, L.C. Alves, R.C. da Silva, A. Kozanecki[1], E. Alves

Sapphire single crystals were implanted at room temperature with 100 keV europium ions up to fluences of 1×10^{16} cm^{-2} aiming at study of damage and Eu ion location after implantation and upon annealing under oxidising or reducing atmosphere up to 1300 ^{o}C.

After implantation an intense red emission indicating the presence of Cr (a natural contaminant) in the samples is observed, along with F-centres. Thermal treatments in air or in vacuum anneal most of the implantation related defects and promote the redistribution of the europium ions. The characteristic emissions due to 4f intra-band transitions in these rare-earth ions become observable (see figure). Detailed lattice site location studies for various axial directions are underway to allow correlating the damage recovery and incorporation of the Eu ions into well defined sites with the intensity and energy of the ion beam induced luminescence.



[1] Institute of Physics Polish Academy of Sciences, 32/46 Lotników Al., 02-668 Warszawa, Poland

Microstructural Studies of Mg doped $SrTiO_3$ Films

A.R.L. Ramos, E. Alves, O. Okhay[1], A. Wu[1], P.M. Vilarinho[1], I.M. Reaney[2], J. Petzelt, J. Pokorny[3]

STO based materials are important for high dielectric permittivity applications and tuneable microwave devices. Recent results have shown that in-plane strain from the substrate can produce room-temperature ferroelectricity in epitaxial STO. The high ε_r at room temperature in these films (nearly 7000 at 10 GHz) and its sharp dependence on electric field are promising for device applications. However this strain-induced enhancement in T_c is attained through the utilization of a (110) $DyScO_3$ substrate and has not been reproduced on silicon based substrates, as required for device applications. Hence, an alternative way to adjust the dielectric response of STO thin films through chemical substitutions deserves further study. The manipulation of the dielectric properties for specific applications is well known in STO single crystals and ceramics, but not in polycrystalline thin films. A-site substitutions in STO lattice with isovalent Ca, Ba and Pb ions induce a low temperature ferroelectric-type anomaly. In spite of predictions, no polar state was reported for Mg doped STO. However, in a previous work of the authors, $Sr_{1-x}Mg_xTiO_3$ (SMT) films displayed increased tuneability at room temperature, not observed in equivalent bulk ceramics, pointing to modification of the lattice polarization. Moreover it was demonstrated that the solid solubility limit of Mg in STO films prepared by sol gel and by pulsed laser deposition (PLD) was higher than in STO ceramics. In order to clarify the role and solid solubility of Mg in STO thin films prepared by sol-gel and deposited on Si/SiO2/TiO_2/Pt substrates, a systematic study of the structure and microstructure was conducted using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM), Rutherford Backscattering Spectroscopy (RBS) and Raman. Results show that the incorporation of Mg and the solid solubility limit of Mg in the A-site of STO lattice of sol gel thin films on silicon platinised substrates is higher than in ceramics and is dependent on the annealing temperature.

[1] Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal
[2] Department of Engineering Materials, University of Sheffield, Sheffield S1 3JD, UK
[3] Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague 8, Czech Republic

Ion implantation and ion beam analysis of MOD deposited oxide films

C. Marques, E. Alves, X. Marko[1], P. Talagala[1], M.B. Sahana[1], R. Naik[1], K.R. Padmanabhan[1]

Dilute magnetic oxide semiconductors are semiconducting oxides substituted with magnetic or other transition elements. The importance of these systems has increased in recent years in view of spintronics and photocatalytic applications. In this work oxide films of TiO_2 and V_2O_5 were deposited by metal organic decomposition (MOD) technique. The thickness, composition, orientation of the film on single crystal substrates (sapphire, Si, MgO) and residual C concentration were measured by Rutherford Backscattering Spectrometry in Channelling mode (RBS/C) and Nuclear Reaction Analysis (NRA). X-ray diffraction and Raman spectroscopy were used for analysis of the structure of the oxide films. The stoichiometric oxide films of appropriate thickness were subsequently doped with elements such as Fe, Co and V either using a suitable metal organic solution or by ion implantation. In ion implantation, the ions are distributed in the sub-surface region of the film. On the other hand, impurities incorporated from solution are expected to be distributed over the entire thickness of the film. The effect of doping on optical and photocatalytic properties is being studied and compared for solution doped films with those doped using ion implantation.

[1] Department of Physics, Wayne State University, Detroit, MI 48202, USA

Ion-implanted magnetic nanolayers of wide band gap semiconductors for spintronics applications

U. Wahl, E. Alves, J. G. Correia, A.C. Marques, C.P. Marques, J.P. Araújo[1], L. Pereira[1]

The project investigates the possibility to fabricate diluted magnetic semiconductors by means of ion-implantation of transition metals into single-crystalline starting materials such as the wide band gap semiconductors GaN and ZnO, and some selected semiconducting oxides such as $SrTiO_3$ and TiO_2.
In first exploratory experiments single crystals of ZnO, GaN and $SrTiO_3$ were implanted with 60 keV ^{56}Fe at fluences of 1×10^{15} cm^{-2} and 5×10^{15} cm^{-2}. RBS/C experiments showed that the implantation damage in ZnO and $SrTiO_3$ can be removed to a large extent using air annealing above 1000°C, while in GaN it is more persistent, especially at higher implantation fluences. Characterizations of the magnetic moments of the samples by means of SQUID have so far only been carried out for samples annealed at 900°C, where they revealed ferromagnetic behaviour in the ZnO and GaN samples and in the 5×10^{15} cm^{-2} implanted $SrTiO_3$ sample. Some of the samples were in addition implanted with small fluences (10^{13}-10^{14} cm^{-2}) of radioactive ^{59}Fe (45 d), followed by emission channelling studies of the lattice location of this isotope as a function of annealing temperature. The majority of Fe was found on substitutional Zn sites in ZnO, substitutional Ga sites in GaN, and at or close to substitutional Ti sites in $SrTiO_3$. The emission channelling experiments also indicated that following annealing up to 900°C the implanted Fe atoms are still located in defect-rich regions which are strained or show considerable mosaicity.

[1] Departamento de Física, Universidade do Porto, 4169-007 Porto.

Investigation of changes in the luminescence and structural properties of nano-SiGe/SiO_2 multilayers due to annealing processes

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]

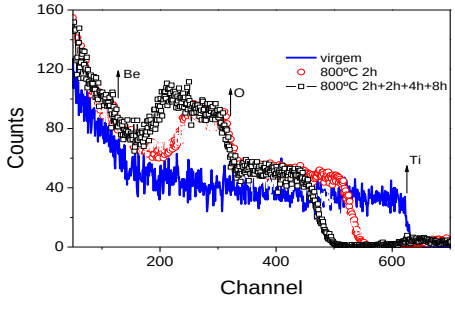
Semiconductor nanoparticles embedded in an oxide matrix are highly interesting for applications in luminescent devices compatible with CMOS technology. A promising method for the production of this kind of structures is the deposition of amorphous SiGe nanoparticles embedded in SiO_2 using Low Pressure Chemical Vapor Deposition at low temperatures, followed by a thermal treatment to crystallize them. These structures exhibit luminescent emission peaking in the blue-violet at 400 nm. Since the luminescence in single layers is limited by the number of nanoparticles that can be placed in a plane, multilayer structures is of high interest to increase the light output. The dependence of luminescence and structural properties (Ge diffusion, nanoparticle diameters) of the multilayer systems on the layer thickness and annealing conditions has been studied using TEM and grazing incidence RBS. The studies revealed that SiO_2 buffer layers with a thickness of at least 12-15 nm are required to suppress the Ge diffusion which is detrimental to the formation of luminescent nanoparticles. The highest luminescence yield was observed after rapid thermal annealing at 900 ºC for 60 s for multilayer structures containing nanoparticles with diameters of about 3.0-4.5 nm and separated by 35 nm thick oxide buffer layers.

[1] Departamento de Tecnología Electrónica, ETSI de Telecomunicación, Universidad Politécnica de Madrid, Spain
[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, Spain

Oxidation studies of beryllides using ion beams

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

To increase the tritium-breeding ratio in the future nuclear fusion reactor, beryllium is expected to be used as a neutron multiplier. Studies have been performed for the use of metallic beryllium in the form of a pebble bed. However, pure beryllium becomes brittle and swells under neutron irradiation, making its use in the form of beryllides a possible alternative. Aiming at a detailed study of its oxidation behaviour, Be-Ti intermetallic compounds with nominal composition Be-5at%Ti and Be-7at%Ti produced at JAERI, were submitted to different air annealings at temperatures of 800 ºC, for periods of up to 16 h. Rutherford Backscattering Spectrometry (RBS) and Particle Induced X-Ray Emission (PIXE) were used with H^+ and He^+ microbeams (~3 µm) in order to access changes in surface topography and monitor the oxide layer formation. Both alloys reveal intra-grain regions with high concentration of impurities (O, Fe and Ni) and Ti depletion and that oxidation occurs preferentially at the Ti depleted (Be rich) regions.
Furthermore in Ti rich zones, oxidation is not due to Ti but to Be oxidation that occurs after Be diffusion to the sample surface (see figure). Results also show that the oxide layer formed in the Be-7at%Ti is larger than the one measured for the Be-5at%Ti sample and that even after 16 h annealing that layer continues to grow.



[1] Instituto de Ciencia de Materiales de Sevilla, Spain
[2] Centro de Física Nuclear da Univ. de Lisboa, Portugal

Defect induced magnetism: magnetism in Ar-implanted ZnO and rutile

R.P. Borges[1], R.C. da Silva, S. Magalhães, M.M. Cruz[1], M. Godinho[1]

The finding of ferromagnetic order in systems that do not include magnetic elements such as HfO_2, along with band structure calculations indicating that cation vacancies may be associated with magnetic moments in materials like CaO and HfO_2, led to the proposal of ferromagnetism based on lattice defects. The defects are hold responsible for the formation of magnetic moments at the molecular orbitals surrounding vacancies and for the formation of impurity bands mediating long range ferromagnetic ordering. This triggered work focused on the role of lattice defects as at least partly responsible for the observed magnetic signal.
Within this context, ZnO and rutile single crystals were implanted with Ar ions with energy of 100 keV and fluences up to 1×10^{17} cm^{-2} and 2×10^{17} cm^{-2} respectively. Ferromagnetic behaviour was observed at room temperature after implantation. Although trace amounts of transition metal impurities were identified in the virgin ZnO crystals, it was shown that they are magnetically inert and cannot account for the observed magnetic behaviour, which was thus assigned to the presence of implantation-induced lattice defects. The ferromagnetic behaviour is suppressed in ZnO after consecutive annealings in air at 400 ºC and 500 ºC. The fact that it disappears after the annealing at 500 ºC can be explained by the annealing out of the implantation defects, confirming the importance of lattice defects towards the magnetic behaviour of ZnO. On the contrary, annealing the as-implanted rutile at 800 ºC in Ar atmosphere for 1 h led to enhancement of the ferromagnetic behaviour. This surprising finding is currently under investigation.

[1] CFMC-Universidade de Lisboa, and Dep. de Física, Faculdade de Ciências, Campo Grande, Ed. C8, 1749-016 Lisboa, Portugal

Structural and magnetic properties of oxides implanted with transition metals – TiO_2 implanted with Co, Ni and Fe: influence of the dopant in the anisotropic magnetic behaviour

J.V. Pinto, M.M. Cruz[1,2], M. Godinho[1,2], N. Franco, E. Alves, R.C. da Silva

We studied the behaviour of the transition ions Co, Ni and Fe introduced in TiO_2, by ion implantation. Single crystals of rutile TiO_2 were doped with magnetic ions Co, Ni or Fe, using ion implantation with fluences in the range of 5×10^{16} cm^{-2} to 2×10^{17} cm^{-2} and energy of 150 keV. The structural and magnetic properties of such samples were studied after implantation and upon thermal treatments in order to understand the role of the dopant and its concentration. As-implanted samples present different magnetic behaviours that are related with the atomic concentration of the implanted species: samples with lower concentrations display paramagnetic behaviour while for higher concentrations ferromagnetic like behaviour is obtained. For intermediate concentration a superparamagnetic regime is found, indicating the formation of nm-sized magnetic aggregates during implantation. After annealing treatments the samples display anisotropic ferromagnetic behaviour at room temperature that is correlated with the rutile structure and dependent on the implanted species. Enhanced electrical conductivity exhibits also anisotropy at low temperatures, following the same general trend as in reduced rutile. No magneto-resistive effects were detected, indicating that there are no polarization effects of the charge carriers. It is suggested that vacancies accommodate at the interface between the aggregates and the TiO_2 host.

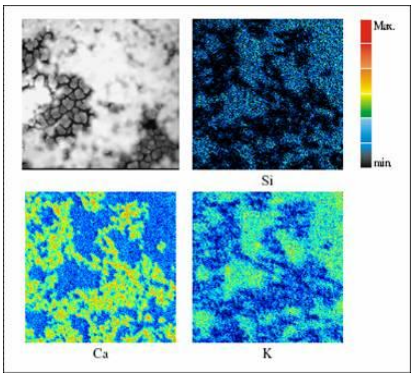
[1] CFMC-Universidade de Lisboa, and Dep. de Física, Faculdade de Ciências, Campo Grande, Ed. C8, 1749-016 Lisboa, Portugal

Characterization of potash-glass corrosion in aqueous solution: the influence of Mn, Fe and Cu ions

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

We continued the investigation of 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 56 mol.% SiO_2, 24 mol.% CaO and 20 mol.% K_2O, and with 1 mol.% of Cu, Mn or Fe oxides added, were prepared. The corrosion products were studied by analysing the glass surfaces after being in contact for different periods with static water or using a stirrer.
The experimental conditions used reproduced well the corrosion processes found in ancient glasses of similar composition weathered through five centuries. Silica rich-layers and Ca-carbonates are always found in the exposed surfaces and more than one such layer develops during the longer immersion periods (see figure). When Cu, Mn and Fe are introduced in the glass matrix a layer richer in the transition metal ion added is formed in the glass surface. Cu-containing glass displays a faster initial dissolution that may be due to its particular oxidation state (2+) and coordination.



[1] Departamento de Conservação e Restauro, Universidade Nova de Lisboa.

Measurement of proton elastic scattering cross sections for light elements – validation of a "bulk sample" method.

A.R. Ramos, N.P. Barradas, E. Alves

The present project aimed at measuring (p,p) elastic cross sections for nitrogen and lithium in the 500-2500 keV energy range and for scattering angles between 160º and 130º. The measurements will be used with existing evaluated cross sections for other light elements, to validate a new automated method of proton elastic cross section measurement. The method will be applied to the determination of cross sections using bulk samples. The research carried out will result in improved data analysis algorithms in existing simulation programs for IBA. The improved algorithm, which accurately calculates proton backscattering spectra in the presence of cross section resonances, constitutes a desirable benchmarking tool for evaluated/measured cross-sections using standard bulk samples.

The following tasks were performed during 2007:

1. Reproducibility tests for the $^{14}N(p,p_0)^{14}N$ cross sections measured during the first year using thin films.
2. Benchmarking of evaluated/measured (p,p) cross-sections in the 500-2500 keV energy range for C, N and Si using bulk samples.
3. Continuation of the measurement of the (p,p) elastic cross sections for Li in the 500-2500 keV energy range using bulk samples.

Advanced data analysis for IBA

N.P. Barradas, M.A. Reis, C. Pascual-Izarra[1]

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. In 2007 the highlight was the conclusion of an intercomparison exercise of the main codes dedicated to the analysis of IBA data, made with support of the IAEA. The results confirmed that available IBA software packages are, within their design limitations, consistent and reliable, and that, in some complex cases, NDF has further capabilities and higher accuracy. The work on integrating PIXE in the NDF package was continued. Seven papers were published in 2007 in international journals.

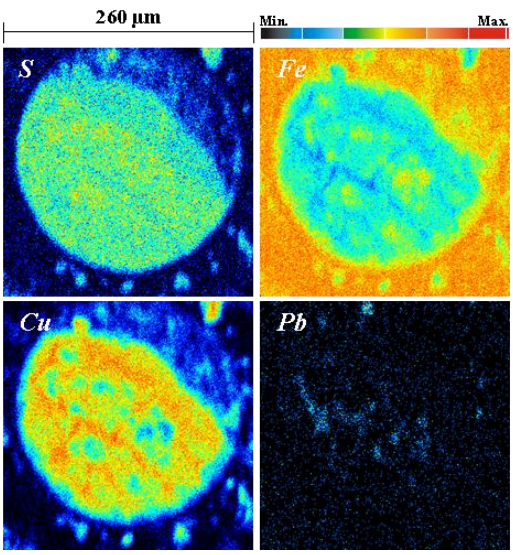
[1] Universidad Autónoma de Madrid, Madrid, Spain.

Characterisation of Roman and modern slag at S. Domingos mine

J. Figueiras[1] *1, A. Mateus*[1]*, A. Pinto*[1]*, N. Neng*[2]*, L.C. Alves, J. Matos*[3]*, J. Nogueira*[2]

Located in the Iberian Pyrite Belt, the S. Domingos mine has been exploited since Roman times. The exploitation generated a large amount of wastes and residues that cause strong environmental impact. The purpose of this work is to study the slag chemical stability under natural weathering and evaluate the possibility of slag re-processing in order to economically recover some of the contained metals.

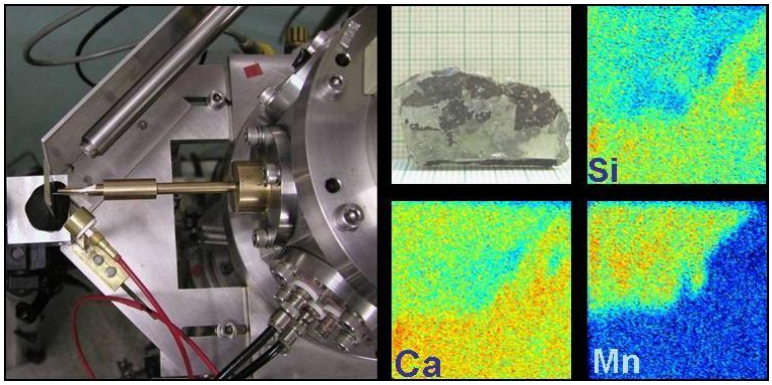
The selected samples were analyzed using several techniques, namely, optical microscopy, SEM-EDS, EPMA, μPIXE, ICP-MS, INAA and image analysis. This work indicates that, in spite of the good mechanical properties of the slag for aggregate use, care should be taken since they may release considerable amounts of metals (see figure). A re-processing of the slag is advised as the amount of some valuable metals in the sulphides and sulphosalts may be of considerable economical interest (Cd 100-400 ppm; In 100-300 ppm; Sn 700 ppm; Sb 200 ppm; Ag 100 ppm; Au 300 ppm).



[1] FCUL/Geology Dept.
[2] FCUL/Chemistry Dept.
[3] IGM/INETI

External microbeam line developments*
P.A. Rodrigues, L.C. Alves, R.C. da Silva

Further developments were achieved with the acquisition and installation of new equipment such as a laser device and video cameras for precise positioning of the target, and a new X-ray detector with fine energy resolution capabilities. These enabled to initiate the study of a group of archaeological Roman glass fragments.



Due to their poor state of conservation, namely delaminating of the glass surface, the use of external beam instead of in vacuum analysis was compulsory. Joining the microbeam capabilities (~70 μm) with the possibility of producing a beam scan, sample surface images were obtained allowing to clearly identifying corroded and clean regions, as corroded areas present increased contents of Mn and Fe (see figure).

This allowed a more representative analysis of the glass bulk composition and the possibility of comparing several fragments as part of the same object, as well as giving clues to their provenance and period of manufacture. The project will be completed with the design of an external target holder comprising a 3-d motorized displacement table with 6 degrees of freedom, 3 continuously driven mm-wise translations for coarse positioning and 3 step-wise micrometer translations for fine positioning.

* Project POCTI/CTM/60685/2004

Upgrade of X-ray laboratory at Physics Department
N. Franco, E. Alves

The main activity of the x-ray laboratory at ITN Physics Department is concentrated on the characterisation of semiconductor materials, in collaboration with several research groups. Modern semiconductor materials used for device fabrication are based on thin multilayer structures and the continuous reduction of the device size puts a lot of pressure on the characterisation techniques, demanding beams with high spatial resolution as well high angular resolution. Thus, the laboratory upgrade with a new high resolution beam line was mandatory and the Bruker-AXS B8Discover X-ray diffractometer showed to be the ideal diffractometer that fulfils these demands. Although, after installation several issues related to beam stability emerged, such as primary beam oscillation and too long warming up times, the problems were solved by 6 months long hard work between ITN and German technicians from Bruker-AXS. The D8Discover shows to be a great advantage in materials characterisation adding new X-ray techniques to the laboratory, e.g. GID (Grazing Incidence Diffraction (planar)), as well allowing decreasing the response time to the collaborators.

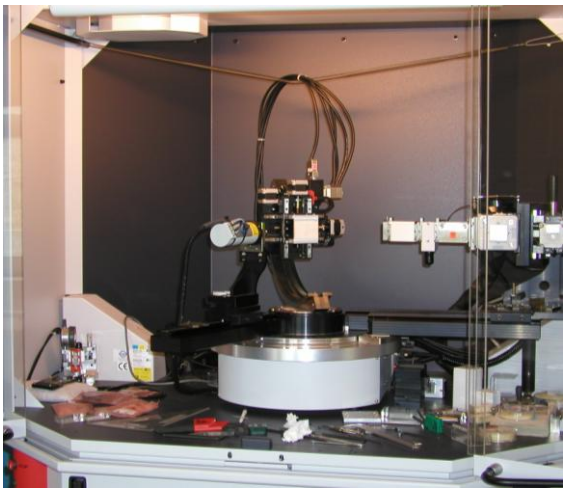


Fig. 1 – Bruker-AXS D8Discover diffractometer

Biomedical Studies

Teresa Pinheiro

The research activities during 2007 within the group of Biomedical Studies make use of focused ion beam techniques to image tissue and cell morphology as well as other micro-analytical techniques to assess elemental composition and molecular indicators of cell/tissue response (e.g., imaging techniques, cell detection techniques along with characterization of signalling molecules, nuclear techniques and mass spectrometry based techniques, among others).

The outcome of past and ongoing research projects in health and disease condition of human populations paved the way to the present activities. The studies on pneumology/environmental health, dermatology and haematology, combining indicators of exposure to pollution sources, the inflammatory response and metabolism, are naturally continuing as confirmed by renewed financial support of private and international entities.

A recently approved project will reactivate environmental health studies and long standing collaborations with Serviço de Pneumologia, Hospital de Santa Maria, and will make use of new technical facilities such as ICP-mass spectrometer that is being installed under the National Program for Scientific Re-equipment. The study will focus on the relationship between professional exposure to chemical agents and EBC (Exhaled Breath Condensate) characteristics, in order to develop a non-invasive human bio-indicator.

The significant funding of several projects in association with the Serviço de Cardiologia, Hospital de Santa Marta, Centro Hospitalar de Lisboa Central, stimulated the research activities to develop a clinical registry of inflammation in acute coronary syndromes and to monitor the alterations of that process during the recovery period. The driving motivation for this work is to improve medical diagnosis for the clinical atheroma. Modern imaging techniques, virtual histology intra-vascular ultrasound (VH IVUS), for the artery wall also assessing plaque composition opened new perspectives of studying the clinical atheroma. Associating the biological characteristics of the plaque with circulating indicators of plaque activity and endothelial function, may have a noteworthy outcome in VH IVUS data interpretation with direct implications in the clinical practice.

These projects will strengthen existing skills in environmental health and molecular cardiology in Portugal, and will promote advanced training for students and create new synergies by involving various research groups from different areas.

The main achievements of the research developed during 2007 are summarised in the following pages.

Researchers

T. PINHEIRO, Aux.
L.C. ALVES, Aux.

Students

P. NAPOLEÃO, Ph.D. student, FCT grant
P. ALMEIDA, M.Sc. student, FC-UL
R. CARVALHO, M.Sc. student, FC-UL

Technical Personnel

R. PINHEIRO, laboratory assistant

Collaborators

R.C. FERREIRA, M.D., Hospital Sta. Marta
M. SELAS, Hospital Sta. Marta
M.C. SANTOS, Aux. Prof., FC-UL
A.M. VIEGAS-CRESPO, Princ. Researcher, FC-UL
A. TURKMAN, Full Prof., CEAFC, FC-UL
M.C. MONTEIRO, Ass. Prof., CESPU, Porto
A. BARREIROS, Aux. Resarcher, INETI
A.B.ALMEIDA, Full Prof., FM-UL/Hospital Sta. Maria
P. FILIPE, Aux. Prof., FM-UL/Hospital Sta. Maria
R. SANTOS, M.D., Hospital Sta. Maria
R.FLEMING., M.D., Hospital Sta. Maria
J.N. SILVA, M.D., FM-UL/Hospital Sta. Maria

New Biomarkers For Human Pathologies

T. Pinheiro and L.C. Alves

A – Endothelial function and plaque activity in acute coronary syndromes

P. Napoleão, R. Cruz Ferreira, M. Selas, M.C. Monteiro, A.M. Viegas-Crespo, A. Turkman[1], V. Andreozzi, R. Carvalho

An increasing body of literature shows that the progressive development of the atherosclerotic plaque and local vascular events that encircle an acute coronary syndrome implicate pro-inflammatory mediators.

We are studying activation and apoptosis associated to endothelial cells and/or platelets by measuring molecules in circulation (signalling molecules, cytokines, adhesion molecules), their expression in platelets and leukocytes, and the microparticles released in those processes. The relationship of virtual histology intravascular ultrasound (VH IVUS)-derived measurements of atherosclerotic plaque with the above indicators of plaque activity and endothelial function are being assessed to establish correlations between plaque composition, patient morphological parameters, cardiac events and plaque progression and regression. A follow-up of acute myocardial infarction (AMI) patients has been evaluated against patients with angiographically normal coronary arteries (controls) and healthy volunteers (reference group). AMI patients are evaluated at 3 time points: at admission (day 0), two (day 2) and 40 (day 40) days after intervention.

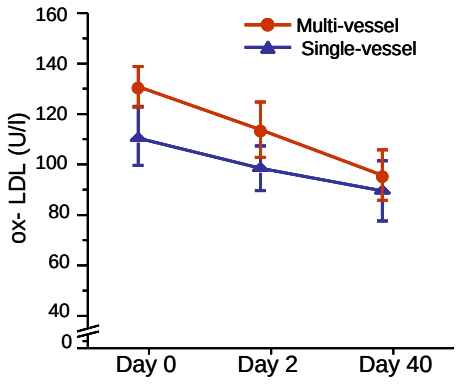


Fig. 1. Disease severity (expressed as no. of vessels involved) and concentrations of circulating ox-LDL from infarct onset to 40 days after.

We expect to obtain new indexes of plaque progression and regression and identification of at-risk patients from a systematic data evaluation of anthropometric, physiological variables, and bio-indicators. The study is supported by Liga de Amigos do Hospital de Sta. Marta and FCT (SFRHI/BD/ 18822/2004).

B – Skin as a tool in metabolic disorders and immune diseases

R. Silva, R. Fleming, P. Filipe, J.N. Silva, A. Barreiros

Skin iron as a diagnosis tool in hemochromatosis

The study used conventional and innovative laboratory tests to differentiate distortions of iron metabolism. Patients were genetically characterized and studied before starting and along the phlebotomy therapy. Nuclear microscopy and nuclear resonance techniques provided iron quantitative imaging and physiological information on skin and liver. Biochemical methods provided hepcidin contents in serum and markers of iron metabolism and organ function. The study is supported by the **projects SPDV 2004-2007 and IAEA CRP 2005-2008**.

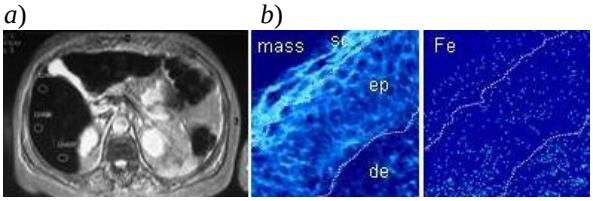


Fig. 2. Iron imaging. a) Magnetic Resonance: dark regions are hypodense liver (Fe = 210 µmol/g); b) Proton Microscopy (~100×100 μm^2): skin layers depicted from mass density image validate epidermal region of Fe deposition (10±3 µmol/g).

Skin barrier* and immune profile *in psoriasis

Psoriasis is a skin disorder characterised by an increased proliferation and disturbed differentiation of keratinocytes. The main objective of the study is to characterise the immune pattern and the markers of the inflammatory cascade, hyperproliferation and keratinisation in the psoriatic lesions of patients with moderate to severe plaque psoriasis. T-lymphocyte profile in responders and non-responders, their activation profile and how it correlates with TNF-a and keratinocyte hyperproliferation and keratinisation, the skin barrier function and the involvement of calcium and other divalent ions distribution in skin strata, are some of the aspects that are being covered in the project. This Project is supported by **SERONO, Fundación Salud 2000 (Research Prize "Investigação Clínica em Psoríase" - 2006-2008)**.

[1] Centro de Estatística Aplicada, FC-UL

Elemental Characterization and Speciation
CEEFI

Miguel A. Reis

The Elemental Characterization and Speciation Group of the LFI (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 was put on particle induced x-ray emission (PIXE) and airborne material. Atmospheric environment related samples like airborne particulate matter and/or biomonitoring samples being different faces of this focus. A tunning of this working line is presently being undertaken in order to cover a broader but more concise focus on small mass samples such as particulate matter (airborne or not), nanoparticles, macromolecules or thin film samples,

Strategically, the group assumes that it is important not to depend exclusively on collaborations neither for sampling nor for data handling processes. Therefore, a strong R&D effort is put on airborne particle sampling and data handling methods. Data handling R&D includes both spectra analysis, as well as environmental data analysis (namely inverse methods for source apportionment).

Taking into account that PIXE is already a matured analytical technique, services are provided to the community in general, and to the scientific community in particular. In this cases, analysis of samples other than small mass ones is carried out, and it is not rare that important spin offs associated to details or specific developments of the PIXE technique, do emerge in this framework.

Within the organics of the Ion Beam Laboratory (LFI), CEEFI is responsible for the maintenance and improvement of PIXE facilities, and assures that, at least, are no losses on the installed capacity occur.

In 2007, the groups' activity was focused on the implementation of the Laboratory for Characterization and Speciation of Aerosols (LCEA), a major equipment upgrade based on a large re-equipment project. Equipment acquisition and installation were tasks using a fair chair of the time. The project contributed to the acquisition of a refurbished Tandetron accelerator where the new PIXE setup for High Energy and High Resolution PIXE is under installation. The first High Energy spectra were obtained and presented at the International PIXE Conference that took place in Mexico.

Apart from this the major lines of work involve: (1) x-ray lines relative intensity studies, these have been shown to present an apparent dependence on the beam energy, which origin is under study and is subject of a PhD thesis in ion beam analysis speciation; (2) improvements on the existing data handling software, including holistic approaches and the recovery of some lines of work that had been abandon in the middle of the 1990 decade (eg: ion ionization cross-sections) which are again becoming an important subject due to the recente developments in both software and hardware (namely fact that a 10eV resolution x-ray EDS detector is about to be installed at ITN as one of the major outcomes from the LCEA project). Finally, the database on airborne element content measurements in Portugal dating back to January 1995 was completed and is being formated for publication during 2008.

Researchers (*)

M.A. REIS, Aux. (Coordinator)

Students

P.C. CHAVES, Ph.D. student, FCT grant

Technical Personnel

R. PINHEIRO

Collaborators

G. DIAS, Graduated (until July 2007)
R. MALVEIRO, Graduated (April to August 2007)
A. TABORDA, Ph.D. Student

(*) Also member of CFNUL.

Micro and Nano-particles Characterization and Speciation

M. A. Reis, P. C. Chaves, N.P. Barradas, A. Taborda, A. Carvalho[1], M. Kavčič[2]

The characterization and speciation of small mass samples like airborne particles, is the basis and central issue of the CEEFI group work. Each of the specific activities of the group therefore converges towards this aim, or emerges from it. During 2007, the main activity besides the operation of an airborne particle sampling unit at ITN campus, was the installation of the Laboratory for the Characterization and Speciation of Aerosols (LCEA), the development of software and the study of Mo and Gd compounds X-ray lines relative intensity as function of the incident proton beam energy. All of the tasks converging to the same goal, namely using particle induced x-ray for determining chemical and/or sample size effects.

Presently almost all major installations planed for LCEA are installed, namely a SO2, CO2, NO, NO2, O3 and gas phase Hg DOAS analyser, working in continuous monitoring, a meteorological station, and the new HEHR-PIXE line, installed on the recently acquired 3MV Tandetron. In the beginning of 2008 the 10 eV resolution POLARIS EDS microbolometer x-ray detector system from Vericold Technologies GmbH, will become operational.

In respect to the study of the Gd compounds it was shown that spectra from pallets of Gd oxide powder do not present the same pattern of variation with the energy of the incident ion beam as 5nm particles of the same material, while these present sometimes patterns similar to those found during the study of pellets of Gd-DOTA, a common MRI contrast agent (see fig. 1).

In the case of Mo, it was shown that the new developed PIXE spectra software was able to provide from the deconvolution of spectra obtained using a Si(Li) detector, results similar to those obtained using a ultra high resolution detector from the JSI, in Slovenia. The same results also showed that different Mo compounds present different patterns for the variation of the x-ray line ratios with the energy of the incident ion beam.

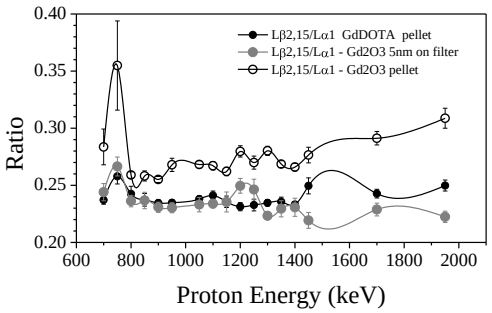


Fig. 1.Change in the ratio of intensity of lines $L_{\beta 2,15}$ and $L_{\beta 1,2}$ in three samples of Gd, as function of the energy of the incident protons. Being transitions to the same L-subshell, this effect is presently unexplainable.

1 Escola Superior de Tecnologias da Saúde de Lisboa, Portugal
2 Josef Stefan Institute, Lubljana, Slovenia

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 European Large Scale Facility where more than 750 isotopes and 80 elements are produced and delivered as ion beams of high elemental and isotopic purity, which is unique in the world. In this context nuclear techniques such as Emission Channeling (EC) and Perturbed Angular Correlations (PAC) provide complementary (atomic scale) information to the material analysis capabilities available at ITN. The ITN-CFNUL infrastructure and related projects are refereed and reevaluated each year within the scope of FCT-supported CERN projects. The scientific work in 2007 was centered in three research subjects that have been approved with beam time by the ISOLDE Scientific Committee:

a) IS453 "Emission Channeling Lattice Site Location Experiments with Short-Lived Isotopes". The lattice sites of impurities in technologically relevant semiconductors (e.g. Si, Ge, ZnO, GaN) and oxides (e.g. $SrTiO_3$, $KTaO_3$) are studied by means of the EC technique. New probes from elements that only possess short-lived radioactive isotopes are now available, as is later detailed in this report.

b) IS390 "Studies of colossal magnetoresistive oxides with radioactive isotopes". PAC is used to study multi-ferroic $RMnO_3$ manganites as a function of element R and temperature to study local phenomena that are correlated with the coexistence of ferroelectricity, ferromagnetism and ferroelasticity.

c) IS360 "Studies of High-Tc Superconductors doped with radioactive isotopes". PAC is used to study the atomic distribution of oxygen dopants at high concentration at the Hg planes of the $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$, high-Tc superconductors. The aim is to learn where O_δ sits (and dopes) depending on concentration. This is accompanied by modern first principle density charge simulations that reveal the importance of spin interactions on site occupancy and lattice relaxation.

With respect to the work topics during 2007, priority was given to the commissioning of the new emission-channeling chamber, the new fast Si pad-detector, the development of the data treatment program for on-line experiments, and first successful data-taking in June 2007. Regarding the EC on-line setup, 2008 will be still a year of experimental consolidation, with the planned integration of a cooling station (30 K-300 K). The overall effort for further development of the EC technique is well justified since the precise lattice location and rms displacements of impurities in crystalline materials are not accessible by more traditional methods. In a different context, radioactive hyperfine techniques are very useful for studying electrical and magnetic properties at the nanoscopic scale. During 2007 an extra physics push was made to learn and handle new state-of-the-art charge density simulation programs that include relativistic and spin interactions to provide a better understanding of systems with strong electronic ⇔ atomic correlations as occurs within the manganites.
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, ISEL as well as from Leuven in Belgium. Presently, seven Ph.D. students, one M.Sc. and one diploma student accomplish their work using this infrastructure, within the scientific proposals and R&D projects, testing new experimental and physics concepts.

Researchers
J.G.M. CORREIA, Princ.
U. WAHL, Princ.
E. ALVES, Princ.

Students
A.C. MARQUES, Ph.D. student, FCT grant
C. SOUSA, Ph.D. student, FCT grant
E.C. RITA, Ph.D. student, FCT grant
J.C.S. AMARAL, Ph.D. student, FCT grant
J.N. GONÇALVES, Ph.D. student, FCT grant
L. PEREIRA, Ph.D. student, FCT grant
S. DECOSTER, Ph.D. student, IKS-Leuven grant
T. MENDONÇA, B.I. fellowship, POCTI
S. COSTA, B.I.I. fellowship, POCTI
M. BARBOSA, Diploma Student FCT projects

R. FERREIRA, Diploma Student

Collaborators
V. AMARAL, Ass. Prof., U. Aveiro
J.P.E. ARAUJO, Aux. Prof., U. Porto
M.R. SILVA, Ass. Prof., IST, Lisboa
J.C. SOARES, Cat. Prof., U. Lisboa
L. REDONDO, Ass. Prof., ISEL, Lisboa
H. HAAS, Emeritus Researcher, ITN
A. VANTOMME, Prof., IKS Leuven
A.L. LOPES, Post-Doc, FCT grant

IS-453 experiment: Emission channeling lattice location studies

U. Wahl, J.G. Correia, A.C. Marques, C.P. Marques, E. Rita, E. Alves, S. Decoster, A. Vantomme, M.R. da Silva, J.P. Araújo, L. Pereira, J.C. Soares, and the ISOLDE collaboration[1]

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 electron emission channelling (EC) from radioactive isotopes. With this technique information is available for very low dopant concentrations and independent from the host lattice elemental composition. The experiments are carried out using the ITN/CFNUL infrastructure installed at CERN's ISOLDE facility.

Results

1. Amphoteric arsenic in GaN

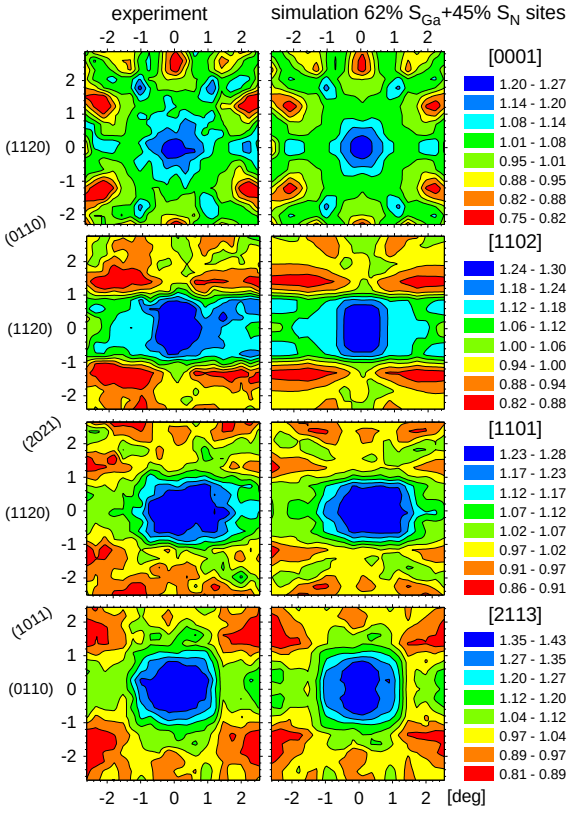


Fig. 1: experimental EC patterns from ^{73}As in GaN (left) and simulations for 62% of As on Ga and 45% on N sites (right).

We have determined the lattice location of implanted arsenic in GaN by means of conversion electron emission channelling from radioactive ^{73}As (80.3 d). Already in the as-implanted state but also following annealing up to 900°C it was found that similar fractions of As occupied substitutional Ga and substitutional N sites. We have thus given direct evidence that As is an amphoteric impurity in GaN, thus settling the long-standing question as to whether it prefers cation or anion sites. The amphoteric character of As provides additional aspects to be taken into account for an explanantion of the so-called "miscibility gap" in ternary $GaAs_{1-x}N_x$ compounds, which cannot be grown with a single phase for values of x in the range $0.1 < x < 0.99$. The lattice location of As in GaN contrasts with its site preference in ZnO where we found it to occupy mainly substitutional Zn sites with only minor fractions on O sites, a fact which can be explained by the smaller size mismatch between As^{3-} and N^{3-} ions (2.22 Å *vs* 1.71 Å).

2. Emission channeling with short-lived isotopes

Following last year's report on the implementation of self-triggering readout chips for position-sensitive Si pad detectors (supported by the ITN Sacavém/CFNUL Lisbon group in collaboration with CERN) and on the development of an emission channelling on-line setup, we report here on first results with this new equipment. The setup was used on-line during the Mn beam time in June 2007, mounted at the LA2 beam line of ISOLDE and equipped with the new detectors, which performed well and allowed to reach data-talking rates above 3 kHz. Two isotopes were successfully used for β^- emission channelling experiments for the first time: ^{56}Mn (2.58 h) and ^{61}Co. While ^{56}Mn was available directly, ^{61}Co was obtained by means of implanting the short-lived precursor isotope ^{61}Mn and exploiting the decay chain ^{61}Mn (4.6 s) $\rightarrow$ ^{61}Fe (6 min) $\rightarrow$ ^{61}Co (1.6 h). We were thus able to determine the lattice location of Mn in GaN and of Co in ZnO in the as-implanted state and following annealing up to 900 °C. In both cases it was found that the transition metals preferred substitutional cation (i.e. Ga or Zn) sites.

Published work

U. Wahl, J.G. Correia, J.P. Araújo, E. Rita, and J.C. Soares: "Amphoteric arsenic in GaN", Applied Physics Letters 90 (2007) 181934/1-3.

[1] CERN, 1211 Geneva 23, Switzerland

IS360 experiment – Oxygen occupancy in $HgBa_2Cu_2Ca_1O_{6+\delta}$ high-Tc superconductors

T. Mendonça, J.G. Correia, H. Haas, M.R. Silva, P. Odier[1], J.P. Araújo, A. Pereira[2], M. Pereira[2], J.C. Amaral, R. Ferreira and ISC[3]

We found evidence for O_δ occupying (unexpected) interstitial positions along the edge of the Hg square in $HgBa_2Cu_2Ca_1O_{6+\delta}$ (Hg1212) on samples heavily doped, under pressure, with oxygen. This was first revealed by an electric field gradient (EFG) with relatively low Vzz and high $\eta \sim 1$ induced at ^{199m}Hg nuclei, measured with Perturbed Angular Correlation (PAC). Then a major effort was made in 2007 to run simulations with a new program, WIEN2k that uses density functional theory with the local spin density approximation. This requires quite large supercells and lengthy computer time for the present physics cases. Since this position for O_δ cannot be stable alone, even if it will reproduce the experimental EFG results, we simulate several oxygen configurations to learn that the stability is ruled by local strong deformations in correlation with the known elongation of the *a* lattice parameter, which can only be properly simulated with the inclusion of spin density functionals. It hints as if oxygen can be promoted to such interstitial abnormal sites if, in adjacent rows the centers of the Hg squares are heavily loaded with oxygen, and extra deformations take place when more oxygen atoms are forced in. Once simulations are completed, this work might explain the origin of controversial diffraction data that hinted such an additional position for the dopant without being able to confirm or explain it.

[1] Lab.Crystalographie, CNRS, Av. des Martyrs 25, F-38042 Grenoble CEDEX 9, France
[2] Dep. of Physics and CICECO, Aveiro University, 3810-193 Aveiro, Portugal.
[3] ISOLDE Collaboration, CERN, 1211 Geneva 23, Switzerland.

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

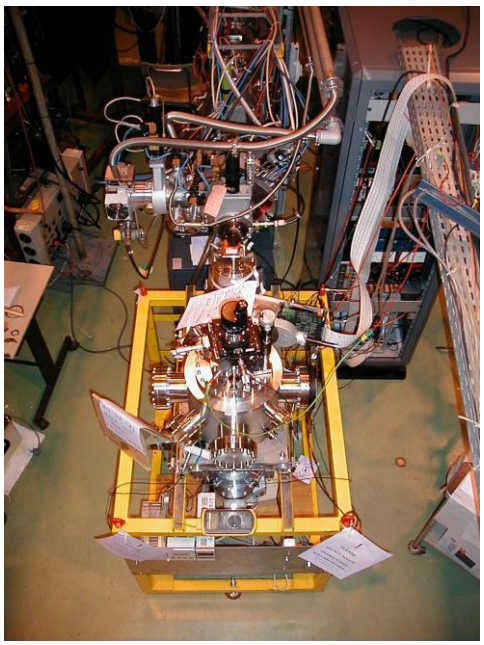
A.M.L. Lopes[1], J.C. Amara1[1], V.S. Amaral[1], J.P. Araújo[2], A. Pereira[2], J.J. Ramasco[2], J.G. Correia, and ISC[3]

A family of multiferroic systems $RMnO_3$ perovskite manganites (R = Eu, Gd, Ho, Y, Er and Lu) have been prepared with the sol-gel technique. On these systems the issue is to understand the microscopic phenomenology that causes coexistence of ferroelectricity, ferromagnetism and ferroelasticity as a function of R and temperature. PAC studies have been performed allover the series to measure the Electric Field Gradient / Magnetic Hyperfine Field of ^{111m}Cd/^{111}cd atoms at R sites, as a function of the ionic radius of the element R and for some cases under different temperature conditions from 10 K to 473 K. The first data and analysis show that there are two competing local configurations on the lattice, from which only one shows a correlation of the η (asymmetry EFG parameter) with transition temperature as a function of R. These first results point to the separation of microscopic phases, maybe associated to local deformations, with the macroscopic properties.

[1] Dep. of Physics and CICECO, Aveiro University, Aveiro, Portugal.
[2] Dep. of Physics IFIMUP and CFP, Porto University, Porto, Portugal.
[3] ISOLDE Collaboration, CERN, Switzerland.

R&D development – new Si pixelated detectors for position sensitive electron detection

A.C. Marques[1], U. Wahl, J.G. Correia, M.R. Silva, P. Weilhammer[2], E. Chesi[2], A. Rudge[2], M. Campbell[3], L. Tlustos[3]



The commissioning of the on-line chamber and fast Si-pad detector has been successfully achieved, with data taking. Looking forward to the future, we have submitted a research proposal to the MEDIPIX detector collaboration at CERN (http://medipix.web.cern.ch/MEDIPIX/) that got approved in early December. These detectors have 256×256 pixels covering 15×15mm^2, self common mode compensation and the bias and full readout is provided via a single USB cable. The collaboration will do a prototype for emission channeling purposes with four of such detectors covering an active surface of 30×30mm^2, that we expect to commission during the second half of 2008. The software is fully developed and can easily be adapted to our type of data analysis.

[1] CFNUL, Lisbon University, Portugal.
[2] CERN, 1211 Geneva 23, Switzerland.
[3] MEDIPIX, CERN, 1211 Geneva 23, Switzerland

Nuclear Reactions

Adelaide Pedro de Jesus

This group has been involved in the experimental study of nuclear reactions relevant to nuclear astrophysics and also to ion beam analytical techniques.

The on-going work is related to the development of the AMS line to study reactions relevant to nuclear astro-physics.

In the short term the work to develop a calibrated PIGE set-up will be extended to a new accelerator line connected to the Tandem 3MV accelerator, creating new perspectives in applied work for Environment, Materials and Health Sciences and Geology.

Researchers (*)
A.P. JESUS, Full Professor (FCT/UNL), Group Leader
J.P. RIBEIRO, Associate Professor (FCUL)
J. CRUZ, Assistant Professor (FCT/UNL)

Technical Personnel
R. MATEUS, Technical Assistant

Students
M. FONSECA, Ph.D. Student, (FCT/UNL)
H. LUÍS, Ph.D. Student, (FCT/UNL)

(*) Also members of CFNUL.

Experimental Study of Nuclear Reactions for Astrophysics

H. Luis, J. Cruz, A.P. Jesus, M. Fonseca, J.P. Ribeiro

Objectives

Nuclear reactions relevant for primordial and stellar nucleo-synthesis usually take place at energies much lower than the Coulomb barrier between the target nuclei and positive projectiles. Its cross sections dominated by the probability of tunnelling through the Coulomb barrier, decrease exponentially, as the energy drops down, achieving values that, for the purpose of an experimental measurement, represent a real challenge. AMS – accelerator mass spectrometry is a technique that has been developed to quantify rare isotopes, achieving for some of them very high sensitivities.

The aim of the present work is the experimental study of reactions relevant for nuclear astrophysics, namely $d(\alpha,\gamma)^{6}Li$ and $^{51}V(^{3}He,n)^{53}Mn$ reactions, through the optimization of the AMS technique to detect and quantify ^{6}Li and ^{53}Mn, products of the referred reactions.

Results

The AMS line (Fig.1) is part of the Tandem accelerator and lines purchased to an Australian laboratory.

The going-on work is related to the assembling, tuning and testing of the AMS line. Due to the high number of parameters involved this task has been very demanding in man-power. The line and the ion source are already assembled; tuning and testing are being done with some carbon spectra already obtained before the accelerating stage (Fig. 2).

In connection to the reactions to be studied targets have been prepared; Ti and Hf have been implanted with deuterium, but the amount obtained was not enough; vanadium foils were bombarded with ^{3}He and the complex gamma-spectra obtained are being analysed.

Future Work

After finishing the tuning and testing of the AMS line, backing materials (for targets) will be tested in order to assess their purity. A nuclear reaction line will be assembled at the Tandem accelerator in order to produce the referred nuclear reactions, whose produtcts will be measured by AMS.

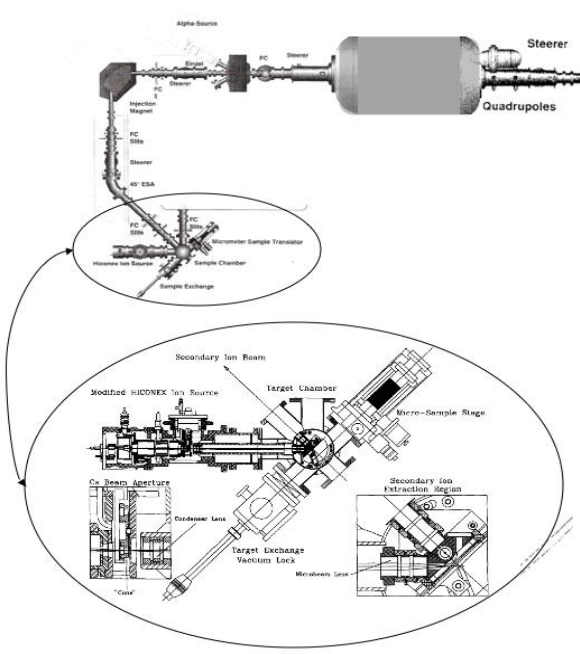


Fig. 1 The AMS line with detail of the ion source.

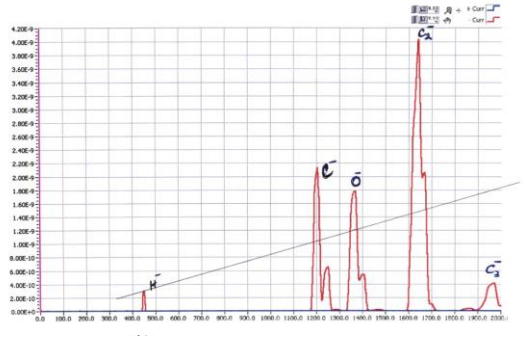


Fig. 2 Carbon spectrum obtained before the accelerating stage.

Calibration of a PIGE Set-up for Al and Mg

M. Fonseca, R. Mateus, A. P. Jesus, H. Luis, J. P. Ribeiro

Objectives

The aim of this work is the extension to Al and Mg of previous work [1-4] in order to install an analytical set-up for light element analysis, based on the detection of the gamma radiation induced by low energy protons, PIGE. This technique will open new perspectives of applied work in environment and health problems.

Results

A precise method based on a code [4] 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 functions for $^{27}Al(p,p'\gamma)^{27}Al$ and $^{25}Mg(p,p'\gamma)^{25}Mg$, were obtained to introduce as input. Thick target gamma yields for several samples containing Al and Mg were measured to be compared with calculated yields. Results for Al have been published [5].

Table 1

Ratios Y_{exp}/Y_{cal} between experimental and calculated γ-ray yields obtained for three different thick samples containing aluminum: Al_2TiO_5, Al_2O_3 and pure Al. Results are given for both 844 keV and 1014 keV γ-emissions of the $^{27}Al(p,p'\gamma_{1,2})^{27}Al$ nuclear reaction. The incident proton beam was fixed at 2.0 MeV, 2.2 MeV and 2.4 MeV.

	Y_{exp}/Y_{cal} - 844 keV emission			Y_{exp}/Y_{cal} - 1014 keV emission		
Thick sample	2.0 MeV beam	2.2 MeV beam	2.4 MeV beam	2.0 MeV beam	2.2 MeV beam	2.4 MeV beam
Al_2TiO_5	1.00	1.00	0.95	1.00	0.99	1.00
Al_2O_3	0.98	0.97	0.93	0.98	0.96	1.00
Al	0.99	0.99	-	1.00	1.00	-

Future work

At energies lower than 2.5 MeV, this work will be concluded by including the case of Be. A nuclear reaction line will be assembled at the Tandem accelerator in order to extend the present work to higher energies and be able to quantify C, N and O.

References

[1] R. Mateus, A.P. Jesus, B. Braizinha, J. Cruz, J.V. Pinto, J. P. Ribeiro, Nucl. Instr. Meth. B 190 (2002) 117-121
[2] R. Mateus, A.P. Jesus, J.P. Ribeiro, Nucl. Inst. and Meth. B 219-220 (2004) 519-523
[3] R. Mateus, A.P. Jesus, J. Cruz, J.P. Ribeiro, Nucl. Inst. and Meth. B 219-220 (2004) 307-311
[4] R. Mateus, A. P. Jesus, J. P. Ribeiro, Nucl. Inst. and Meth. B229, 302-308 (2005)
[5] R. Mateus, M. Fonseca, A.P. Jesus, H. Luís, J.P. Ribeiro, *Nucl. Inst. and Meth*.B, doi:10.1016/j.nimb.2007.11.042 (*in press*).

Condensed Matter Physics

Fernanda Margaça

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 particular samples. Special polymeric materials have been investigated in collaboration with groups from the Universities of Aveiro and Coimbra, Laboratoire Léon Brillouin (CEA-CNRS-Saclay), KFKI, Budapest, and the Budapest Neutron Centre. During 2007 the main effort was put into the characterisation of hybrid materials and co-polymers prepared by gamma irradiation using the ^{60}Co source of UTR.

The systems studied were: (i) hybrids prepared from mixtures of a polymer (PDMS) and various alkoxides, with emphasis in the elemental and topographic characterization and RBS analysis of various samples prepared using irradiation methods; (ii) development of new copolymers (HEMA grafted on LPDE thin films) suitable for bioapplications. Here, sample preparation conditions were correlated to the grafted material structure and the hydration level achieved by the final product, and toxicity studies were conducted. Tests of Biocompatibility (haemolysis and tromboresistance) are also being carried out. Work on these systems is resumed in an MSc thesis defended in 2007and a PhD thesis completed in 2007.

The Group has also been 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. Shortage of resources, both human and financial, is preventing the proper development of the activity in this area.

As concerns human resources both the staff and the students were recently significantly reduced. Frederico Carvalho, senior researcher and founder of the group, had reached retirement age in 2006. Although he continues to contribute to current activities the long due implementation of a plan of selected recruitment of scientific personnel has become more pressing.

This situation has been aggravated by the exit of two students in the end of the first half of 2007. David Silva left as he found a better professional position outside of the Institute and the MsC student Susana Gomes left at the end of the FCT grant, after having finished her Master thesis.

As concerns the financial resources, the neutron scattering instruments situation is also particularly difficult. This type of instruments installed at reactors require a set of equipments and components that are, generally expensive items, to be able to tailor the neutron beam, eliminate the undesired background and collect the data, in a suitable and efficient way. This becomes particularly critical when the source has low flux. During 2007 the core of the Portuguese Research Reactor, RPI, has been converted from HEU to LEU. It is predicted that this change will have a significant impact in both the total thermal neutron flux and on the signal to noise ratio. Work will proceed, in the instruments installed at RPI, to determine how far these are affected.

The Group’s work has been supported by funds from FCT, IAEA, ITN and income from services.

Researchers
F.G. CARVALHO, Senior[1]
F.M.A. MARGAÇA, Princ.
A.N. FALCÃO, Princ.
L.M.M. FERREIRA, Aux.
C.M.M. CRUZ, Aux. (20%)
J.S.NEVES, Aux. (20%)

Students
S. GOMES, B.I. Grantee, POCTI [2]

Technical Personnel
D. SILVA, Laboratory Assistant[3]

Collaborators
I.M.M. SALVADO, Dep. of Glass and Ceramics Engineering, UIMC, University of Aveiro,
M.H. GIL, Dep. of Chemical Engineering, Faculty of Sciences and Technology, Coimbra University

[1] Retired
[2,3] Left in end of June

Novel Way to Control PDMS Cross-linking by γ Irradiation

F.M.A. Margaça, S.R. Gomes, A.N. Falcão, L.M. Ferreira and I.M.M. Salvado

Objectives

The purpose was to investigate the properties of the cross-linked PDMS network obtained from the gamma-irradiation of a mixture of PDMS and the silicium alkoxide TEOS.

Results

Samples were prepared by γ-irradiation of a mixture of polydimethilsiloxane, PDMS, and tetraethylortosilicate, TEOS, in varying concentrations. The obtained materials are monolithic, flexible and transparent. It was confirmed that, for this type of mixture, the mass of the irradiated materials approach that of the PDMS used in the preparation stage as the drying stage proceeds [1]. Thus, most of TEOS evaporated and only a very small part was retained in the dried sample. X-ray diffraction was carried out in dried samples and showed that they are amorphous. The thermal behaviour has also been studied by using Differential Scanning Calorimetry (DSC) and Thermal Gravimetric Analysis (TGA).

Fig.1. Thermograms of xPDMS (1-x) TEOS samples.

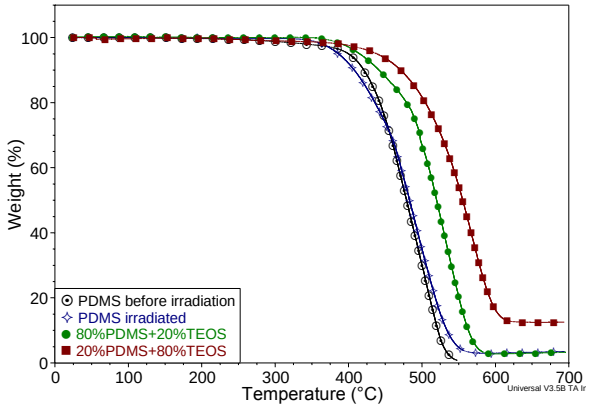
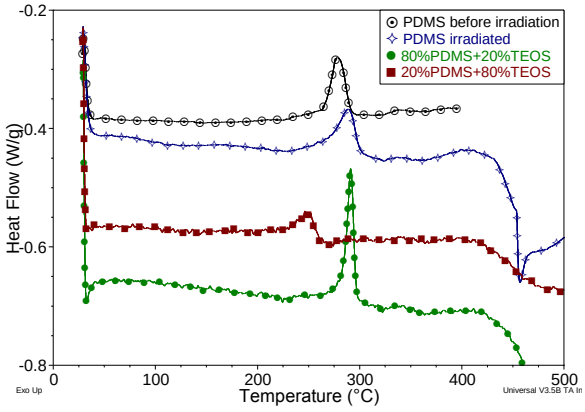
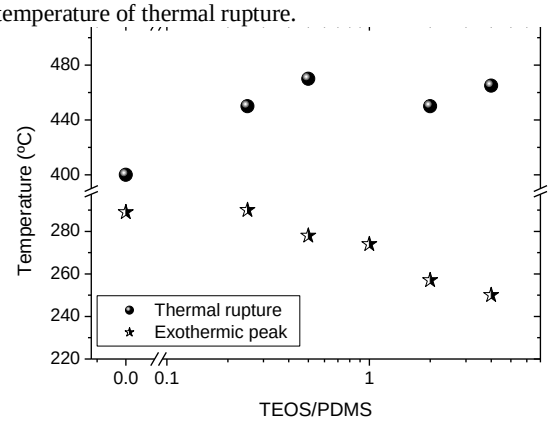


Fig.2. DSC plots for the same set of samples.



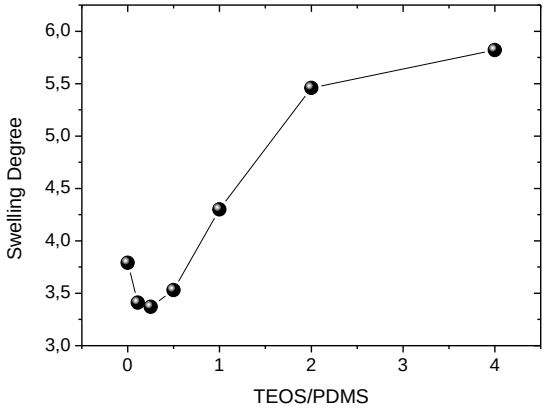
DSC and TGA curves show that the thermal behaviour depends on the presence of TEOS.

Fig.3. Variation of the exothermic peak position and temperature of thermal rupture.



The temperature necessary to promote the thermal rupture increases, by 50 ºC, when TEOS is used. As TEOS evaporates almost completely during the drying stage, the increase in this temperature seems to be related to the increasing strength of the PDMS cross-linked network. The exothermic peak, that is associated to chain ordering, occurs at T < 300 ºC and its value decreases as the TEOS content increases. This shows that TEOS facilitates the spatial ordering of PDMS chains in the sample.

Fig.4.Variation of the swelling degree with TEOS.



Although most of TEOS evaporates after precursors irradiation, its presence has a major impact in thermal properties as well as in the swelling properties of the material prepared by γ-irradiation.

The latter showed that PDMS cross-linked network strongly depends on the TEOS content present during the irradiation process. This provides a new way to control PDMS cross-linking by γ-irradiation.

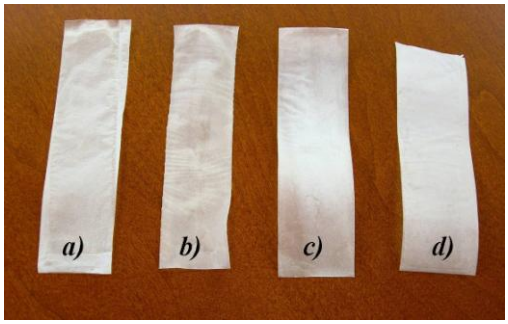
Published Work

S.R. Gomes, F.M.A. Margaça, L.M. Ferreira, I.M. Miranda Salvado, A.N. Falcão, *Nuclear Instruments and Methods B* **265** (2007) 114-117.

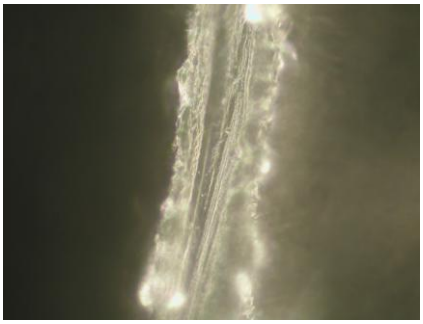
Hemocompatibility Evaluation of LDPE Based Copolymeric Films Obtained by Gamma Irradiation

L.M.Ferreira, A.N. Falcão, M.H. Gil

Using 2-hydroxyethyl methacrylate (HEMA) as grafting monomer, we have optimized the preparation of new grafted copolymeric Low Density Polyethylene (LDPE) based films by gamma radiation, using a ^{60}Co source. The physical and chemical properties observed in these new copolymeric films show that they are very promising materials for multiple bioapplications. In this way we started the hemocompatibility evaluation *in vitro* of the films according to standards ISO 10993-4 and 10993-5. Two types of blood interactions are being studied: hemolysis and thrombogenicity. This work is being conducted in collaboration with the *Laboratório Nacional de Investigação Veterinária* (LNIV).
According to ASTM F 756-00 standard, materials can be classified according to their hemolytic index. When this parameter is between 0 and 2%, the material is classified as "nonhemolytic". If hemolysis reaches values between 2 and 5%, the material is classified as "slightly hemolytic". However, when materials induce hemolysis values upper than 10%, they are classified as "hemolytic". Although it is not possible to define an absolute scale for this effect, by definition a blood compatible material must be "nonhemolytic". The results obtained for the new PE-g-HEMA films reach a maximum of 2% of hemolytic effect, which classify them as "nonhemolytic" and therefore suitable for direct contact with blood. A detailed assessment of thrombogenicity is still being done.
Future work involves the conclusion of thrombogenicity study and the evaluation of the general citotoxicity of the films. The final aim of the research under way is the registration of a National Patent for this new polymeric material.



PE-g-HEMA grafted films *a)* 7,5 kGy, 237%; *b)* 9 kGy, 403%; *c)* 10,5kGy, 166%; *d)* 12 kGy, 163%



PE-g-HEMA cross-section view

Polymer Characterization Laboratory

The *Polymer Characterization Laboratory* (LCP) is a multifunctional unit located at the Physics Department. Initially created in straight collaboration with IAEA, as a tool of the Portuguese Cobalt-60 Facility (UTR) for quality control of the industrial irradiation services of polymer made devices (electric insulators, medical devices, etc), gradually began to increase its R&D activity as a result of the increasingly collaboration with the Dep. of Chemical Engineering, Faculty of Sciences and Technology of Coimbra University. The installation of new experimental resources for materials testing is in course. This new laboratory, *Laboratory of Materials Mechanical Tests,* is being equipped with a *Universal Mechanical Assays Machine* and a *Thermal Press*.

Neutron Spectrometers at the Portuguese Research Reactor

F.M.A. Margaça, A.N. Falcão, J.S. Neves, C.M.M. Cruz, D.M.P.S. Silva, F.G. Carvalho

The situation of the diffractometers ETV and DIDE remained unchanged during 2007. As concerns the small angle neutron scattering instrument, EPA, test work on the measurement of signal-to-noise ratios was halted due to the malfunctioning of the water pump in the circulation system of the neutron diffuser in the beam tube D2. The pump was dismantled and proved to be irreparable. It was replaced by a new one that had to be acquired. Meanwhile the RPI core has been converted from HEU to LEU. It is predicted that this change will have a significant impact in both the total thermal neutron flux and on the signal to noise ratio. Work to determine how far these are affected is underway.

Radiation Technologies: Processes and Products

M. Luísa Botelho

Radiation Technologies: Processes and Products is an interdisciplinary group that uses the holistic approach as the key to conceptualize a research or a service. This interdisciplinarity, using Biology, Chemistry and Physics science, allows the study of a subject from various angles and methods unified by a common goal: the validation of methodologies to understand the subject of study.

The group *modus operandi* permits a constant connection with Industries, Universities and other Research groups applying its "way of knowing" in response to requested services, as a collaborator in a research project or in the transmission of knowledge. The group activities focus on the delineation, development, validation and application of technologies and processes in various fields, such as Environment, Food and Pharmaceutics. As a fundamental part of the validation studies, Risk Analysis is being applied as a process management tool either in production lines of studied products (*e.g.* food, devices and pharma-ceuticals) or in environmental control (*e.g.* hospitals rooms and pharmaceutical industries).

In the scope of ITN mission the group is solicited by the authorities or private industries to undertake a consultant role on sterilization and decontamination procedures mainly applying ionising radiation. The group also develops work with the National and International normalization, standardization and certification bodies (IPQ, CEN and ISO).

Being aware of society's current needs and the demand of Quality, Innovation and Development, the upgrading and renewal of facilities are being carried out in the scope of project REEQ/996/BIO/2005. In the course of this project, modelling tools (Monte Carlo simulations) have been applied to the pre-upgrading phase of ionizing radiation equipments (*e.g.* gamma experimental facility). Other domain of this project has been the design of a renewed layout of an existing building transforming it in an interdisciplinary laboratory with controlled environment in order to assist new applications for radiation technology, among others. These facilities together with the inclusion of automation/robotic systems, in a further stage, have as main purpose to allow researchers of National and International Institutions and Industries to develop radiation technologies and/or to suppress the need of environmental control areas (clean areas) for their work.

The Group's main R&D activities are focused at employing ionising radiation technologies to new processes and applications in Agriculture, Food, Pharmaceutical, Wastewater Treatment and other areas. In order to improve our understanding of the Radiation effects in products integrated methodologies composed by Analytical Methods of Biology, Microbiology, Chemistry and Physics are being used. Molecular Biology new trends based on PCR technique are being developed as a diagnostic tool (*e. g.* potential pathogenic micro-organisms) and as well as fingerprinting methods to assess the bio-diversity profile of environmental samples.

Training and "know-how" diffusion are one of the main issues of this Group reflecting in the attainment of academic degrees (Graduation, M.Sc. and Ph.D.) and in the dissemination of obtained results in the scientific community (publications, workshops and conferences).

The financial support of the group is based on projects, sponsored by National (e.g. FCT, AdI) and International (e.g IAEA) science foundations and expertise services to Industrial Companies.

Researchers
M.L. BOTELHO, Aux., Group Leader
S. CABO VERDE, Post-Doc

Students
A. BELCHIOR, MSc student, ITN grant
A. MENDES, undergraduate student.
L. ALVES, BIC grantee, ITN grant
R. CLEMENTE, undergraduate student, AESBUC grant
R. MELO, Ph.D. student, ITN grant
T. SILVA, BIC grantee, LM grant
N. MESQUITA, graduate student from Coimbra University

Technical Personnel
H. MARCOS, system operator, ITN

Collaborators
A. SANTANA and P. PINTO, ESAS Professors
C. CANTO E CASTRO, ITN Network Manager
J. BRANCO, Chemistry Dep., ITN Researcher
J.P.LEAL, Chemistry Dep., ITN Researcher
P. MATOS, Technical Director of CHIP,S.A
J. MANTEIGAS; Physics Dep., ITN Researcher
J. TRIGO, INIAP Researcher
P. FONSECA, Aveiro University Researcher
P. MAZARELO and S. XISTO, LM Researchers
P. VAZ, DPRSN Dep., ITN Researcher
R. TENREIRO, DBV-FCUL Prof. Aux./ICAT
A. PORTUGAL, Coimbra University Professor

Applied Research a link to Industry

S. Cabo Verde, L. Alves, A. Belchior, T. Silva, R. Melo, H. Marcos, M. L. Botelho

Objectives

Applied research is related with the practical application of knowledge, material, and/or techniques directed toward a solution to a specific requirement. In this scope, the Radiation technologies: processes and products Group has been requested to apply its experience to respond to Industry either as in contracted service or in a partnership. 1) One of the performed study objective was to validate the radiation sterilization process for a product denominated "Globone®" (requested service by Ceramed). This product is a medical device intended to be used as bone implant shielding. 2) As member of a partnership with the TradeLabor several studies were developed aiming the evaluation of air quality of National Hospitals and Offices.

Results

1) In order to accomplish the sterilization level aimed for the product Globone®, some previous studies were needed in order to develop techniques that validate the irradiation process. This validation procedure was divided in two parts: I – Establishment of the Sterilization Dose for the product (D_{min}) and II - Evaluation by FTIR of product material compatibility to γ radiation (D_{max}). The establishment of the Sterilization Dose (D_{min}), *i.e.* gamma radiation dose necessary to achieve a Sterility Assurance Level (SAL) of 10^{-6}, was based on Method VD_{max}^{25} - substantiation of 25 kGy described in the International Standard EN ISO 11137-2:2006. To ascertain the maximum radiation dose (D_{max}) to be applied to the product without changing significantly its chemical composition (*e g.* hydroxyapatite and tricalcium phosphate properties) was used the technique Fourier Transform Infrared Spectroscopy (FTIR). The product sampling plan was representative of that subjected to routine processing and conditions. The whole irradiation process was completed in the Co-60 facility (UTR) under exploitation of CHIP and located in ITN. The irradiation was performed in a calibrated place (dose rate = 2.9 kGy/h) that is comparable to the whole irradiation process in the irradiation chamber. The irradiation geometry was planned in a way that minimized the Dose Uniformity (D_{max}/D_{min}). Routine dosimetry (Perspex, Harwell) were used to monitorize the product's absorbed dose. The validation of the bioburden determination method was performed by artificial contamination of product samples with known concentrations of a *Bacillus pumilus* E601 culture and allowed the calculation of a correction factor of 1.4. The validated bioburden determination method was applied to 10 product samples from 3 different production batches. The obtained results pointed out to a higher dispersion in product bioburden values intra than inter batches that could be explained by the found contamination peaks. The analysis of results obtained from the division of bioburden values into contamination classes suggested that bioburden frequency values for the product Globone® do not follow a normal distribution. The natural microbiota of the product was morphologically and biochemically characterized. The most frequent morphological types of microorganisms (genus *Staphylococcus* and *Bacillus*) found in the Globone® product point out to personnel and environmental contamination. These results highlights the importance of the identification of production line critical control points and of the implementation of preventive actions based on a chart control, in order to lower and homogenizes the product's bioburden. The verification dose experiment was based on the estimated product bioburden and the Sterilization Dose of 25 kGy was found to be adequate to guarantee a probability of non sterile Globone® product and its inner package less than one per million ($SAL=10^{-6}$). The FTIR analysis of irradiated product samples (n = 3) at four distinct doses (25, 35, 50 and 100 kGy) indicated that there was no significant difference between the profiles of Globone® samples. This study performed to Ceramed was audit by an international entity. A similar work is being developed to other bone product (Bonelike®) from Medmat Innovation Industry. In a near future it is intended by the group to certify the validation procedure of sterilization process of health care products. This will be possible due to a new multidisciplinary laboratory of controlled air environment that is being projected under the REEQ/996/BIO/2005, and will be accredited by ISO 17025.

2) In the evaluation of air quality, namely airborne contamination, the experimental methodology relied on air sampling methods. The quantification of the number of colony forming units (cfu) was performed by a biocolector (MAS®100) and by sedimentation plates. These two air sampling methods were used with the goal of estimating the number of viable particles that remains suspended in the air (MAS®100) and to detect microorganisms of large dimensions (> 5 μm), which tend to settle by gravity (sedimentation plates). The sampling plan consisted in several air collections, in different places of each analysed room, in order to assure the representativity of the studied parameters. The results analyses are based on the correlation between the counts of viable microorganisms and particulate matter (physical parameters measured by TradeLabor) in indoor air. Due to the lack of legislation and limits for microbiological air contamination in health care facilities, for each client (e.g. Hospitals, clinics) are suggested recommendations in order to improve de indoor air quality. In terms of R&D a database is being developed that reflects typical microbial levels in a variety of indoor air environments. This microbial data will be correlated with measurement of physical parameters, HVAC system information and cleaning and disinfection procedures. The development of such a database would allow legislative bodies to begin to make prudent regulations regarding microbiological quality of indoor air.

Published work

Internal Reports to Ceramed – Part I and II, Sep. 2007.

Internal Reports to: IBMC, Hospital da Luz, June 2007; Hospital dos Covões June 2007, Clínica dos Poetas July 2007, Escritórios Mercer, Hospital Fernando Fonseca.

.

R&D in Physical and Chemical Field

A. Belchior, R. Melo, P.Vaz[1], J. Bran[1], L. Peralta[2], S. Cabo Verde, L. Alves, , T. Silva, V. Folgado, M. L. Botelho

Concerning the use of ionising radiation, dosimetry represents an important tool in the physical field. In order to evaluate the absorbed dose values, as well as the evaluation of the dose distribution (uniformity) in a product being irradiated, several dosimetric studies have been carried out. Ideally, the product should be uniformly irradiated, however, in practice this uniformity is difficult to achieve. Regarding this, Monte Carlo codes PENELOPE and MCNPX have been used for simulating the dose rate distribution in a ^{60}Co gamma irradiator, in order to carry out the spatial dose distribution in a certain irradiation position. Simulated results were validated comparing them to dose measurements performed with a Fricke solution and thermoluminescence dosimeters which are standard dosimeters widely used in radiation processing for calibration purposes. The agreement between the simulated values and the measurements indicates the effectiveness of both codes in performing dose measurements. In the chemical field, the effect of ionising radiation on the structure of different compounds was evaluated. The influence of the chloroanisoles on the wine cork taint is well known and it is difficult to reduce its effect. Physical-chemical pre-treatments, before and after gamma irradiation, were applied on cork samples to understand its impact on chloroanisoles concentration. Sensorial and analytical studies were undertaken. Preliminary results point out that physical-chemical pre-treatment with different solvents leads to the decrease of chloroanisoles concentration on the cork samples. Analytical techniques have to be optimized to increase the precision of the detection methods.

[1] DPRSN and Department of Chemistry ITN; [2] Physics Department, FC-UL

Microbiological application of ionising radiation

S. Cabo Verde, L. Alves, A. Belchior, T. Silva, A. Mendes, N. Mesquita[1], A. Portugal[1], M. L. Botelho

The ability of ionising radiation to inactivate microorganism is being researched and applied in the sterilisation/disinfection of several products. The establishment of a sterilisation/disinfection dose is based on a validated procedure that relies on the follow up of the line production up to the end of the process. In this context the sterilisation dose of medical devices was estimated for a bone implant shielding and is being carried out for a synthetic bone graft. This integrated approach is also being applied in a research project with the University of Coimbra aiming a disinfection process of a book archive using the gamma radiation. The population of fungi isolated from the books seemed to follow exponential inactivation kinetics in a surrogate substrate. In the food technology field it was studied the applicability of gamma radiation as an alternative treatment for raw milk under the scope of a graduation thesis. The results suggested that a range of doses between 1.5 and 10 kGy could be applied in the hygienisation of raw milk without significantly affect its protein profile. The environmental sustainability is other research subject of continuous interest, namely the use of ionising radiation as an optimisation tool of wastewater treatment. The influence of dose rate in the inactivation of microbial populations was studied in domestic wastewater samples during an IAEA training of a Morocco PhD student. The data obtained pointed out to an absence of a dose rate effect probably due to the high levels of radiosensitive microbiota such as the coliforms. At the genetic level, the microbial biodiversity at several radiation doses is being assessed by molecular methods under the scope of an IAEA training at Copenhagen University/Denmark. The gamma inactivation response of enteric viruses in wastewater samples are being also investigated in the development of a post-doc project. These studies are under progress.

1 University of Coimbra.

Risk Analysis Studies

T. Silva, S. Cabo Verde, P. Mazarelo[1], S. Xisto[1], M. L. Botelho

The study developed under the project LPM/MDN PIDDAC "Study of microbiological environment in operating rooms of HMP for the prevention of cross infection" aims the typification of strains isolated from surgical room environment in order to construct a data base. The methodology used focused the microbiological evaluation of the environment of a surgical room of HMP quantitatively (colony forming units) and qualitatively (phenotypic and genotypic characterization of isolates). The sampling plan involved collections of air with a biocolector MAS100 and sedimentation plates (before, during and after surgeries), metal surfaces and dermic and washing solutions. The average air bioburden were 10^2 cfu/m^3 for MAS100 and 10 cfu/plate for sedimentation plates with a slight increase of air bioburden values after surgery. The microbiological contamination of metal surfaces and dermic and washing solutions point out to be negligible (<1 cfu), except for a hand washing solution (10^3 cfu/ml). From all types of analyzed samples 76 isolates were phenotypically characterized and the most frequent (> 40 %) isolated morphological type was the gram positive cocci. The majority of isolates (> 44 %) were found to be resistant to iodopovidone and alcohol solutions used in the disinfection of patients. A simple and rapid chloroform DNA extraction protocol was evaluated and found out to be efficient in 51% of the isolates. For the other isolates lysozime DNA extraction method is being applied. Molecular biology methods, namely PCR typing techniques will be applied to all isolates in order to assess their genetic similarity.

1 Military Laboratory of Pharmaceutical and Chemical Products.

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 physics parameters, measurement of neutron cross--sections;
2. Modelling of gas discharges;
3. Development of software for control;
4. Design of electronic instrumentation for nuclear applications;
5. Instrumentation and technical assistance.

Modelling of radiation fields, calculation of neutron physic parameters

Monte Carlo calculations have been carried out in the framework of the EUROTRANS Project (IP EUROTRANS, 516520), the CANDIDE Project (Coordination Action on Nuclear Data for Industrial Development in Europe, 036397), and the n_TOF Collaboration (ITN participation in the n_TOF-phase 2 experiment at CERN).

Measurement of neutron cross-sections

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

Modelling of gas discharges

1. The PLASMAKIN chemical kinetics software package was updated: The libpk library was extended to provide access from C programs and a Python extension module was developed to provide access to libpk from Python programs.
2. The study of the electron kinetics in Ar-X [< 2%] (where X is H_2, N_2, O_2 or H_2O) mixtures with application on GDS (Glow Discharge Optical Emission Spectroscopy) has continued with the characterization of Ar and Ar-H_2 mixtures.

Design of electronic instrumentation

- One "Radioscan" Gamma Isotope TLC Analyser for measuring and recording radioactivity levels, on labels or strips, to be used in TLC and HPLC at ITN/DPRSN;
- Three "6 Channel Micro-Current Source", multiple precision current source, used in electrochemical, electromagnetic and electronic experiments, at ITN/ /Química.

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. Plasma Physics Center/Gas Electronics Group, IST;
3. Research Institute for Solid State Physics and Optics, Budapest, Hungary.

Researchers
J. MANTEIGAS, Aux., Group Leader
C. CRUZ, Aux.
I.F. GONÇALVES, Aux.
J. NEVES, Aux.
N. PINHÃO, Aux. (40%)

Students
C.M. CARRAPIÇO, Ph.D. Student, IST
C. SANTOS, M.Sc. Student, FC-UL

Technical Personnel
T. JESUS, Electronics Technician
N. INÁCIO, Electronics Technician
M. CABAÇA, Mechanical Technician

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

J.B. Manteigas, J. Neves, C. Cruz

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) Collaboration in the installation of the "Ion Beam Laboratory – TANDEM 3 MV" at the Physics Sector.

(ii) Collaboration on the acquisition, construction and installation of the LCEA (Characterisation and Speciation of aerosols Laboratory Project (REEQ/ /377/FIS/2005).

(iii) Collaboration on the upgrading of the Radiation Technology Unit (UTR) (Project REEQ/996/BIO/ /2005).

(iv) Technical support (development of electronic circuits) to be used in "Perturbed Angular Correlations experiments" at the RPI (Project POCTI/FIS/ /58498/2004).

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

Summary of the more relevant Services/Equipments rendered in 2007

Activity	Qty	Client
Laboratory equipment for the determination of radioactive element traces by electrodeposition	1	UNIWERSYTET GDANSKI (Poland)
	1	HASSAN GHEETH (Germany)
	1	THAILAND INSTITUTE OF NUCLEAR TECHNOLOGY (Thailand)
	1	AIEA (Sri Lanka)
- *Electrodeposition cells*	1	CENTRE NATIONAL DES SCIENCES ET TECNOLOGIES NUCLEARES (Tunisia)
Personal Radiation Dosemeter Equipment	1	SOPORCEL
- *Technical assistance*	4	DIRECÇÃO GERAL DE NAVIOS BASE N. DE LISB. ALFEITE
	4	DIRECÇÃO GERAL DE NAVIOS BASE N. DE LISB. ALFEITE
	1	DIRECÇÃO GERAL DE NAVIOS BASE N. DE LISB. ALFEITE
	4	DIRECÇÃO GERAL DE NAVIOS BASE N. DE LISB. ALFEITE
	1	ITN/RPI
	1	ITN/RPI
	1	ORTOGNATICA
Technical assistance to - *Source Containers*	1	INSTITUTO SUPERIOR DE AGRONOMIA
	1	INSTITUTO SUPERIOR DE AGRONOMIA
	6	SN SEIXAL - SIDERURGIA NACIONAL SA
	1	SN SEIXAL - SIDERURGIA NACIONAL SA
Measuring and control of sources activities	5	EMA 21 - GRUPO PORTUCEL/SOPORCEL – FIGUEIRA DA FOZ
	20	EMA 21 - GRUPO PORTUCEL/SOPORCEL – FIGUEIRA DA FOZ
	19	EMA 21 - GRUPO PORTUCEL/SOPORCEL – CACIA
	6	EMA 21 - GRUPO PORTUCEL/SOPORCEL – FIGUEIRA DA FOZ
Prices including TAX (VAT)		**Total Amount: 18 593,81€**

Participation of ITN in the n_TOF phase 2 experiment
P. Vaz, I.F. Gonçalves, C. Cruz, J. Neves, C. Carrapiço, C. Santos, L. Ferreira, L. Távora[1]

The n_TOF phase2 project is the continuation of the involvement of ITN in the activities of the n_TOF Collaboration. The intention of the n_TOF Collaboration is to build a second n_TOF beam-line and a new experimental area (EAR-2) using a shorter flight path (20 meters), with lower backgrounds and count rates in the detectors, making possible the extension of measurements to higher energies and the availability of a higher neutron flux (a factor of 100).
A team of researchers of ITN has been involved in Monte Carlo simulation activities, data analysis and development of electronics for the BaF2 calorimeter. ITN is strongly involved in collaboration with CIEMAT-Madrid, INFN-Bari and CEA, Saclay, in the following areas: Monte Carlo simulation(I) - full and detailed simulation of the geometry of the new experimental area, computation of the particle fluxes, assessment of the backgrounds, with the usage of the state-of-the-art Monte Carlo codes MCNPX and GEANT-4; Monte Carlo simulation studies (II) - continuation of the studies to simulate the response of the BaF2 calorimeter, calibration and efficiencies on a module-by-module basis; Data analysis (I) - continuation of the analysis of the following data sets: Au-197, Np-237, Pu-240, initiated during 2005, using the BaF2 calorimeter; Electronics developments for the DAQ and the BaF2 calorimeter.

[1] Centro de Instrumentação / U. Coimbra

Development of an open source software package for plasma physics modelling
N. R. Pinhão

The PLASMAKIN chemical kinetics package has been extended to support new reaction processes and expanded with new modules. Presently the package includes a chemical kinetics library, an electron kinetics library solving the electron Boltzmann equation in the classical two-term expansion and a Python extension module. Work is underway to extend the electron kinetics library to include a density gradient method and to include in the package a database for species and reaction. The project was moved to Source forge (http://plasmakin.sourceforge.org).

Electron kinetics in gas mixtures used for Analytical Glow Discharge Optical Emission Spectroscopy
Z. Donkó, M. J. Pinheiro, N. R. Pinhão, P. Hartmann

The electron energy distribution functions in pure argon and argon-H2 mixtures have been studied. The numerical methods used include a two-term Boltzmann solver, a density-gradient expansion and a Monte-Carlo method. Two different sets of electron collision cross sections for hydrogen have been tested and the transport parameters obtained have been compared with experimental values