Physics and Accelerators Unit

Physics and Accelerators Unit

Eduardo Alves

During the year 2008 and within the framework of the Re-Equipment programme, several researchers and technicians of the Unit were pretty much involved in the upgrading and installation of new experimental equipments or facilities.

In addition, the research activities covering different topics in Advanced Materials, Environment, Health and Biomedical Sciences followed the approved time schedule and were supported exclusively by externally funded projects. Along with the scientific achievements the post graduated formation was maintained with the engagement of graduated students in the research activities, leading to M.Sc. and Ph.D. theses. The strategic collaborations with Institutions and Universities worldwide were strengthened and were fundamental to maintain the high scientific production of the Unit. The following laboratories and Groups are responsible for the R&D activity:

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

2 – High Temperature Materials Laboratory (MA^3T) equipped with a high-resolution, high-temperature diffractometer (*Hotbird*), particularly adapted to solve difficult problems in advanced materials (*e.g.* materials for the electronics industry, high temperature alloys for fusion applications) and a high resolution diffractometer to study low dimensional single crystalline structures. The research activity in the laboratory is merged with the Advanced Materials Research Group.

3 – 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.***

4 – 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.***

5 – Condensed Matter Group is focused in the processing of hybrid materials and the modification of new polymeric materials by gamma-irradiation using the ^{60}Co (UTR) source as well as in their characterization using a wide range of techniques. The R&D work on these materials progress in collaboration with groups in Aveiro, Saclay and Budapest. The activities will be presented under ***Condensed Matter Physics.***

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Researchers

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Administration and Informatics

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Advanced Materials Research

Eduardo Alves

The Advanced Materials Research Group (GIMA) runs most of the experimental facilities at the Ion Beam Laboratory (IBL) being responsible for the operation of the accelerators - a 2.5 MV Van de Graaff accelerator equipped with a nuclear microprobe and external beam facility and a 3 MV tandem accelerator with a 30 µm lateral resolution Accelerator Mass Spectrometry (AMS) system - and the Danfysik S1090 ion implanter.

The recent research work of the group has been focused on the study of advanced materials with high technological impact, e.g. wide band gap semi-conductors and nanostructures. Wide bandgap semiconducting (III-nitrides) and oxide (ZnO) materials are the base of an emerging class of optoelectronic devices operating in the visible wavelength range of the electromagnetic spectrum being under intense research worldwide. The potential of these materials for spintronics applications is also being investigated. Our work aims at the optimization of the implantation conditions of magnetic and optically active dopants in these materials.

Other exciting study is being carried out in quantum dot (QD) multilayered structures. An intense research of the structural properties and Rare Earth doping of GaN/AlN QD layers continued in collaboration with Universities of Aveiro and Grenoble.

The work in insulators comprise the modification of the optical and structural properties of α-Al_2O_3 as well as the study of nanoprecipitates formed in rutile by high fluence implantation doping with transition metals.

Taking advantage of the potential of ion beam techniques to study thin films and multilayers, important work continued on the characterisation of magnetic thin films for magnetic spin valves, tunnel junctions, and functional oxynitride coatings, in collaboration with INESC and University of Minho.

The activities under the technology programme of the European Fusion Development Agreement (EFDA), in association with the Centro de Fusão Nuclear of the Instituto Superior Técnico was focused on the study of beryllium intermetallics, the characterisation of the new Eurofer (ODS) steel and the study of surface erosion and ^2H retention in W and Mo irradiated under ITER working conditions.

In addition to the research activities the group reinforced is commitment with the training of graduate students, through the supervision of new M.Sc. and Ph.D. thesis. Also worth to be mentioned were the two new researchers joining the group under the Ciência 2007 programme.

All the referred activities are funded by projects, both European and National (FCT), either in collaboration with other Institutions or lead by members of the group. Of particular importance are the new projects funded by the EC, *"FEMaS-Fusion Energy Material Science"*, EURATON 7th Framework Programme for Nuclear Research and Training, Grant agreement No 224752-CA, (2008-2011) and *"Support of Public and Industrial Research Using Ion Beam Technology (SPIRIT)"*, Grant agreement No 227012-CP-CSA-Intra planned to start next 2009/03/01.

These 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 and its international recognition in the field of processing and characterization of advanced materials with ion beams.

The scientific output of the group in 2008 was:

Publications (peer reviewed journals): 49
Conference and workshop contributions: 3 invited, 24 oral and 14 posters.
Running projects: 21

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Damage build-up and annealing of Eu-implanted GaN

K. Lorenz, N. Franco, S. Magalhães, N. Barradas, E. Alves, I. M. Roqan[1], R. W. Martin[1], K. P. O'Donnell[1], F. Gloux[2], P. Ruterana[2], M. Bockowski[3], D. J. As[4], M. Panfilova[4]

Objectives

Rare earth doped GaN is widely studied with respect to applications in electroluminescent devices. Eu-doped GaN with its characteristic red emission arising from the intra-4f shell transitions of trivalent Eu^{3+} is of special interest because the efficiency of conventional GaN-based LEDs and lasers is high in the blue spectral region but is strongly quenched in the green and red.

Ion implantation is a powerful tool to introduce controllable impurity concentrations at precise depths below the surface with the added capability to dope selective areas. However, it creates lattice damage which may affect the optical properties due to the introduction of non-radiative decay paths. High temperature annealing is usually necessary to remove the implantation damage and thereby activate rare earth ions optically.

Results

The implantation damage build-up in wurtzite phase GaN (W-GaN) was studied in detail using a combination of Rutherford Backscattering Spectrometry/channelling (RBS/C) and transmission electron microscopy (TEM). Four regimes could be identified (Fig. 1): In the low fluence regime strong dynamic annealing keeps the damage accumulation rate low. The retained damage consists mainly of point defect clusters and low concentrations of basal and prismatic stacking faults. For medium fluences (regime II), implantation damage increases steeply; an increasing number of stacking faults is observed. In regime III the damage in the bulk of the samples, in particular the production of stacking faults, saturates while the damage at the surface increases further. Above a threshold fluence of 2-3×10^{15} Eu/cm^2 a highly damaged surface layer is formed consisting of randomly oriented nanocrystallites and voids.

Previously it was shown that a thin AlN layer grown on top of GaN successfully protects the GaN surface from dissociation during high temperature annealing

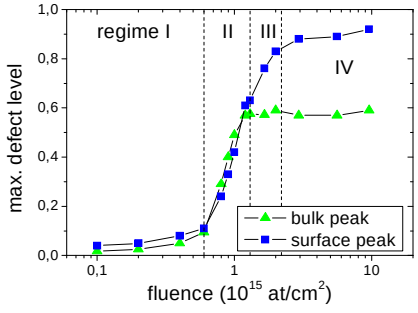

Fig. 1: Damage build-up curve for 300 keV Eu-implantation into W-GaN: The relative defect level at the maximum of the surface and bulk damage peak in RBS/C spectra as a function of the fluence.

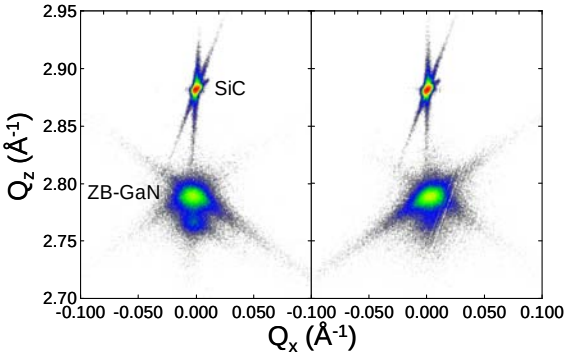

Fig. 2: X-ray diffraction reciprocal space maps around the (002) lattice point of ZB-GaN after implantation of 1×10^{14} at/cm^2 (left) and 1×10^{15} at/cm^2 (right) Eu ions at 300 keV.

and a strong increase of Eu-related luminescence with annealing temperature up to 1300 ºC was observed for samples implanted with a fluence of 1×10^{15} Eu/cm^2. Interestingly, for lower fluences the highest luminescence intensity is found at lower annealing temperature due to the sensitive balance of implantation defect removal and defect formation during annealing despite the AlN-capping. This defect formation could be suppressed by performing the annealing at extreme nitrogen overpressure of 1 GPa which led to an exponential increase of luminescence intensity up to temperatures as high as 1450ºC for a sample implanted with 1×10^{13} Eu/cm^2. This sample only showed one major Eu luminescence centre while a second, possibly defect related centre, is usually observed for higher implantation fluences.

Furthermore, Eu-implantation of cubic (zincblende) GaN (ZB-GaN) was investigated.

The implantation damage causes an expansion of the lattice parameter (Fig. 2), similar to what is observed in W-GaN. Unlike the case of W-GaN no preferential surface damage was observed. However, ZB-GaN is partially converted to W-GaN during high temperature annealing. Eu was found on a high symmetry interstitial site in contrast to W-GaN where Eu occupies near-substitutional Ga-sites. Optical activation was achieved after annealing and different Eu emission lines could be assigned to Eu-centres residing within W-GaN inclusions and Eu-centres in cubic ZB-GaN.

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Rare Earth implantation of AlN for light emission from IR to UV

K. Lorenz, E. Alves, T. Monteiro[1], M. Peres[1], F. Gloux[2], P. Ruterana[2]

Rare Earth (RE) doped group-III nitride semiconductors (GaN, AlN, InN and their alloys) attract much research interest due to their unique optical properties with narrow and temperature stable emissions ranging from infrared to ultraviolet. As host for REs, AlN with its large band gap allows energetically high lying RE levels to be exploited and to decrease thermal quenching of the luminescence.
In this work Eu ions were implanted into AlN with a wide fluence range from 10^{14} to 10^{17} at/cm^2. The damage build-up was investigated by Rutherford Backscattering/channelling (RBS/C) revealing sigmoidal shaped damage build-up curves that indicate efficient dynamic annealing. Strong ion channelling effects were observed when the implantation was performed along the <0001> direction of the wurtzite lattice. Compared to random implantation the range of the implanted ions doubles and the defect density is reduced efficiently. For the highest fluence and random implantation a buried amorphous layer is formed which was confirmed by transmission electron microscopy analysis. After annealing all samples show bright Eu-related photoluminescence (PL) in the red spectral region. The PL intensity is strongly dependent on the lattice damage, being higher in samples implanted with low fluences and in channelled geometry.

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Defect studies and optical activation of Yb doped GaN

K. Lorenz, E. Alves, S. Magalhães, M. Peres[1], T. Monteiro[1], A. Kozanecki[2], M. E. G. Valerio[3]

Wide band-gap semiconductors, particularly III-nitrides, became one of the most studied materials during the last decades. These compounds are the base of a new generation of optoelectronic devices operating in the UV-Blue region of the electromagnetic spectrum. Incorporation of rare-earth (RE) ions into nitrides creates new routes to build all-nitride electroluminescent devices, using the sharp intra-4f^n transitions of these elements. The introduction of the RE ions in the nitride lattice during the growth or by ion implantation creates defects which influence the optical behaviour of the doped region.
In this work we report the results on Yb implanted GaN. A combination of techniques (Rutherford backscattering/Channeling and Photoluminescence) was used to assess the mechanisms responsible for the optical and structural behaviour of the doped materials. Lattice site location experiments showed that Yb is incorporated into positions slightly displaced from the Ga-site. Clearly the optical activity of the RE could be enhanced by orders of magnitude reducing the number of non-radiative recombination paths related with defects.

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Free electron behavior in InN

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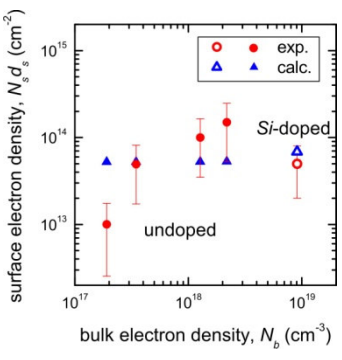
We have used precise measurements of the Optical Hall effect in InN using magneto-optical generalized ellipsometry at IR and THz wavelengths, which allows decoupling of the surface accumulation and bulk electron densities in InN films by non-contact optical means and further to precisely measure the effective mass and mobilities for polarizations parallel and perpendicular to the optical axis. We have performed studies of InN films with different thicknesses, free-electron densities, surface orientations and polarities, which enable an intricate picture of InN free carrier properties to emerge. Electron accumulation is found to occur at polar, semi-polar and non-polar surfaces of wurtzite and zinc-blende InN and the surface charge shows distinct dependence on the bulk free-electron density (see figure). Striking findings on the scaling factors of the bulk and surface electron densities with film thickness points to an additional doping mechanism or different evolution of dislocation density from currently accepted picture and suggest that the complexity of the surface chemistry might have been underestimated in the existing models.



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Structural and compositional analysis of near-lattice matched $Al_{1-x}In_xN$/GaN (0.08<x<0.21) epitaxial layers

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

The ternary alloy AlInN is attracting much research interest due to the possibility of growing it lattice matched to GaN for an InN molar fraction of ~17-18%. However, the growth of AlInN is rendered difficult by problems of phase separation during epitaxial growth, driven by a large disparity in cation sizes as well as by differences in thermal properties of the binary constituents, leading to a wide immiscibility region. A large number of AlInN/GaN bilayers with alloy layer thicknesses from 20 nm to 200 nm were grown using metal organic vapour phase epitaxy. The InN content, ranging from 8 to 21%, was controlled by means of the growth temperature. The structural properties were studied using Rutherford Backscattering/channelling spectrometry (RBS/C), X-ray diffraction (XRD) and atomic force microscopy (AFM). For nearly all samples the InN content measured *directly* by RBS is lower than that determined from XRD measurements assuming Vegard's rule, indicating a deviation of the AlInN/GaN system from this empirical law. The surface for closely lattice matched samples was smooth with RMS roughness values as low as 0.3 nm. Lower InN contents cause an increase of V-shaped pits on the surface relaxing tensile strain while higher InN contents lead to the formation of three dimensional islands. Detailed analysis of XRD rocking curves showed that the quality of the GaN buffer layer is a critical parameter for the AlInN film quality in agreement with TEM results revealing that most threading dislocations are formed inside the GaN layer and continue in the AlInN film.

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Unintentional impurities and dislocations in InN films and their role for the unintentional n-type conductivity in InN

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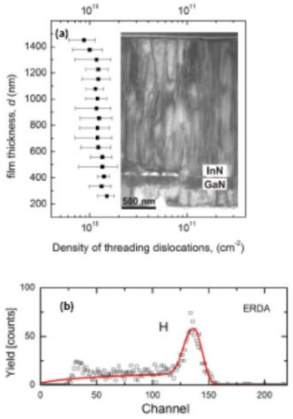
We have studied the unintentional impurities profiles and the evolution in the dislocation density in InN films with different free electron concentrations and using different nucleation schemes. The goal is to unravel the cause for the unintentional doping mechanisms in InN, which is a key issue to enable further progress in the InN based technology. We found that the dislocation densities are similar in InN films with free electron concentrations that differ by more than an order of magnitude, indicating that dislocations associated with native defects could not play a decisive role for the unintentional conductivity in InN (top figure). We also found significant amount of H in the films being much larger at the surface than in the bulk (bottom figure). Surprisingly, the amount of H is estimated to be larger in the films with lower free electron concentrations, both in the bulk and at the surface. On the other hand, no O (>0.1 at%) could be detected in the InN films but some traces of C are detected in the films, specifically for those with low free electron concentrations. Our results further suggest that minimizing the amount of O in combination with H passivation might be a successful route for enabling p-type doping of InN.



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Lattice parameters and E_2 phonons in $In_xAl_{1-x}N$

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The lattice parameters of InxAl1-xN in the whole compositional range using first-principle calculations were studied. Deviations from Vegard's rule are obtained via the bowing parameters, $\delta a = 0.0412 \pm 0.0039$ Å and $\delta c = -0.060 \pm 0.010$ Å, which largely differ from previously reported values. Implications of the observed deviations from Vegard's rule on the In content extracted from x-ray diffraction are also inferred. We also combine these results with x-ray diffraction and Raman scattering studies on InxAl1-xN nanocolumns with $0.627 \leq x \leq 1$ and determine the E2 phonon frequencies versus In composition in the scarcely studied In-rich compositional range.

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Structural and optical properties on thulium-doped LHPG-grown Ta_2O_5 fibres

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Structural, spectroscopic and dielectric properties of thulium-doped laser-heated pedestal Ta_2O_5 as-grown fibres were studied. Undoped samples grow preferentially with a single crystalline monoclinic structure. The fibre with the lowest thulium content (0.1 at%) also shows predominantly a monoclinic phase and no intra-$4f^{12}$ Tm^{3+} recombination was observed. For sample with the highest thulium amount (1.0 at%), the appearance of a dominant triclinic phase as well as intraionic optical activation was observed. The dependence of photoluminescence on excitation energy allows identification of different site locations of Tm^{3+} ions in the lattice. The absence of recombination between the first and the ground-state multiplets as well as the temperature dependence of the observed transitions was justified by an efficient energy transfer between the Tm^{3+} ions. Microwave dielectric properties were investigated using the small perturbation theory. At a frequency of 5 GHz, the undoped material exhibits a dielectric permittivity of 21 and for thulium-doped Ta_2O_5 samples it decreases to 18 for the highest doping concentration. Nevertheless, the dielectric losses maintain a very low value.

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Gallium oxide waveguiding nanowires doped with luminescent elements

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Monoclinic gallium oxide (β-Ga_2O_3) presents the widest band gap among the transparent semiconductor oxides oxides, around 5 eV, while still behaves as a semiconductor due to the presence of a native donor band. Besides, it has a fairly high refractive index in the visible range, about 1.85-1.91, which makes it a promising material for waveguiding purposes.
In this work we study the doping of β-Ga_2O_3 nanowires either by diffusion or ion implantation. The spatial and spectral properties of the luminescence from individual wires was studied both by cathodoluminescence (CL) in a SEM and micro-photoluminescence (micro-PL) in an optical microscope. Luminescence sharp peaks and broad bands from the dopants in the visible and infrared ranges of the spectrum are observed in single nanowires. Homogeneous luminescence yield along the nanowires is shown in the CL images. Waveguiding of the light emitted by the luminescent ions in the nanowires is shown in the micro-PL images. The shape of the characteristic broad red Cr^{3+} luminescence spectrum at room temperature depends on the dimensions of the wires when their width is of the order of the emission wavelength. Luminescence from several rare earth ions has also been obtained and several emitting centers have been identified. Waveguiding of external blue, green and red light which does not excite the luminescent centers was also observed in the nanowires.

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Tuning of oxidation states in the $LaNiO_{3-\gamma}$ perovskite around the insulator-metal transition

N. Franco, R.. M. C. da Silva, B. Berini[1], N. Keller[1], B. Pigeau[1], Y. Dumont[1], E. Popova[1]

The $LaNiO_{3-\gamma}$ perovskite has been studied during its reoxygenation process at the reversible insulator-metal transition by spectroscopic ellipsometry for different pressures and temperatures conditions. First, it was demonstrated that the reoxygenation dynamics increases with both increasing pressure and temperature. Considering the temperature dependent experiments, two regimes of kinetics have been identified: a slow reoxygenation dynamics at low temperature (below 523 K) and fast dynamics above 623 K. Second, contrary to our expectations, the reoxygenation process of a preliminary reduced sample is completed after a sufficient time delay even for the smallest investigated temperature of 473 K or oxygen pressure of 0.03 μbar, respectively. Modeling the change in extinction coefficient as a function of time during the reoxygenation, it was found that the oxygen diffusion coefficient varies from $4.2x10^{-14}$ to $1.1x10^{-13}$ cm^2/s depending on the temperature (473 K to 523 K). This oxygen diffusion constant is similar in magnitude order to those observed in the YBCO superconductor. At the light of these investigations, a pulsed oxygen injection was used, allowing a control of the injected oxygen quantity and by consequence, it was possible to precisely tune the oxidation state for a $LaNiO_{3-\gamma}$ film between the reversible reduced sample and the stoichiometric compound. ***In situ*** ellipsometry measurements are simultaneously performed to follow changes in optical constants.

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

U. Wahl, E. Alves, R.C. da Silva, J.G. Correia, A.C. Marques, K. Lorenz, L. Pereira[1], J.P. Araújo[1], M.M. Cruz[2], R.P. Borges[2], M. Godinho[2], M. Peres[3], A.M.L. Macatrão[3], T. Monteiro[3]

This project investigates the possibility to fabricate diluted magnetic semiconductors by means of ion-implantation of transition metals or rare earths into single-crystalline starting materials such as the wide band gap semiconductors GaN and ZnO, and some selected semiconducting oxides such as $SrTiO_3$, $BaTiO_3$, $KTaO_3$, and TiO_2. The role of defects created during implantation as a possible source of magnetism or as a prerequisite in modifying the magnetic properties of the implanted impurities is addressed as well.

During this year single crystals of ZnO and $SrTiO_3$ were implanted with the stable isotopes ^{55}Mn, ^{56}Fe, ^{59}Co and ^{58}Ni at various fluences ranging from 1×10^{15} cm^{-2} to 1×10^{17} cm^{-2} and implantation energies of 60 keV or 200 keV. In addition some ZnO samples were implanted with high fluences (>1×10^{17} cm^{-2}) of N or Ar. Following thermal annealing treatments at various temperatures up to 1250°C and the RBS/C results showed that the crystalline structure of 1×10^{16} cm^{-2} or lower fluence implanted ZnO and $SrTiO_3$ (figure) almost fully recovers from implantation damage through annealing in air above 1000°C. The study of the macroscopic magnetic moments of the samples as a function of measurement temperature and applied magnetic field by means of SQUID is currently under way at the Universities of Lisbon and Porto. Preliminary results indicate magnetic moments related to the presence of ferromagnetism in some of the samples, with its intensity depending on the chosen implantation conditions and annealing procedures. Superparamagnetic behavior was observed in high-fluence Ni implanted ZnO indicating the formation of magnetic nano-aggregates, whereas Co and Mn implanted ZnO seems to be mostly paramagnetic. The optical properties of some of the ZnO:Fe samples were characterized using photoluminescence at the University of Aveiro and intraionic Fe^{3+}-related emission found in all cases.

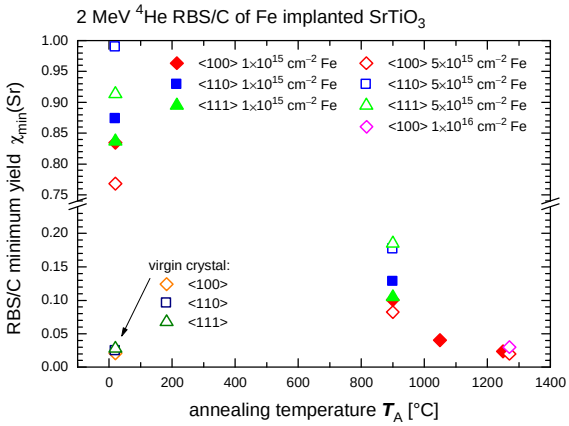

Figure: RBS/C minimum yields from Fe-implanted $SrTiO_3$ single crystals as a function of implanted fluence and annealing temperature (30 min in air).

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

M.M. Cruz[1], M. Godinho[1], U. Wahl, E. Alves, R.C. da Silva

We extended previous work to the investigation of the behaviour of the transition ions Co, Ni and Mn introduced in ZnO by ion implantation. Single crystals of ZnO were doped with magnetic ions Co, Ni or Mn, using ion implantation with fluences in the range of 1, 2, 5×10^{16} cm^{-2} to 1×10^{17} cm^{-2} and energy of 150 keV. The structural and magnetic properties of such samples were studied after implantation. 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 only for the highest implantation fluence superparamagnetic behaviour was observed, indicating formation of nm-sized magnetic aggregates. Study of the behaviour of the implanted ZnO crystals upon thermal treatments is under way in order to understand the role of the dopant and its concentration, in particular the occurrence or absence of magnetic anisotropy in correlation with the orientation of metallic aggregates in the ZnO structure.

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

R.P. Borges[1], M.M. Cruz[1], M. Godinho[1], N. Franco, R.C. da Silva

The finding of ferromagnetic order associated with lattice defects triggered research focused on the role of lattice defects as the source of magnetic moments and their relation to magnetic ordering. Within this context rutile and ZnO single crystals were implanted with Ar or N ions with energy of 100 keV and fluences up to 1×10^{17} cm^{-2} and 2×10^{17} cm^{-2} respectively. In both materials 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. In rutile, no impurities other than the implanted species were detected. Consequently the ferromagnetic behaviour is attributed to defects created during implantation. The ferromagnetic behaviour is suppressed in ZnO after consecutive annealings in air at 400 ºC and 500 ºC. Annealing the Ar-implanted rutile single crystals at 800 ºC induced partial recovery of the lattice structure and a decrease of the measured ferromagnetic moment, while it did not change significantly for rutile implanted with nitrogen. The observed evolution in temperature can be explained by the annealing out of implantation defects, confirming their importance towards the magnetic behaviour of ZnO and rutile. Study of similar systems formed by implantations with 200 keV ions is also under way in order to assess the influence of denser, deeper implantation damage.

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Structural and optical properties of nitrogen doped ZnO films

E. Alves, N. Franco, N. P. Barradas, F. Munnik[1], T. Monteiro[2], M. Peres[2], J. Wang[3], R. Martins[3], E. Fortunato[3]

Zinc oxide is getting an enormous attention due to its potential applications in a variety of fields such as optoelectronics, spintronics and sensors. The renewed interest in this wide band gap oxide semiconductor relies on its direct high energy gap (E_g~3.437 eV at low temperatures) and large exciton binding energy ZnO. However to reach the stage of device production the difficulty to produce in a reproducible way p-type doping must be overcome.

In this study we discuss the structural and optical properties of ZnO films doped with nitrogen, a potential p-type dopant. The films were deposited by magnetron sputtering using different conditions and substrates. The composition and structural properties of the films was studied combining X-ray diffraction (XRD), Atomic force microscopy, Rutherford backscattering (RBS), and heavy ion elastic recoil detection analysis (HI-ERDA). The results show an improvement of the quality of the films deposited on sapphire with increasing RF power with a preferentially growth along the c-axis. The ERDA analysis reveals the presence of H in the films and a homogeneous composition over the entire thickness. The photoluminescence of annealed samples evidences an improvement on the optical quality as identified by the well structured near band edge recombination.

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Temperature behavior of damage in Sapphire implanted with light ions

E. Alves, C. Marques, G. Sáfrán[1], Carl J. McHargue[2]

In this study we compare and discuss the defect behavior of sapphire single crystals implanted with different fluences (1×10^{16} to 1×10^{17} cm^{-2}) of carbon and nitrogen with 150 keV. The implantation temperatures were RT, 500 ˚C and 1000 ˚C to study the influence of temperature on the defect structures. For all the ions the Rutherford backscattering-channeling (RBS-C) results indicate a surface region with low residual disorder in the Al-sublattice. Near the end of range the channeled spectrum almost reaches the random indicating a high damage level for fluences of 1×10^{17} cm^{-2}. The transmission electron microscopy (TEM) photographs show a layered contrast feature for the C implanted sample where a buried amorphous region is present. For the N implanted sample the Electron Energy Loss Spectroscopy (EELS) elemental mapping give evidence for the presence of a buried damage layer decorated with bubbles. Samples implanted at high temperatures (500 ºC and 1000 ºC) show a strong contrast fluctuation indicating a defective crystalline structure of sapphire.

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Ge-Nanocrystal Formation and Oxide Matrix Evolution during Annealing of LPCVD-SiGeO Films

A.Kling, A. Rodríguez[1], B. Morana[1], T. Rodríguez[1], J. Sangrador[1], M. I. Ortiz[1], C. Ballesteros[2]

Group-IV semiconductor nanocrystals in oxide matrices are important for applications of optoelectronic devices compatible with standard CMOS technology. It has been previously shown that Low Pressure Chemical Vapor Deposition (LPCVD) at low temperatures (400ºC -500ºC) and subsequent annealing of SiO_2:Ge single and multi-layers enables the formation of Ge-nanocrystals that show blue-violet luminescence. The present study focuses on the behavior of oxygen deficient SiGeO layers that may allow the formation of Si and/or SiGe nanoparticles. Layers deposited with various gas flow ratios were annealed at temperatures between 600ºC and 1100ºC to segregate possible excess of Si and Ge in the form of nanoparticles. The composition depth-dependence of the as-deposited oxide layers and its evolution during annealing was investigated by grazing incidence RBS. Further Transmission Electron Microscopy was used in order to study the formation of nanoparticles and complement the RBS results. For low GeH_4:Si_2H_6 flow ratios and deposition temperatures of 450 ºC or lower, the deposited film consists of a SiO_2 matrix incorporating Ge. After annealing of the samples with SiO_2 matrices at temperatures of 600 ºC or higher, quasi-spherical isolated Ge nanocrystals with diameters ranging from 4.5 to 9 nm are formed. In the samples deposited with low flow ratios, the original SiO_2 matrix holds its composition.

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Memory effect on CdSe nanocrystals embedded in SiO2 matrix

E. Alves, N. P. Barradas, S. Levichev[1], A. G. Rolo[1], M. J. M. Gomes[1], P. Basa[2], Zs. J. Horváth[2], A. Chahboun[3]

Atom-like energy levels within quantum dots with enhanced interaction of zero-dimensional electron states promises novel quantum devices for future logic and memory applications. CdSe nanocrystals (NCs) have recently attracted enormous attention because of both their light-emitting and charge storage abilities. Memory effects in the electronic transport in CdSe NCs prepared by organic techniques have been observed and characterised. Recently an optical memory effect has been obtained in SiO_2 structures containing CdSe NCs prepared by ion beam synthesis. In this work, we studied CdSe NCs embedded in SiO_2 grown by RF-sputtering technique and post annealed.

A memory effect (flat-band voltage shift) has been first obtained in SiO_2/CdSe NC structures. The composition and the thickness of the CdSe/SiO_2 films were estimated by spectroscopic ellipsometry, Rutherford Backscattering (RBS), and Scanning Electron Microscopy (SEM). The electrical and memory behaviour were studied by capacitance-voltage (C-V) and memory window measurements. Three different samples have been studied: two SiO_2 layers with different CdSe content and a reference sample without CdSe NCs. The structures were grown on p-type Si and electrical contacts were deposited on both sides of the wafers by evaporation of Al. The typical C-V characteristics obtained on samples A, B and C are presented in the figure. Samples with embedded CdSe NCs exhibited memory effect, while no shift of the C-V curve for the SiO_2 reference sample (A) was obtained, a significant shift of the curves on the left during the forward scan was observed for samples B and C. This negative voltage shift due to negative bias (related to the metal electrode) can be attributed to hole injection from the substrate, or to an electron emission from CdSe NCs.

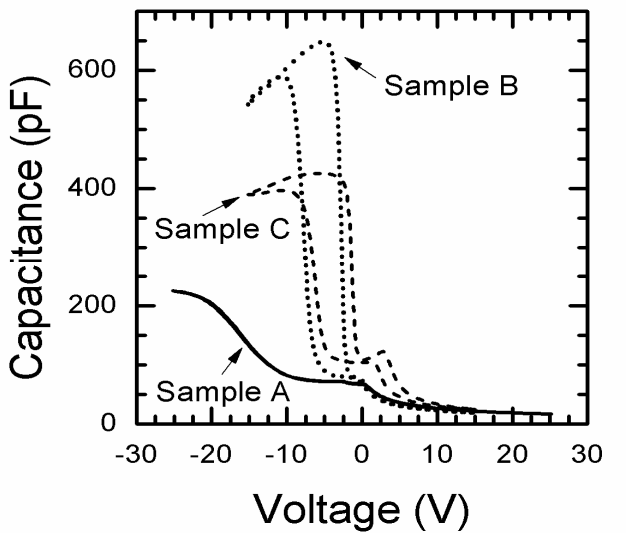

Figure: C-V behaviour of the reference SiO_2 film (A) and with CdSe NCs (B and C).

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Microstructure characterisation of ODS-RAFM steels

R. Mateus[1], P.A. Carvalho[1,2], D. Nunes[1,3], L.C. Alves, N. Franco, J.B. Correia[3], H. Fernandes[1], C. Silva[1], R. Lindau[4], E. Alves

New Reduced Activation Ferritic Martensitic (RAFM) ODS stuls are being developed for fusion reactors study of different RAFM ODS Eurofer 97 batches were preformed with a nuclear microprobe and scanning and transmission electron microscopy. X-ray elemental distribution maps obtained with proton beam scans showed a homogeneous composition of all the batches within the proton beam spatial resolution and, in particular, point to a homogeneous distribution of ODS (yttria) nanoparticles along the Eurofer 97 matrix. This assumption was partially confirmed by transmission electron microscopy, with the observation of the nanoparticles over the entire matrix in one of the samples. Scanning electron microscopy coupled with energy dispersive spectroscopy made evident the occurrence of enriched chromium carbide precipitation. Precipitates occurred preferentially along GBs in three of the batches and have a globular shape on the last one, which points to the existence of different thermo-mechanical histories. Additional electron backscattered diffraction experiments revealed crystalline textures and the ferritic structure of the ODS steel samples.

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Production and Characterisation of Titanium Beryllides with Fine-Grained Structure

N. Franco, L. C. Alves, E. Alves, P. Kurinskiy[1], A. Moeslang[1], A. A. Goraieb[2]

Within the frame of the European Helium Cooled Pebble Bed (HCPB) blanket development, a considerable effort is developed to the qualification of ceramic breeder and beryllium neutron multiplier pebble beds. As the tritium inventory of beryllium pebbles has a main impact on the attractiveness and safety of the entire HCPB blanket, a major goal of the materials development is to maximize the tritium gas release under operating conditions. Preliminary investigations revealed that beryllides like $Be_{12}Ti$ may be much more suitable as neutron multiplier in future fusion power plants compared to pure beryllium. Titanium beryllides promise faster tritium release, much smaller swelling and better compatibility with stainless steel. However, considerable work is still required to develop efficient production methods for beryllide pebbles. During the last 6 years the firm GVT (Goraieb Versuchstechnik), located in Forschungszentrum Karlsruhe (FZK), in collaboration with FZK scientists has carried out a number of manufacturing tests aimed to produce titanium beryllides with fine grains. Microstructural analyses revealed that fabricated specimens consist, mainly, of titanium beryllides and have fine-grained structure.

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Nuclear fusion materials: Deuterium retention in W*

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

Profiting from its fine thermal properties, W is expected to be used as a plasma-facing component on a Nuclear Fusion Reactor. Besides, during the deuterium(D)-tritium(T) reactor operation, it is desirable that the materials facing the plasma may present low hydrogenic retention. W has been reported as having low hydrogenic solubility but all the experiments have been done in conditions were the ion flux densities are very low when compared to the ones expected in a nuclear fusion reactor. In this work, poly-crystalline samples were exposed in the linear plasma generator Pilot PSI, to high flux densities ($\sim 10^{24}$ D/m^2.s) and the final sample D distribution profile measured with nuclear reaction analysis while the total D content compared with thermal desorption spectroscopy. It should be noticed that the nuclear reaction analysis allowed obtaining information on small sample areas (~ 1 mm^2) and then establishing correlation with attained sample surface temperature, measured by pyrometry. The most important result is that W targets, in fact, retain very little D, and that there is no clear dependence with the incident ion fluence. However there are indications that low surface sample temperature (1000K – 1600K was the measured experimental temperature range) may significantly increase the D retention and further work is then needed.

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Structural and mechanical properties of AZOY thin films deposited at room temperature

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Transparent oxide semiconductors have been investigated intensively for basic optoelectronics devices like Thin Film Transistor (TFTs). Integration of oxides with different funcionalities promise new possibilities for technological developments. Transparent conducting Al-doped ZnO films were deposited on glass and electroactive polymer substrates (poly vinylidene fluoride-PVDF), (by dc and pulsed dc magnetron sputtering). The films were deposited at room temperature varying the argon sputtering pressure, after optimizing other processing conditions. All ZnO:Al films are polycrystalline and preferentially oriented along [002] axis. Electrical resistivity around $3.3x10^{-3}$ □.cm and optical transmittance at 550 nm of ~85% have been obtained in AZOY films deposited on glass while a resistivity of $1.7x10^{-2}$ □.cm and transmittance at 550 nm of ~70% has been attained in similar coatings on PVDF. Resistivity seems to be strongly influenced by the roughness of the PVDF substrate. As shown in Fig. 6b, the film thickness has influence on both resistivity and transmittance. Increasing film thickness yields a reduction in the film resistivity. This phenomenon is associated with the crystallinity improvement as thickness increases, the concomitant increase of carrier mobility [Aga04] and with the increase of film thickness itself. As reported by other authors, the resistivity of thin films is affected by surface roughness of the substrate. Indeed the high roughness of the substrate leads to a non uniform morphology in the film [For03]. Likewise, high surface roughness increases the multiple reflections, leading to a reduction of the overall transmittance.

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Chemical and electronic structure influence on the electrical behaviour of decorative zirconium oxynitride thin films

E. Alves, N. P.Barradas, P. Carvalho[1], J. M. Chappé[1], L. Cunha[1], F. Vaz[1], C. Rousselot[2], J. P. Espinós[3], A. R. González-Elipe[3]

The goal of this study was the investigation of decorative zirconium oxynitride, ZrO_xN_y, thin films prepared by dc reactive magnetron sputtering, using a 17:3 nitrogen to oxygen ratio gas mixture. The colour of the films changed from metallic-like to very bright yellow-pale and golden yellow for low gas mixture flows (from 0 to about 9 sccm) to red-brownish for intermediate gas flows (values up to 12 sccm). With further increase of the reactive gas flow, the samples showed a significant decrease of brightness values and the colour changed from red-brownish to dark blue (samples prepared with 13 and 14 sccm).

The films deposited with gas flows above 14 sccm showed only apparent colorations due to interference effects. This change in optical behaviour from opaque to transparent (characteristic of metallic to insulating-type materials), promoted by the change in gas flows injections, revealed that significant changes were occurring in the films characteristics (namely in the type of bonds and structural arrangements) and thus opening new potential applications for the films, beyond those of purely decorative ones. Taking this into account, the electrical behaviour of the films was investigated as a function of the reactive gas flow and correlated with the observed chemical, electronic and structural features, which could reveal their potential to be used in electrically-based applications. The dependence of the composition with the flow rate was measured by RBS and indicated in the figure.

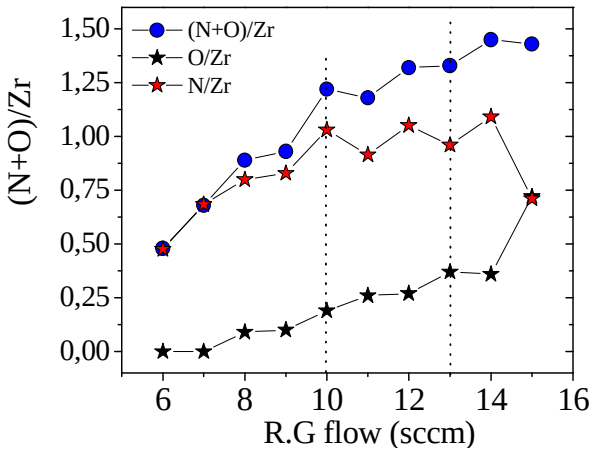

Figure: Composition dependence of the zirconium oxynitride films with the reactive gas flow.

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Structural and optical characterization of Er implanted sapphire
C. Marques, R.C. da Silva, E. Alves

Rare-earth doping of insulating and semiconductor materials is a common method for producing systems with tuned optical properties. The optimum optical performance is highly dependent on the concentration of the doping species as well as on the local environment surrounding these ions. In this work, sapphire crystals were implanted at RT with a low fluence of Er ions, to a maximum concentration of 0.1 at. %. After implantation RBS-C measurements reveal a considerable amount of radiation defects with some Er ions already in regular lattice sites of the host matrix. The optical emission measured by IBIL shows a weak IR line, characteristic of Er transitions. Annealing in air at 1573 K removed the radiation damage almost completely, the fraction of Er ions in regular sites increasing to 50 %. The characteristic emissions are now very intense, with all transitions visible. XRD analysis revealed the presence of Er_2O_3 with <111> parallel to c-axis of sapphire. On the other hand, similar annealings in vacuum produce less extensive crystalline recovery and comparatively lower intensities of the characteristic emissions. The optical absorption spectra at this stage showed what may be a surface plasmon resonance band of Al nano aggregates in the UV region. This may be explained by the lower enthalpy of formation of Er_2O_3 as compared to Al_2O_3, leading to Al dislodging and aggregation.

N-doped photocatalytic titania thin films on active polymer substrates
C.J. Tavares[1], S.M. Marques[1], S. Lanceros-Méndez[1],F. Munnik[2], T. Girardeau[3], J.-P. Rivière[3], E. Alves, N.P. Barradas

Active polymer substrates have found their way in the semiconductor industry as a base layer for flexible electronics, as well as in sensor and actuator applications. The optimum performance of these systems may be affected by dirt adsorbed on its surface, which can also originate mechanisms for the degradation of the polymer. In this collaboration we studied titanium dioxide (titania) semiconductor photocatalytic thin films deposited by unbalanced reactive magnetron sputtering on one of the most applied and investigated electroactive polymer: poly(vinilidene fluoride), PVDF. In order to increase the photocatalytic efficiency of the titania coatings, a reduction of the semiconductor band-gap has been attempted by using a nitrogen doping. Rutherford Backscattering Spectroscopy was used in order to assess the composition of the titania thin films, whereas Heavy Ion Elastic Recoil Detection Analysis provided the evaluation of the doping level of nitrogen. X-ray Photoelectron Spectroscopy provided valuable information about the cation-anion binding within the semiconductor lattice. The photocatalytic performance of the titania films have been characterized by decomposing an organic dye illuminated with combined UV/visible light.

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Characterization of Roman Glasses of historical interest with external PIXE and PIGE
P.A. Rodrigues, M. Vilarigues[1], L.C. Alves, R.C. da Silva

Archaeological campaigns in the site of the Roman *villa* of Quinta da Bolacha at Amadora, Portugal, which was discovered in 1979 during prospection of a Roman aqueduct, provided a recollection of many different types of materials and objects. The archaeological works that followed allowed identifying sealed contexts attributed to the 3rd and 4th centuries AD, together with revolved contexts of uncertain dating. In general, the unearthed objects and the available historical information consistently point to the 3rd and 4th centuries AD as the main occupation periods of the *villa*.
Seeking to materially define those moments, glass fragments recovered from the different contexts were analysed non-destructively by ion beam techniques. Because of their poor state of conservation, namely the delamination of the surfaces, the museological objects could not be analysed in vacuum, making the external beam analysis a better and only option for their study. Combination of the PIXE and PIGE techniques in the newly available external microbeam analytical end-station allowed establishing a clear correlation between the composition of the fragments and their contexts of origin. Grouping by similarity of composition further allowed associating some fragments from one of the revolved contexts to well defined ones.

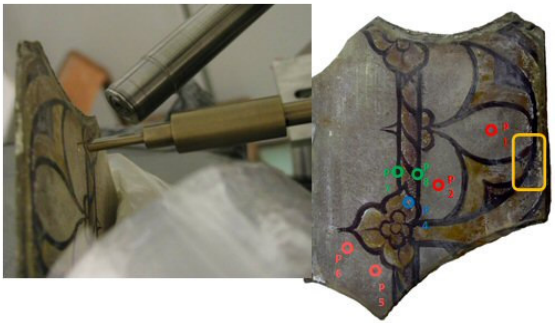

Fig.: Experimental mount and glass fragment sample analysed in the external beam. Coloured dots indicate analysed spots.

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Studies in mineralogy and cultural heritage using focused ion beams*

J. Figueiras [1], A. Mateus [1], A. Pinto [1], L.C. Alves, J. Matos [2], J. Mirão [3], T. Ferreira [3], D. Rosa[2], M. Ondina Figueiredo [2], T. Silva [2], D. Oliveira [2], M. Pereira [4], T. de Lacerda-Aroso [4], M. Vilarigues[5]

In addition to the work performed in the biomedical and material science fields, focused ion beams have been applied in the study of geological/mineralogical and cultural heritage materials, in collaborations with the Univ. of Lisboa, Univ. Nova of Lisboa, Univ. of Évora, Univ. of Minho and INETI.
In the mineralogy field the work involved the characterisation of old mine slag for the evaluation of the amount of valuable metals and also of pyrite ore characterisation in terms of Indium contents and possible type of mineral bearing it.

In the cultural heritage field work, other than the one performed with the external beam, was done in the study of 17th century ceramic wall tiles and of 17th century Arraiolos tapestries. The purpose of this last study was to analyse the tapestry fibres in order to identify the mordants used by the Arraiolos dyers as well as the composition of the different dyes. In what concerns to the ceramic wall tiles, analysis were performed in order to identify the pigments originating the different colours (yellow, blue, white).

* Projects POCI/CTE/61700/2004 and PTDC/CTE-GIN/67027/2006.
[1] Univ. of Lisboa;
[2] INETI.;
[3] Univ. of Évora;
[4] Univ. of Minho;
[4] Univ. Nova of Lisboa.

External microbeam line setup*

P.A. Rodrigues, M. Vilarigues[1], L.C. Alves, R.C. da Silva

The new external microbeam analytical end-station became fully operational and available on a routine basis. The installation of a laser-assisted target positioning system with micrometer precision stages, of a He flow system for reducing beam scattering and lower energy X-rays attenuation, along with use of a HPGE detector for simultaneous PIGE analysis, extended its capabilities, allowing a more reliable determination of low Z elements, in particular the quantitative determination of Na as a complement to PIXE analysis. This is of particular importance for the analysis of glass matrices as in the case of a number of archaeological Roman glass fragments of historical importance which characterisation could be better established by the experimental determination of the Na contents.
In collaboration with the Restoration and Conservation Department of Universidade Nova de Lisboa, the new external microbeam line setup system was also applied in the study of stained glasses from the Mosteiro da Batalha, both for the characterisation of the bulk material and the identification of the colour pigments and decorations used, allowing to obtain clues concerning the manufacturing processes and techniques. Extending this work to museological and non-museological glasses existing in Portugal and dating from the XV century to the present is under way.

* Project POCTI/CTM/60685/2004
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Artificial neural networks for real time in-situ RBS analysis

N.P. Barradas, D. Smeets[1], J. Demeulemeester[1], A. Vantomme [1], A. Vieira[2], C. M. Comrie[3], C. Theron[4]

Real time RBS characterization, i.e. performing the analysis during thin film growth has been applied to sputter processes, implantation studies, diffusion experiments and solid phase reactions. In the case of a solid phase reaction for example it has been demonstrated that kinetic parameters such as the apparent activation energy and the diffusion coefficient can be obtained from a single real-time RBS measurement. However, the large number (thousands) of RBS spectra obtained during a typical real-time RBS experiment and the time consuming analysis associated with that has until now obstructed the real breakthrough of this technique. We revived the Artificial Neural Networks work that we had developed years ago, to solve this issue. Entire systems are solved after a few days of work, as opposed to months previously. One paper was published in 2008 in Applied Physics Lettes, and several are under preparation.

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AMS Line Software and Hardware upgrade

N. Franco, H. Luís, E. Alves

Since the recent acquisition, by ITN physics department, of a Tandetron accelerator from the CSIRO lab in Australia, there has been an effort to upgrade and modernize some of the dated features of the system, namely the computer control system as and the hardware controller (DACs) that was by today standards obsolete. So there was a complete replacement of the old Apple based system to a newer PC Windows based system. The control software developed using the LabVIEW programming language was fully rebuild and reviewed from Apple OS, new facilities were introduced like the control of new lines, e.g. ^{14}C line, as well the data analysis. The upgrade of the DACs to a 16 bit resolution and Ethernet based communication allow the improvement of the resolution of the controllers, the addiction of new controllers and the system reliability.

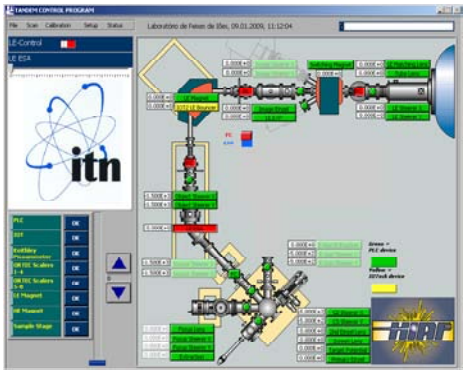

Fig. 1 – Computer interface showing the Control Program.

A new AMS facility installed at the ITN

H. Luís[1,2], N. Franco, L. Gasques[2], M. Fonseca[1,2], A. P. Jesus[1,2], E. Alves[2]

AMS (accelerator Mass spectrometry) is an extremely valuable tool for the detection of certain nuclides and measurement of their concentrations down to levels that can be within the 10^{-12} to 10^{-15} range. This sensitivity makes it popular in many fields of science, such as nuclear physics and astrophysics, geology, archaeology, medicine and several others. In the last year the first results in the micro-AMS system were obtained. The micro-AMS system at the physics unit is based on a 3 MV Tandetron accelerator and has the ability to perform AMS using a micro-beam that allows the study of isotopic ratios within samples with a very high spatial resolution. Its main features are a specially adapted HICONEX source and a fast bouncer system. In the past year the computer control system was updated, and also a lot of work was done in terms of the alignment of the beam transport system, and the resolution of several problems related to the complexity of the system. Several beams have been tested, including carbon, sulphur and gold, however since the ^{32}S beam is the most easy to obtain we have mainly used it in the test of the several components of the system. Some of the test results obtained with sulphur beam is shown in the figure. The system will be fully operational once the instabilities affecting the last section of the beam transport system after the HE Magnet were fixed.

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Advanced data analysis for IBA

N.P. Barradas, M.A. Reis, C. Jeynes[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 2008 we continued the application of the joint RBS and PIXE analysis capabilities to real cases, revealing the power of such a combined approach. Also, a new model was developed to routinely calculate the influence of the pulse height defect effect in energy spectra. We developed a method to determine non-Rutherford cross sections from simple RBS spectra using Bayesian inference data analysis. Six papers were published in 2008 in international journals.

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Biomedical Studies

Teresa Pinheiro

The research activities during 2008 within the group of Biomedical Studies make use of focused ion beam techniques to image tissue and cell morphology, and other micro-analytical techniques to assess elemental composition and molecular indicators of cell/tissue response.

The fruitful association with researchers within ITN (UQR and Reactor), with researchers outside ITN, of other national laboratories and universities, enabled us to build a true multidisciplinary team.

Also, the instrumental panoply used provides unique analytical capabilities. High-resolution biological imaging with particle beams, elemental analysis with ICP-mass spectrometer, and molecular discrimination with flux cytometry are examples of knowhow developed and combined to reach specific milestones.

Collaborative work carried out, developed skills and the outcome of past research projects paved the way to the present activities.

Ongoing projects focus non-invasive human bio-indicators of pathology and environmental exposure, which can be:

- molecules and microparticles in circulation and body fluids or adhesion molecules, receptors, cytokines, that are expressed in cells to study coronary artery disease;
- Exhaled Breath Condensate (EBC) as a new indicator of exposure to pollutants;
- Nuclear Microscopy and MRI images of Fe in skin and liver in human metabolic disorders;
- images of the atheroma (IVUS-VH - intra-vascular ultrasound virtual histology) associated to specific markers to treat patients with coronary disease in real-time;

Continued funding on areas such as cardiology and environmental health had strengthened existing skills, promoted advanced training for students and created new synergies by involving various research groups from different areas.

The main achievements of the research developed during 2008 are summarised in the following pages.

Researchers

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L.C. ALVES, Aux.

Students

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Biomarkers in Coronary Syndromes

P. Napoleão[3], R. Cruz Ferreira[1], M. Selas[1], A. Toste[1], M.C. Monteiro[2], A.M. Viegas-Crespo[3], A. Turkman[4], V. Andreozzi[4], R. Carvalho[+], A. Borges[+], L.G. Borges[+] & T. Pinheiro

Objectives

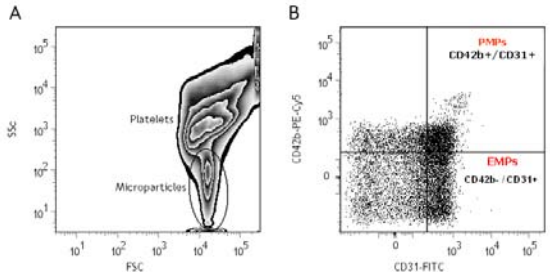
To study new bioindicators of endothelial dysfunction and thrombotic potential in coronary artery disease aside with clinical and biochemical data. Patients with myocardial infarction were assessed at the onset of the thrombotic event previous to intervention and along the recovery period.

Results

Cytokines, soluble and expressed forms of adhesion molecules, and microparticle production were measured. Changes of paramenters measured were monitored over time together with inflammatory markers and specific indicators of myocardial damage. The influence of confounders, such as medication intake, in the measured parameters variations over time was also assessed.

Special attention has been dedicated to microparticles produced by activated endothelial cells, blood cells and platelets in the acute myocardial infarction (AMI).

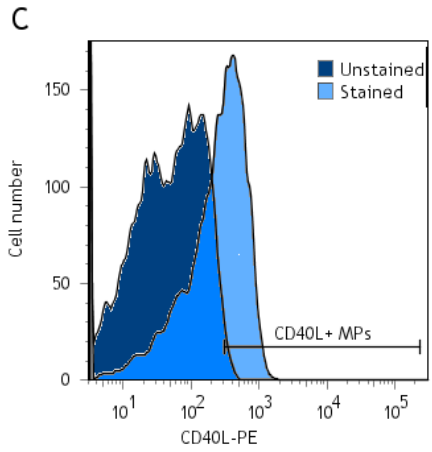
Micropaticles were defined according to morphological characteristics (size and roughness) based on light scattering properties (forward scattering - FSC and side scattering – SSC), and localized below platelets. The representative flow cytometry zebra-plot (contour and density) – A, shows the microparticles region - elliptic area.



In the flow cytometry fluorescence scattergram (B) Platelet microparticles, PMPs (right upper quarter) and endothelial microparticles EMPs (right lower quarter) subsets can be identified using specific labelling antibodies fluorescent in specific fluorescence bands, such as CD31-FITC and CD42b-PE-Cy5.

Fluorescence histograms can be then produced to quantify the positive events of interest. Therefore the expression of membrane-bound molecules such as CD40L, P-selectin, E-selectin, etc. can be quantified.

As exemplified in (C) the surface CD40L-positive-MPs can be selected after unstained sample background set-up. The number of microparticles expressing this molecule can be then estimated in stained samples by counting positive events and measuring fluorescence intensity (CD40L-PE).



The associations found between the microparticle-bound CD40L and CD62E+ with CD40L expression on platelets, on CD4+ and on CD8+ T lymphocytes, at the acute event and in the follow-up, highlighted the complex interplay of CD40L in thrombosis, inflammation and endothelial damage/dysfunction.
The time dependent-variations of soluble CD40L levels and the expression of CD40L on platelets observed in AMI patients, point out differential individual behaviour that may be relevant in AMI prognosis.
In the continuation of these studies, emphasis will be put on apoptosis and plaque macrophagic activity. Assembling all the information collected within the collaborative work, between ITN and Hospital de Santa Marta, will contribute to improve indexes of plaque progression and regression, identification of at-risk patients, and the validation of prognostic value of CD40L in AMI evolution.

Published work

P. Napoleão et al, Serial changes of oxidized-low-density lipoprotein associated with culprit vessel in ST-elevation myocardial infarction – a promising marker? Rev. P. Cardiol. (in press);

P. Napoleão et al, Platelet and endothelial status in AMI. in: 77th EAS Congress European Atherosclerosis Society Proceedings in Ather. Suppl. (in press);

P. Napoleão et al, Oxidized LDL levels associate with culprit vessel in AMI. in: ESC2008 European Society of Cardiology Congress Proceedings (in press).

[1] Hospital Sta. Marta EPE, Serv. Cardiologia
[2] CESPU, Porto
[3] Centro de Biologia Ambiental, FC-UL
[4] Centro de Estatística Aplicada, FC-UL
[+] MSc. Students

B – Skin iron as a diagnostic tool in hemochromatosis

T. Pinheiro, L.C. Alves, R. Fleming[1], R. Silva[2], P. Filipe[2], A. Barreiros[3]

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. There are currently two papers in press.

[1] Hospital de Sta Maria, Serv. Imuno-hemoterapia
[2] Hospital de Sta Maria, Serv. Dermatologia/FM-UL
[3] INETI, Lisboa

C – Exhaled Breath Condensate: A tool for noninvasive evaluation of pollutant exposition?

M. Almeida, T. Pinheiro, A. Bugalho de Almeida[1], S. Garcia[2], A. Barreiros[3],M. F. Araújo, M. Santos, M.C. Freitas, L.C. Alves, P. Félix, C. Franco[4], B. Batista[4]

The aim of the present study is to investigate whether Exhaled Breath Condensate (EBC) can be employed for a better risk assessment among human exposed to toxic pollutants, using industries processing lead. The project is a joint initiative of ITN units UFA and UR, together with the Instituto de Soldadura e Qualidade and the Hospital de Santa Maria. The primary objective is to develop a new non-invasive human bioindicator that could be applicable for professional exposition. During 2008 industries were selected according to the project objectives: number of workers exposed, handled metals, workers shifts, industry localization and industry and workers interest on the project. EBC sampling was tested in voluntaries to establish the better methodology to sample, store and analyse the EBC. Preliminary tests were also made in workers along the working shift to define the most representative sampling time.
EBC chemical characterization are being performed by TXRF in INETI and by ICP-MS in ITN, the latest recently installed under the Programa Nacional de Re-Equipamento. This collaborative work with the Environmental and Analytical Chemistry Group of ITN and LAAQ/INETI will enable methodology validation and perform inter-laboratory exercise for analytical performance comparison.

[1] Hospital de Sta Maria, Serv. Pneumologia/FM-UL
[2] Inst. de Soldadura e Qualidade
[3] INETI, Lisboa
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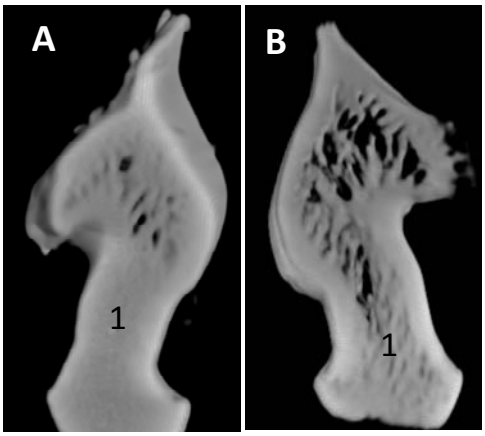
D –Nuclear Microscopy and X-ray micro-computed tomography

I. Gomez-Mollila[1], M.D Ynsa[2],L.C. Alves, T. Pinheiro

X-ray micro-computed tomography (µCT) is an excellent tool to examine the morphology of a sample in a non-destructive way, making its inner structure visible.
Rendered reconstructed data of a sample taken from an healthy (A) and an osteoporotic (B) bone slice can be depicted in figure. The osteoporotic sample presents a higher degree of porosity (trabecular bone – 2) in comparison to the healthy bone.



Nuclear microscopy provides quantitative information about the elemental distribution and concentration. Both can be used as complementary techniques in order to get more information about the samples. Osteoporosis will be the major biomedical application.
In order to achieve conclusive quantitative results on densities, a monochromatic source has been used for µCT studies. For this, a project has already been approved at HARWI II beam line, Hasylab DESY: *Density changes in femoral bones from rats under osteoporosis preventive treatments.*

[1] Univ. Dresden, Germany
[2] CMM, Univ. Autónoma de Madrid

Elemental Characterization and Speciation
CEEFI

Miguel A. Reis

The Elemental Characterization and Speciation Group of the IBL (CEEFI), carries out R&D work on ion beam based nuclear analytical techniques aiming at elemental composition characterization, as well as the establishing of ion beam based instrumental speciation methodologies.

So far, the main focus was put on particle induced x-ray emission (PIXE) applied to the characterization of airborne material. A tuning of this working line is presently being undertaken in order to cover a broader but more concise focus on small mass samples. Still, the recently installed aerosol characterization set, that includes a DOAS system (operational since 2007), a meteorological station (operational since January 2008), online in the Portuguese Meteorological Institute Urban Stations Network and a PM10 and PM2.5 sampling station is kept operational.

Nanoparticles and other particulate matter (airborne or not), as well as macromolecules and thin film samples, do now come into the scope of the group application work. This orientation is also connected to recent results on potential health impact issues identified by the group, which fit into a new research context of study of physical mechanisms behind airborne nanoparticles toxicology.

Strategically, the group assumes that it is important not to depend exclusively on collaborations neither for sampling nor for data handling processes. Therefore, effort is put on airborne particle sampling and data handling methods.

Given that PIXE is a matured analytical technique, services are provided to the community in general, and to the scientific community in particular.

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

In 2008, 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 installation and test tasks used a fair chair of the available time. Following the acquisition of the ITN-IBL Tandetron accelerator in 2007, a new High Resolution and High Energy PIXE (HRHE-PIXE) setup was made operational in 2008 and the first high resolution EDS X-ray spectra were obtained using the POLARIS microcalorimeter detector produced by Vericold Tech. GmbH.

The present lines of work involve: (1) ion induced X-ray lines Relative Yield Ion Energy Dependence (RYIED) studies, an effect shown to contain information on both emitters speciation as well as physical dimensions (size) of the emitters container, which is now the subject of two ongoing PhD programs; (2) improvements on the existing spectra data handling software, including holistic approaches to data from other IBA techniques; (3) calculations of ion impact ionization cross-sections, a recovery of work started on the 1990 decade, which regained major importance in face of the latest developments in the field, in particular the new capacities of the 15eV resolution POLARIS X-ray EDS detector; (4) the maintenance of the ITN PM10 airborne particles sampling station, which already lead to the identification of potential important public health impact conditions

Researchers

M.A. REIS, Aux. (Group Leader)
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A. TABORDA, Ph.D. Student, FCT Grant

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L. CARVALHO, Ass. Prof., CFA-UL, FC-UL
M. MOTA, Graduation Student (from Jul. 2008)
R. TEIXEIRA, Graduation Student (from Dec. 2008.

High resolution EDS and Characterization and Speciation of Micro and Nano-particles

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

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 2008, the main activities besides the operation of the airborne particle sampling unit at the ITN campus, were: (a) the installation of the Laboratory for the Characterization and Speciation of Aerosols (LCEA), including the POLARIS microcalorimeter detector; (b) the development of software for spectrum data handling; (c) the study of the Gd_2O_3 nanoparticles RYIED ; and (d) bibliographic research aiming at understanding the state of the art regarding mechanisms for nanoparticles toxicology. All of the tasks converging to the same goal, namely using particle induced X-ray for determining chemical and/or sample size effects, and eventual consequences and/or uses of that information. This work being partially a process to deepening the level of data handling of preliminary works presented at the PIXE conference held in Mexico in 2007, showed to be a task leading to greater developments than expected. Combining this fact with the commissioning of all LCEA equipments resulted on delays on reaching the final level of the works, and therefore to delays on publication of results.

Nevertheless, several important results were obtained like the commissioning of the POLARIS detector in which it was possible to achieve a 14 eV resolution at 2.345 keV of Pb-$M_{\alpha 1}$ line, as shown in the Pb M-shell X-ray spectrum in Fig. 1, and 26 eV at 17.479 keV of Mo-$K_{\alpha 1}$ line, 0.6% and 0.15% respectively.

Besides this important instrumental and operational results, it was also possible to identify plausible mechanisms for a cause/effect relation between high PM2.5 chlorine measurements at ITN and a surge in diabetes incidence in Portugal in 2004/2005, as well as plausible explanations for the physics behind the similarity between Gd_2O_3 5nm particles RYIED pattern and that for Gd-DOTA. An ***a priori*** strange result, since it is different from the RYIED pattern found for a powder pellet of Gd_2O_3. This raw data result presented at the International PIXE Conference held in 2007, and mentioned in the 2007 ITN Report, has lead to some very important conclusions that will be made public in the beginning of 2009, and have strong implications regarding the potential of the PIXE-RYIED method proposed in 2005 [Reis et al., NIM B229 (2005) 413-424].

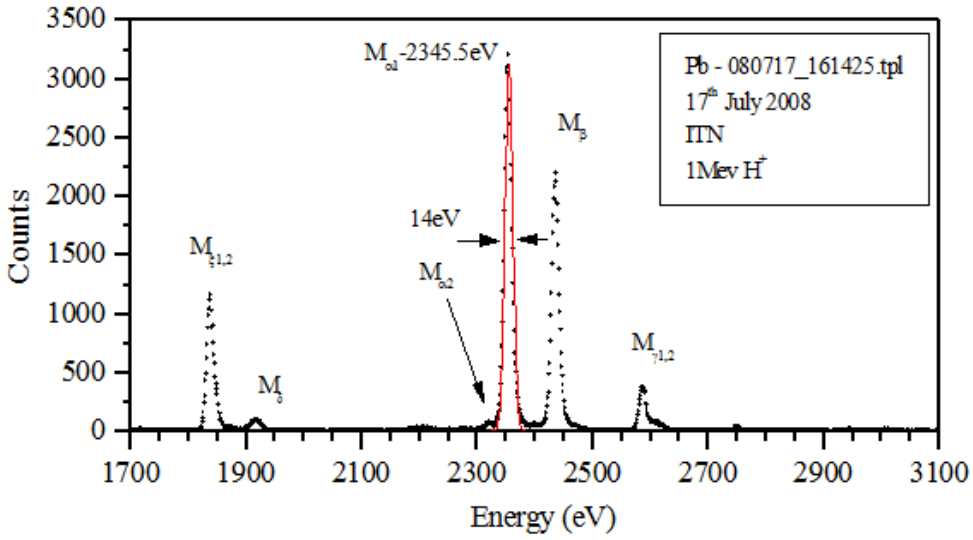

Figure: Detail on the spectrum of Pb M lines obtained using the POLARIS detector at ITN and the Python digital ADC code specifically written for the purpose at ITN.

[1] Escola Superior de Tecnologias da Saúde de Lisboa, Portugal

Materials Characterization with Radioactive Nuclear Techniques

João Guilherme Martins Correia

A **laboratory infrastructure** on materials characterization is maintained and developed at ISOLDE-CERN by researchers 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 ion beam laboratories. 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 2008 was centered in three research subjects approved by the ISOLDE Scientific Committee:

a) IS453 "Emission Channeling Lattice Site Location Experiments with Short-Lived Isotopes". The lattice sites of impurities in scientifically and 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. Elements of interest, which can only be characterized by using their short-lived isotopes are now detectable.

b) IS390 "Studies of colossal magnetoresistive oxides with radioactive isotopes". PAC is continuously used to study a large variety os multi(anti)ferroic $RMnO_3$ (R = rare-earth) manganites and cromites $ACrO_2$ (A = Ag,Cu) as a function of the elements R, A, and of temperature. By combining PAC data with first principle simulations (f.p.s.) of charge density distributions on these materials, local phenomena that correlate the coexistence of ferroelectricity, ferromagnetism and ferroelasticity are studied.

c) IS360 "Studies of High-Tc Superconductors doped with radioactive isotopes". PAC was 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 was to learn the O_δ atomic configurations depending on concentration and temperature. This project was closed in 2008 after finishing f.p.s. of charge density distributions that allowed to interpret the experimental data, revealing that the oxygen atomic configurations change with temperature above and below Tc. An extensive paper will be published in 2009.

2008 was a year of consolidation and new achievements on R&D projects. The new emission-channeling chamber using the fast Si pad-detector setup was refined and reused with success. There we have further implemented a cooling station (50 K – 300 K) and first low temperature test EC experiments were successfully achieved with ^{111}In implanted into InP. Additionally, first electron tests on a highly pixilated 256x256 14x14mm^2 Si detector (MEDIPIX) were done with a source of 73As: ZnO sample.

In a different context, the radioactive hyperfine technique PAC was very useful to study at the nanoscopic scale electrical and magnetic properties. 2008 was a rich year in both experimental, with new materials being studied, and simulation achievements. We point the fact that our group is now able to use, autonomously, complex charge density simulation programs, which are essential providing the data interpretation on the studied systems.

Of interdisciplinary nature, these activities integrate and initiate 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. On 2008 one PhD student defended her thesis, one is finishing the writing, six other PhD and three MSci students performed their work using this infrastructure within the scientific proposals and R&D projects.

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E.ALVES, Princ.

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T. MENDONCA, Ph.D. Student, FCT grant
E.C. RITA, Ph.D. Student, FCT grant
A. PEREIRA, Ph.D. Student, FCT grant
J.N. GONÇALVES, Ph.D. Student, FCT grant
C. SOUSA, Ph.D. Student, FCT grant
L. AMORIM, M.Sc. Student FCT projects
M. BARBOSA, M.Sc. Student FCT projects
G. OLIVEIRA, M.Sc. Student FCT projects

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M.R. SILVA, Ass. Prof., IST, Lisboa
J.C. SOARES, Cat. Prof. Emeritus, U. Lisboa
L. REDONDO, Ass. Prof., ISEL, Lisboa
H. HAAS, Emeritus Researcher, ITN
A. VANTOMME, Prof., IKS Leuven

IS-453 experiment: Emission channeling lattice location studies

U. Wahl, J.G. Correia, L. Amorim, C.P. Marques, A.C. Marques, E. Alves, S. Decoster[1], A. Vantomme[1], M.R. da Silva[2], J.P. Araújo[3], L. Pereira[3], and the ISOLDE collaboration[4]

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 channeling (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. Lattice location of implanted Er in Ge

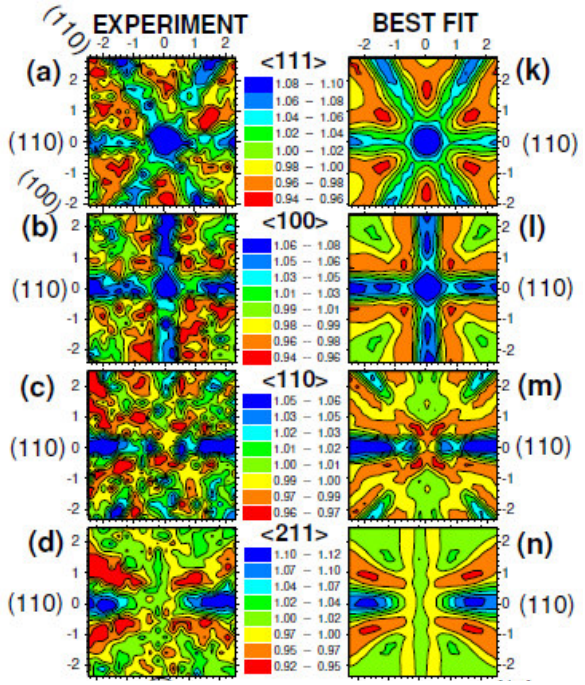

Figure: Experimental EC patterns from ^{167m}Er in Ge (left) and simulations for a combination of 20% of Er on T , 16% on BC and the rest on random sites (right).

We have used conversion electron emission channeling to determine the lattice location of ^{167m}Er (2.28 s) in Ge after 60 keV room temperature implantation of the precursor isotope ^{167}Tm (9.25 d). We found direct experimental evidence of Er atoms located on the tetrahedral interstitial site (T) and on the bond-centered (BC) site. Whereas Er is expected to occupy the interstitial T site in a diamond crystal structure (as was previously determined from emission channeling in the case of ^{167m}Er Si), the observation of bond-centered Er in Ge is more surprising and believed to be related to the so-called Er-vacancy defect in the split-vacancy complex configuration, which is formed when an Er atom pairs with a Ge double-vacancy. Such complexes have been theoretically proposed to exist for a number of oversized transition metal impurities in Ge and our results strongly suggest that these predictions also apply to the case of rare earths.

2. Emission channeling with short-lived isotopes

Using our new emission channeling on-line setup which is equipped with a fast position-sensitive Si pad detector and was commissioned in 2007 followed by its first on-line run at the ISOLDE facility, a second set of lattice location experiments with short-lived radioactive isotopes were done during this year's Mn beam time. We were able to determine the lattice sites of implanted ^{56}Mn (2.6 h) in ZnO, Ge and GaAs, and of ^{61}Co (1.6 h) in GaN during the run. We found that Mn in ZnO prefers substitutional Zn sites and Mn in Ge substitutional Ge sites. Mn in GaAs occupies substitutional sites as well, but distinguishing between Ga and As sites will only be possible after careful analysis due to the very similar nuclear charges of these two elements. While ^{56}Mn was implanted directly, for the study of Co in GaN we exploited the decay chain ^{61}Mn(4.6 s) $\rightarrow$ ^{61}Fe (6 min) $\rightarrow$ ^{61}Co (1.6 h), i.e. ^{61}Mn was implanted and after a waiting period of 30 min lattice location was done on ^{61}Co. We found that Co occupies substitutional Ga sites in GaN. In addition, by means of using the decay chain ^{59}Mn (0.71 s) $\rightarrow$ ^{59}Fe (45 d), we prepared samples of $SrTiO_3$ and $KTaO_3$ doped with ^{59}Fe, for which the lattice location of Fe is being determined during the following months.

Published work

S. Decoster, B. De Vries, A. Vantomme, U. Wahl and J.G. Correia: Experimental evidence of tetrahedral interstitial and bond-centered Er in Ge, Appl. Phys-Lett. 93 (2008) 141907.

[1] Inst. voor Kern- en Stralingsfysica (IKS), Katholieke Univ. Leuven, 3001 Leuven, Belgium.
[2] Centro de Física Nuclear da Univ. de Lisboa (CFNUL), e IST.
[3] Dep.de Física, Univ. do Porto, 4169-007 Porto.
[4] CERN, 1211 Geneva 23, Switzerland.

IS390 experiment – Studies of local phase transitions on multiferroic compounds.

T.M. Mendonça[1], A.M.L. Lopes[2], J.N. Gonçalves[3], G. Pereira[1], V.S. Amaral[3], J.P. Araújo[1], A. Pereira[1], C. Sousa[1], J.C. Amaral[3], M. Barbosa[1], J.G. Correia

In 2008 we have published in a PRL a detailed study of the electric field gradient (EFG) across the $Pr_{1\_x}Ca_xMnO_3$ phase diagram and of its temperature dependence. The EFG behaves differently on samples outside or inside the charge order (CO) regime. In particularly, the EFG temperature dependence evidences a new and discontinuous phase transition occurring over the broad CO region of the phase diagram. Such prominent features revealed to be associated with polar atomic vibrations, which eventually lead to spontaneous local electric polarization below the CO transition. Following the same experimental procedures we are now looking in detail at the temperature dependence of the EFGs on multiferroic systems $YMnO_3$ and $EuMnO_3$ and of the newly synthesized $AgCrO_2$ as a function of temperature down to 10 K. The aim is to study other cases where there is coexistence of magnetic and electric polarization along the phase diagrams, looking forward to find the extension, looking at the nature of the different local regimes. For all samples the data is excellent, in the sense that it has enough precision for evidencing local transitions at different regions of the phase diagrams for each sample. Again these results point the coexistence of multiple microscopic phases, somehow hindered at measurements of only macroscopic properties. The data is presently under analysis, refining the fits and performing first principles calculations of the EFGs for different local arrangements.

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R&D development – concept design, manufacture and commissioning of a cooling station for EC studies

L.M. Amorim, M.R. Silva[1], U. Wahl, J.G. Correia, N. Ferrão[1], C. Mendes[1], M. Campbell[2], L. Tlustos[2]

Since about ten years that lattice location experiments with the EC technique have not been performed at low temperatures. In spite of the fact that one of the old goniometer setups is equipped with a He flow cryostat, there were several inhibiting factors for regularly doing such experiments: 1) it is very heavy (~50kg), requiring the use of a crane each time samples need to be changed or the cryoshield needs to be turned to cope with the sample axis, 2) it is actually installed on a building without He recovery line and 3) it cannot be mounted on-line. With the commissioning of the new fast detector and on-line chamber the motivation to go below RT become very appealing, where the samples could be implanted at cryogenic temperatures to study annealing stages of impurities below RT. Furthermore, on materials with low structural symmetry we might attempt to probe the anisotropy of vibrations, or position r.m.s shifts of the elements / impurities as a function of temperature, e.g., upon electric and magnetic phase transitions. Successfully cases of such experiments would be of great interest on probing microscopic local effects. With these aims in mind we have developed and successfully commissioned a cooling station using a closed cycle He refrigerator and a cryogenic shielding system that is coupled to our "all-day-use" simple goniometer. In this first approach we could achieve a sample temperature down to 50K. We have studied a first test case prepared by ion implantation of ^{111}In on InP. Once In is a member of the lattice it was easy to anneal out the implantation damage at 300^{o}C. Additionally, since InP has a low Debye temperature it is expected (as were measured) large variations of the vibration r.m.s. amplitudes as a function of temperature from RT down to 50K. The data is presently under analysis but, as new information from these experiments, we guess so far that on systems with low Debye coefficients, i.e., large r.m.s vibration amplitudes the dechanneling plays a stronger effect than what is actually considered in the present manybeam EC simulations. 2009 will be a year of analysis, experiments, and consolidation and improvement of the low temperature system, aiming to achieve 30K.

Still on the field of EC R&D, we report first EC tests of electron detection with a MEDIPIX 256x256 channels, 14x14mm^2, 300μm thick detector. We used a ^{73}As : ZnO source and nicely measured the EC electron anisotropy spectrum for the face axis <0001> for the 42 keV electrons. A tentative spectrum using only 12keV electrons was done, with some channeling effect being visible, but the probable detection of x-rays and the lack of knowledge of how should look such low energy electron spectra hindered further conclusions. New tests using TIMEPIX (energy resolved detectors) will be further done on 2009 on a special chamber developed by us, equipped with a cooling system on real experimental conditions.

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[2] 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 astrophysics.

Also a new line has been installed in the new Tandem 3MV accelerator, for nuclear reaction studies both for fundamental nuclear physics and nuclear astrophysics and for applied PIGE work.

Researchers

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(*) Also members of CFNUL.

Experimental Study of Nuclear Reactions for Astrophysics

H. Luis, J. Cruz, D. Galaviz, L. Gasques, A.P. Jesus, M. Fonseca, J.P. Ribeiro

Objectives

Following its experimental work in nuclear reactions relevant for primordial and stellar nucleosynthesis (hydrogen burning) [1,2], the group is focusing now in later stages of stellar nucleosynthesis, namely alpha, carbon and oxygen burning and p-process. Some of the studies will proceed within international collaborations, making use of facilities such as ERNA, FAIR, ISOLDE. Other studies will be conducted at ITN, taking advantage of the heavy ion beams available at the 3 MV Tandem accelerator and of the accelerator mass spectrometry (AMS) line.

In the short term, studies will be made of the oxygen+oxygen fusion reaction and in relation to the AMS technique our aim is the study of reactions that lead to the production of ^{10}Be and ^{26}Al, also in order to open new perspectives of applied work.

Results

A new reaction line has been installed at the 3 MV Tandem facility. During this year, alignment and vacuum tests were performed. The line is now ready for operation with a Ge (HP) detector and PIP particle detectors.

In relation to the AMS line some technical difficulties have retarded the predicted plans. Realignment and reassembling of some parts were necessary to improve the beam intensity and stability.

Future Work

During 2009, sulphur isotopic ratios will be remeasured to complete the tests of the AMS line (fig. 1 and 2), namely to assess the bouncing system, and afterwards a period of target testing and preliminary nuclear reaction measurement will follow. In relation to the recently assembled reaction line, target testing and preliminary nuclear reaction measurement of the oxygen+oxygen fusion reaction will proceed.

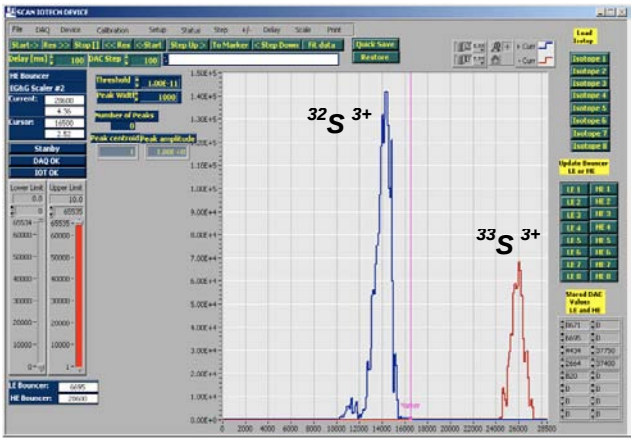

Fig. 1 Part of the mass spectrum of a sulphur target.

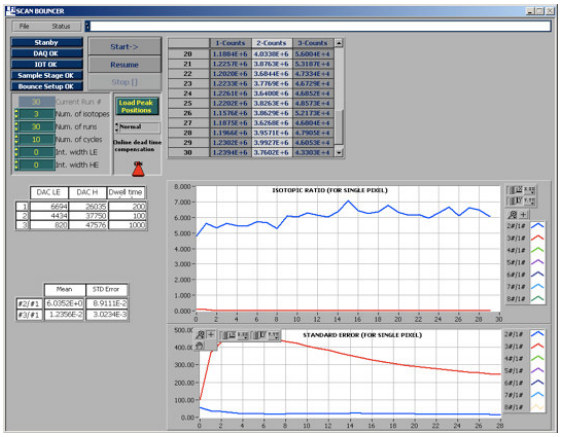

Fig. 2 Labview control of the bouncing system, showing ratios relative to mass 34 isotope of the 33 and 36 isotopes.

Published Work

LUNA Collaboration; D. Bemmerer, F. Confortola, A. Lemut, R. Bonetti, C. Broggini, P. Corvisiero, H. Costantini, J. Cruz, A. Formicola,;Zs. Fülöp, G. Gervino, A. Guglielmetti, C. Gustavino, Gy. Gyürky, G. Imbriani, A. P. Jesus, M. Junker, B. Limata, R. Menegazzo, P. Prati, V. Roca, C. Rolfs, D. Rogalla, M. Romano, C. Rossi-Alvarez, F. Schümann, E. Somorjai, O. Straniero, F. Strieder, F. Terrasi, H. P. Trautvetter, Nuclear Physics A779, 297-317 (2006).

J. Cruz, H. Luis, M.Fonseca, Z. Fülöp, G. Gyürky, F. Raiola, M. Aliotta, K. U. Kettner, A. P. Jesus, J. P. Ribeiro, F. C. Barker, C. Rolfs, Journal of Physics G 35, 014004 (2008).

Development of a PIGE Set-up
M. Fonseca, R. Mateus, L. Gasques, A. P. Jesus, H. Luis, J. P. Ribeiro

The aim of this work is the extension to all light elements of previous work 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.

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 already been published [5] and the analysis of Mg (gamma spectrum in figure) was concluded (preliminary results in table).

A nuclear reaction line was assembled at the 3 MV Tandem accelerator in order to extend the present work to higher energies and be able to quantify C, N and O.

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. The main effort has been made to characterise the hybrid materials and co-polymers prepared by gamma irradiation using the ^{60}Co source of UTR.
The systems studied involved hybrids prepared from mixtures of a polymer (PDMS) and different metallic alkoxides. Characterization of selected samples prepared by gamma irradiation continued, making use of a wide range of techniques, most of them available at ITN.

During 2008 the main work on the development of new copolymers (HEMA grafted on LPDE thin films) suitable for bioapplications was concluded. The sample preparation conditions were correlated to the grafted material structure and the hydration level achieved by the final product, and toxicity studies were finished. Tests of Biocompatibility (haemolysis and tromboresistance) were completed. Work on this system has been summarised in a PhD thesis that was submitted to the University of Lisbon in December 2008.

The Group had 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, has been preventing the proper development of the activity in this area. In the last two years the human resources both the staff and the students have been considerably reduced. As concerns the financial resources, the neutron scattering instruments situation became particularly difficult. This type of instruments installed at any reactor source require a set of equipments and components that are generally expensive items, to be able to tailor the neutron beam, to eliminate the undesired background radiation and to collect the data, in a suitable and efficient way. This becomes particularly critical when the source is a low flux reactor.

As concerns the small angle scattering instrument, extensive work had been done to optimise its installation at RPI. However the actual signal to noise ratio was found to be too low to carry out meaningful measurements. During 2007 the reactor core was converted from HEU to LEU which further contributed to lower that ratio value. In 2008 it became clear that no further progress could be made to overcome this problem unless a few technical solutions were implemented. The matter of fact was presented to the Board of the Institute.

Given the considerable funding required and the current financial difficulties of the Institute, the decision was made to temporarily set aside the project of the small angle neutron scattering instrument at the Portuguese research reactor. Characterization of the prepared materials using small angle neutron scattering will continue to be carried out in foreign neutron scattering centres.

Three proposals for small angle scattering measurements have been presented to European neutron scattering centres. Those proposed at the Budapest Neutron Centre in Hungary and at the Laboratoire Léon Brillouin in France have already been approved.

Researchers

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C.M.M. CRUZ, Aux. (20%)
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Collaborators

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Progress in the characterization of hybrids obtained by γ-irradiation

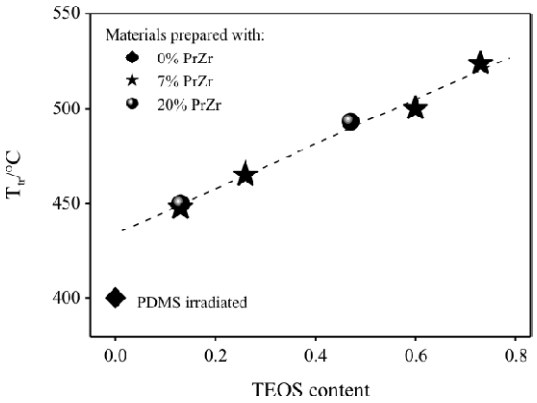
F.M.A. Margaça, L.M. Ferreira, A.N. Falcão and I.M.M. Salvado

Objectives

To characterize organic-inorganic hybrid materials prepared using the gamma-irradiation from the ITN ^{60}Co source from a mixture of composition x polydimethylsiloxane (PDMS) (100-x) Alkoxide, in order to investigate the microstructure and properties.

Results

The alkoxides used as precursors were tetra orthosilicate (TEOS) and Zr-isopropoxide (PrZr). All the obtained materials were monolithic and transparent after drying in air. They have been studied using different techniques. The detailed measurements and results have been presented and published [1-4]. In the following a few of those results are shown.



Figures 1 show the behaviour of the hybrid material rupture temperature, T_{tr}, which is associated to the breaking of the polymer chains into volatile fragments and marks the rupture of the structure. It was found that this temperature increases linearly with the TEOS content in the hybrid materials prepared with PrZr.

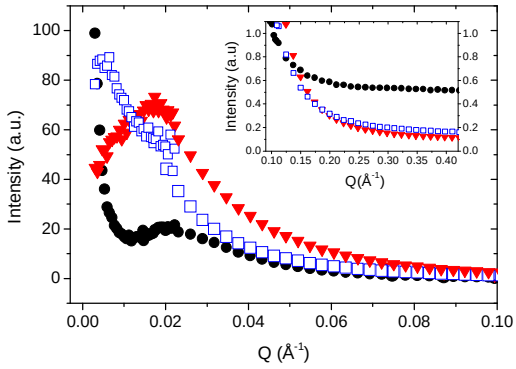


Figure 2 shows Small Angle Neutron Scattering (SANS) data for the 20%PDMS+73%TEOS+7%PrZr sample dried at room temperature (●) and after heat-treatment at 450 ºC (□) and 600 ºC (▼). The insert shows the intensity at large Q before subtracting the incoherent scattering.

The SANS data revealed the mass fractal nature of the inorganic oxide regions structure. It also showed that, although the presence of PrZr is required to obtain a stable hybrid, the increase in its content leads to a less dense mass fractal oxide structure. The slope values of the spectra linear descents revealed that the oxide domains develop via reaction-limited aggregation. The size and the fractal density of the inorganic oxide regions increase with the TEOS content.

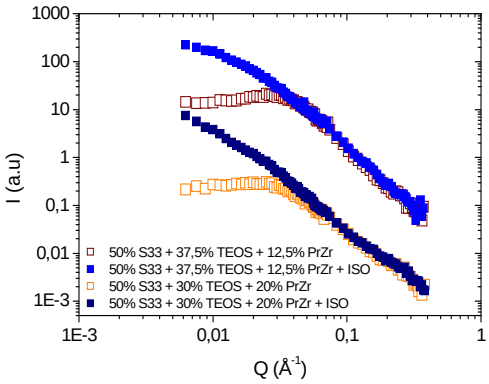


Figure 3 shows the SANS intensity obtained from samples with 50%PDMS and varying contents of TEOS and PrZr prepared with and without further addiction of isopropanol. It was observed that the further addition of isopropanol in the preparation stage causes the inorganic fractal structure to extend over a much larger volume in the samples so prepared. This effect needs further investigation and work is in progress.

Published Work

S.R. Gomes, F.M.A. Margaça, L.M. Ferreira, I.M. Miranda Salvado, J.P. Leal, C. Marques, E. Alves, L.M. Ferreira and A.N. Falcão, Elemental and RBS analysis of hybrid materials prepared by gamma irradiation, Nucl. Inst. Meth. Phys. Res. B, 266 (2008) 288-294.

S.R. Gomes, F.M.A. Margaça, D. Faria Silva, L.M. Ferreira, I.M. Miranda Salvado, A.N. Falcão, Novel Way to control PDMS Cross-linking by Gamma Irradiation, Nucl. Inst. Meth. Phys. Res. B, 266 (2008) 1105-1108.

S.R. Gomes, L.M. Ferreira, F.M.A. Margaça, I.M. Miranda Salvado and A.N. Falcão, Thermal analysis of hybrid materials prepared by gamma irradiation, J. Therm. Anal. Cal., Online First: Oct. 2008, Doi:10.1007/s10973-008-9223-8

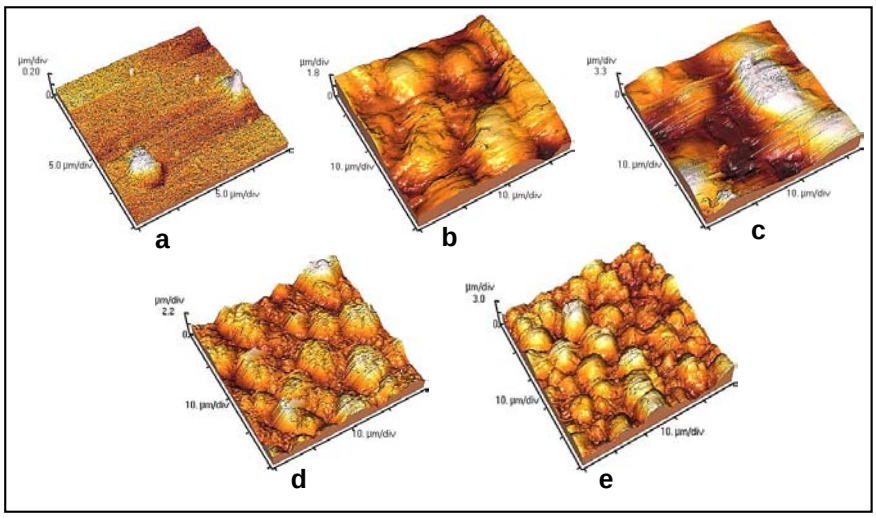
S.R. Gomes, F.M.A. Margaça, I.M. Miranda Salvado, A.N. Falcão, L. Almasy and J. Teixeira, SANS investigation of PDMS hybrid materials prepared by gamma-irradiation, Nucl. Inst. Meth. Phys. Res. B 266 (2008) 5166–5170.

Modification of Polyethylene by Grafting Copolymerization Induced by Gamma Radiation – Its Application in Biomaterials Field

L.M.Ferreira, A.N. Falcão, J.P. Leal, M.H. Gil[1], L.Cerqueira, A. Rodrigues, C. Marques, H. Ferronha[2] and I. Correia[2]

The R&D work on the preparation of a new grafted copolymeric polyethylene based materials by gamma irradiation technique, using the ITN ^{60}Co source, was concluded. The PE-g-HEMA films prepared exhibit a good mechanical behaviour associated with a maximum hemolytic effect of 2%, which, according to ASTM F 756-00 standard, classify them as "nonhemolytic" material and therefore suitable for direct contact with blood. The copolymeric films reveal other good properties such as their porous and rough surface.

These are essential conditions for cell bio-interaction for linkage and/or cell proliferation. Furthermore, these are important characteristics too for physical or chemical immobilization of active biomolecules (enzymes, drugs, tromboresistentes agents, etc).



The work developed in this research project is reported in detail in the PhD thesis of Luís M. Ferreira, which was submitted to University of Lisbon in December 2008. The descriptive documentation process for registration of a National Patent for the new polymeric material is under way.

[1]Univ. Coimbra / Dept. Chemical Engineering.
[2]LNIV (National Laboratory of Veterinarian Research).

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 pharmaceuticals) or in environmental control (*e.g.* hospitals rooms and pharmaceutical industries).

In the scope of ITN mission the group is requested 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 cope with 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 achievement 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

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S. CABO VERDE, Post-Doc

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R. MELO, Ph.D. Student, ITN Grant
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J. REIS, Ph.D. Student from Évora University
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Radiation Technology in Chemistry

R. Melo, J.P. Leal, J. Branco, Erzsebet Takacs[1], A. Bechior, S. Cabo Verde, M. L. Botelho

The radiolysis phenomenon caused by ionizing radiation (γ; β) applied to the environmental remediation of wastewater foreseen a promising treatment technology. The chemistry behind this process is essential to improve substantially our basic understanding of the radiation chemistry of recalcitrant compounds (reactions, pathways, and rates) in various systems. Gallic acid (GA) is a biorecalcitrant phenolic compound and could be considered as a model pollutant of the wastewater generated in the cork boiling process. The aim of the present research is the evaluation of γ and β radiation as emerging oxidation technologies. The evaluations of rate constants as well as the establishment of the partial contributions of the direct and radical reactions pathways to the global process are being studied. The studies performed in the Institute of Isotopes, Budapest showed that the GA is almost degraded (~86%), at 60 kGy, in the LINAC accelerator at 360 kGy/h. The HPLC measurements showed three main radiolytic products. The •OH and e^-_{aq} radicals attack were studied using pulse radiolysis technique. The spectral characteristics of the intermediates formed in •OH and e^-_{aq} reactions are different. Results are being analysed to better understand the degradation mechanism of such compound. Other Chemical field of study was the effects of gamma radiation on human haemoglobin structure evaluated by UV-VIS spectroscopy. Results pointed out to different degradation response of haemoglobin at lower dose rate (27 Gy/h) and at higher dose rate (270 Gy/h) which there was a decrease of the intensity against an increase of the haemo groups, respectively.

[1] Department of Radiation Chemistry, Institute of Isotopes, Budapest, Hungary.

Radiation Technology in Physics

A. Belchior, R. Melo, S. Cabo Verde, M. Goulart[1], D. Marcos[2], P. Vaz[1], R. Sarmento, J. Cardoso[1], I. Gonçalves, M. L. Botelho

Monte Carlo methods and computational tools provide evidence not only in support of the assessment of dose distributions but also in shielding calculations in industrial processing facilities. Regarding this, MCNPX has been used to calculate the dose rate values of several positions in the Unit of Radiation Technologies (UTR), in order to carry out the effectiveness of the variance reduction techniques, concerning shielding verification. Simulated results were compared with ionizing chamber values (LMRI, ITN) and taking into account some disagreement in the results, the methodology is being developed, namely with an attempt of a better definition of the irradiator and chamber geometry. A study concerning the low dose effect on human mature red blood cells was done by means of necrosis and apoptosis induction. Due to exposure to gamma radiation (5, 10, 20 and 30 kGy) red blood cells show lactate dehydrogenase release in the medium. The % of specific lysis is time dependent – increases with time of incubation (until 72h), after that shows a significant ($P < 0.05$) decrease. In apoptosis, control values determination were higher than experimental levels, which means that red blood cells die by necrosis and the quantification was due to the presence of haemoglobin on medium.

[1] Unit of Radiological Protection and Safety, ITN.
[2] Sociedade Avanço, S.A., Tercena, Portugal.

Radiation Technology in Microbiology

S. Cabo Verde, T. Silva, J. Santos[1], J. Vinjé[2], S. J. Nascimento[3], M. L. Botelho

The environmental persistence of infectious microorganisms is a current issue that questions the efficacy of available disinfection methods. In this scope two studies were developed. One, a research project, aimed to assess the inactivation response to common disinfectants (50 - 90% Ethanol and 1000 - 5000 ppm of Bleach) of two surrogates' models for human norovirus (murine norovirus – MNV and feline calicivirus – FCV). The virus infectivity was estimated using three different methods (Plaque assay, Tissue Culture 50% Infectivity Dose – $TCID_{50}$ and Quantitative Real-time PC–qRT-PCR) for comparison purposes. FCV (> 4 log titer decrease) point to be more sensitive than MNV (max 4 log titer decrease) to the assayed disinfectants. Based on the obtained results ethanol solutions point out to be more efficient (4 log decrease) than bleach (2 log decrease) in the inactivation of MNV. FCV was not detected when bleach solutions were used and a 5 log titer decrease was verified with ethanol treatment. qRT-PCR suggested to follow up the MNV inactivation response when compared with the plaque assay (ratio<2), the gold-standard method to measure virus infectivity. $TCID_{50}$ method point out to be a potential method to measure the inactivation of norovirus. The other study refers to a partnership between RTPPG and the company TradeLabor. This service pretended to evaluate the number of viable particles in several national health care services. The air bioburden ranged between $1 – 10^2$ ufc/m^3 and in the majority of cases the obtained values were not in consonance with the ISO room classification, suggesting that correction actions need to be made in the health routine disinfections procedures.

[1] TradeLabor.
[2] Center of Disease Control and Prevention.
[3] Faculdade de Farmácia, Univ. Porto.

Nuclear Instruments and Methods

João B. Manteigas

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

1. Modelling of radiation fields, calculation of neutron physic parameters, measurement of neutron cross-sections;
2. Modelling of gas discharges;
3. Development of software for control and data analysis;
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 on 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 the CERN, was carried out.

Modelling of gas discharges

1. A code for the simulation of atomic emission spectra in plasmas was developed and included in the PLASMAKIN plasma modelling package. The code is able to deal with all relevant line broadening processes and with radiation trapping under complete frequency redistribution conditions.
2. The effect of small admixtures of molecular gases on the electron kinetics in argon, with application on GD-OES (Glow Discharge Optical Emission Spectroscopy) was studied. The molecular gases studied included H_2, N_2, O_2 and H_2O in concentration up to 10%.
3. The study of the oxidation of methane in DBD (dielectric barrier discharges) was started. Two discharge reactors were built and the conversion efficiency of methane and the selectivity for H_2, CO and CO_2 studied.

Development of software for control and data Analysis

1. A system for control of gamma spectrometry equipment was developed. The system uses a client-server architecture based on the EPICS system for instrument communication and control and allows the remote control of a multichannel acquisition board.
2. The effect of interference on measurements and on critical and detection limits was studied and applied to the simultaneous measurement of gross alpha and beta activity measured either with gas proportional counters or with liquid scintillation counting.

Design of electronic instrumentation

- Triple Power Supply/Readout System, "Mass Flow Controller", designed to control 3 Mass Flow Meter/Controller from Bronkhorst® High-Tech B.V., Holland, *in-situ* and remotely.
- Optimization of Gamma Isotope TLC Analyser, "RadioScan" (for measuring and recording radioactivity levels, on label or strips) and upgrading of "Portable Gamma Level Indicator" – DNG-P.

Instrumentation and Technical Assistance

The main objectives are the development of equipment for ITN 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 was involved in the following collaborations:

1. n_TOF collaboration, a consortium of 40 laboratories in Europe and USA;
2. International project EU 5th FP IP-EUROTRANS, collaboration with CIEMAT (Spain) and others.
3. Research Institute for Solid State Physics and Optics, Budapest, Hungary.
4. Plasma Physics Centre / Gas Electronics Group, IST;
5. ISEL, Department of Automation and Electrotechnical Engineering.

Researchers

J. MANTEIGAS, Aux., (Group Leader)
C. CRUZ, Aux.
I. F. GONÇALVES, Aux.
J. NEVES, Aux.
N. PINHÃO, Aux.(90%)

Students

C.M.CARRAPIÇO, Ph.D. Student, IST (IG)
A. JANECO, Project Grantee (NP)
R.P.F. MENDES, Graduation Student, FC/UL (NP)

Technical Personnel

T. JESUS
N. INÁCIO
M. CABAÇA

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

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

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 corrective and preventive maintenance of the "Ion Beam Laboratory – TANDEM 3 MV" at the Physics Sector.

(ii) Collaboration with CIEMAT (Spain) in the framework of international project EU 5th FP IP-EUROTRANS. In order to minimize noise susceptibility of experiments, some technical work on grounding and shielding was carried out at Yalina facility on the Joint Institute of Power and Nuclear Research, Sosny, Minsk, Belarus.

(iii) Collaboration on Automation-Robotic of the Multidisciplinary Laboratory of Controlled Areas ("Concurso Nº2/ITN/REEQ/2008").

(iv) Collaboration on the construction of the Multidisciplinary Laboratory of Controlled Areas ("Concurso Nº3/ITN-REEQ/2008").

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

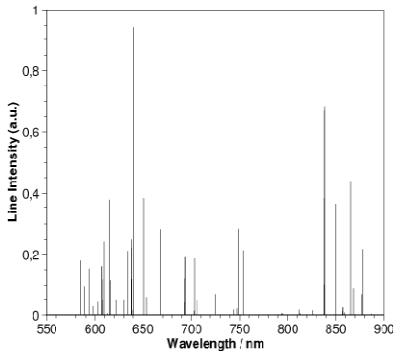
Summary of the more relevant Services/Equipments rendered in 2008

Activity	Qty	Client
Laboratory equipment for the determination of radioactive element traces by electrodeposition	1	UNIWERSYTET GDANSKI (Poland)
Personal Radiation Dosemeter Equipment	2	FARMA APS
	2	PREVINAVE (República Popular de Angola)
	2	J. ROMA, LDA.
	2	Instituto de Ciências de Materiais de Barcelona (6 Channel Micro Current Sources)
Electronic Nuclear Instrumentation	1	PREVINAVE – República Popular de Angola (Portable Level Indicator)
Technical Assistance to Nuclear Equipment	1	ITN/UPRSN (RADIOSCAN)
	1	ITN/UCQR (Mass Flow Controller)
	1	ITN/UPRSN
	1	Direcção Geral de Navios
	20	EMA 21 – PORTUCEL/SOPORCEL (Figueira da Foz)
	6	SIDERURGIA NACIONAL SA (Seixal)
Prices including TAX (VAT)		**Total Amount: 17 300,18€**

Participation of ITN in the n_TOF phase 2 experiment at CERN (3rd year)
I.F. Gonçalves, P. Vaz, C. Cruz, J. Neves, C. Carrapiço, R. Sarmento, L. Távora[1]

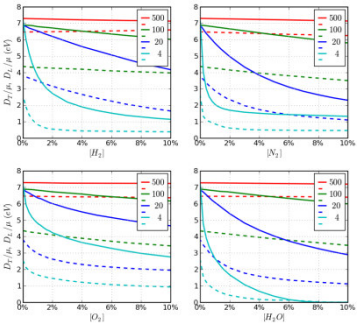
The n_TOF phase2 project is the continuation of the involvement of ITN in the activities of the n_TOF Collaboration. The intention of the n_TOF Collaboration is to build a second n_TOF beam-line and a new experimental area (EAR-2) using a shorter flight path (20 meters), with lower backgrounds and count 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 INFN-Bari and CEA, Saclay, in the following areas: Monte Carlo simulation - 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; Data analysis (I) - continuation of the analysis of the following data sets: Au-197, Np-237, Pu-240, taken during 2005 using the BaF2 calorimeter.The data analysis was initiated in 2006 and it is foreseen that will continue till 2009; Electronics developments for the DAQ and the BaF2 calorimeter.

Development of open source software for the simulation of atomic emission spectra
N. R. Pinhão



We developed a software code for the simulation of atomic emission spectra of discharge plasmas in either plane-parallel or cylindrical geometries. Line profiles take account of combined natural, Doppler and pressure broadening effects. Pressure broadening includes van der Walls collisions, resonance broadening and quadratic Stark broadening from collisions with charged species (electrons and ions). The resulting combined line profiles are approximated by the sum of a Voigt profile with a correction term. Radiation trapping is taken into account assuming complete frequency redistribution. The code has been included in the Open Source PLASMAKIN package for plasma modelling.

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

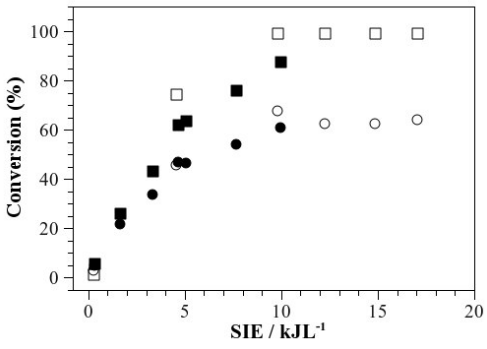


The electron kinetics in argon with small admixtures (from 0% up to 10%) of molecular gases (H_2, N_2, O_2 and H_2O) was studied. Electron energy distribution functions, transport parameters and reaction rates were compared using three different numerical methods: a two-term Boltzmann equation solver, a density gradient expansion for the Boltzmann equation and a Monte-Carlo method. The results show a strong influence of small amounts of admixture (< 1%) in low electric field. As the field increases this influence becomes less important.

Development of a distributed system for data acquisition and treatment in gamma spectrometry
R. P. F. Mendes, N. R. Pinhão

A system for remote control of gamma spectrometry equipment was developed. The system uses a client-server architecture based on the EPICS system for instrument communication and control over TCP/IP. Data acquisition is done on a PC running a real-time Linux kernel, acting as a server, and equipped with a multichannel acquisition board. Data treatment can be done in any PC running a client application. The project has included the development of a Linux device driver for the EG&G 916A multichannel board.

Oxidation of methane using CH_4/O_2/He and CH_4/CO_2/He mixtures in dielectric barrier discharges
J. Branco, N. R. Pinhão, A. Janeco, A. G. Ferreira, L. Redondo, A. P. Gonçalves



The oxidation of methane in non-thermal plasma produced in a dielectric barrier discharge (DBD) has been studied in two different systems: one with a needle-to-plane (dielectric) geometry and another one with cylindrical geometry. A maximum value for CH_4 conversion of 70% was obtained with a mixture of CH_4/O_2/He and a Specific Input Energy (SIE) of 10 kJ/L. This study is integrated in the project "*Coupling catalysts and a non thermal plasma for low temperature decomposition of organic volatile compounds"*, discussed elsewhere.

Effect of Interference on Detection Limits for the Simultaneous Measurement of Gross Alpha and Beta Activities
N. R. Pinhão, J. Abrantes

The effect of interference on measurements and on critical and detection limits was studied, developed for the case of two mutually interfering analyte and applied to the simultaneous measurement of gross alpha and beta activity measured either with gas proportional counters or with liquid scintillation counting. A new and simple criteria for the detection threshold in the presence of interference was proposed. The detection limit was split into a component independent of interference and characterizing the measurement process, and a term dependent on interference.