Advanced Materials Research

Eduardo Alves

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

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

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

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

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

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

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

The scientific activity of the group in 2005 materialized in:

Publications (peer review journals): 50
Conference and workshop contributions: 8 invited talks, 17 talks and 46 posters.
Running projects: 23

Research Team

Researchers (*)

E. ALVES, Aux., Group leader (90%)
R.C. da SILVA, Aux.
L.C. ALVES, Aux. (75%)
N. BARRADAS, Aux. (20%)
A.R. RAMOS, Aux. (10%)
A. KLING, Aux. (10%)
U. WAHL, Post-Doc fellow, FCT
K. LORENZ, Post-Doc fellow, EC
V. CORREGIDOR, Post-Doc fellow, EC

Students

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

Technical Personnel

J. ROCHA
F. BAPTISTA
P. PEREIRA

Collaborators

M.R da SILVA
L. REDONDO
S. PEREIRA
A. RODRIGUES, IEFP fellowship

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

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

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

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

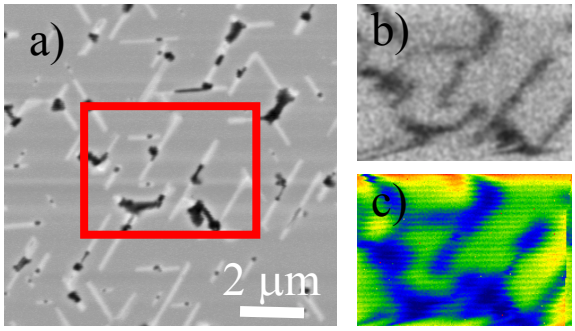

Figure 1: a) BSE image of a Eu-implanted GaN sample after annealing at 1200 ºC; b) the corresponding N-compositional mapping obtained with WDX and c) CL mapping of the integrated intensity from the $^5D_0$-$^7F_2$ transition corresponding to the same area showing decreased N-content and CL intensity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

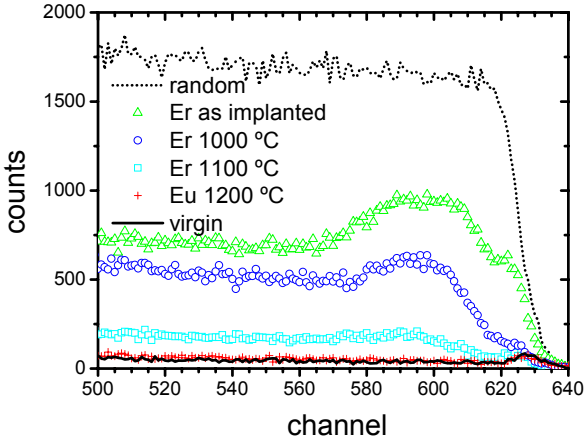

Figure 2: Typical random and <0001> aligned RBS spectra of Er and Eu implanted GaN after annealing at different temperatures.

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

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

Transparent thin film transistors based on indium oxide semiconductor

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

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

[1] Dep. de Ciência dos Materiais, FCT-UNL, 2829-516 Caparica, Portugal
[2] LMSCE, Complexo I-IST, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[3] Dep. de Física, IST, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[4] ICEM/Dep. de Física, FC-UL, 1749-016 Lisboa, Portugal

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

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

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

[1] Project POCTI/CTM/60685/2004

Structural, optical and magnetic properties of ion implanted ZnO

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

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

[1] Departamento de Física, Universidade de Aveiro
[2] Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, Portugal
[3] Departamento de Física, Universidade do Porto
[4] Department of Physics, University of Jena

Structural and Magnetic properties of oxides implanted with transition metals

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

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

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

Characterization of potash-glass corrosion in aqueous solution

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

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

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

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

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

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

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

Microstructural Studies of PZT Thick Films Directly Deposited on Cu Foils

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

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

[1] Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, Portugal
[2] Materials Research Center, North Carolina State University, Raleigh, USA
[3] Department of Engineering Materials, University of Sheffield, Sheffield S1 3JD, England, UK

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

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

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

[1] Faculdade de Ciências da Universidade de Lisboa, Dep. de Física
[2] Department of Physics, University of Warwick, Coventry

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

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

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

[1] Departamento de Física, Universidade de Aveiro
[2] Faculdade de Ciências da Universidade de Lisboa, Dep. de Física
[3] Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Damage behaviour of multilayer structures

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

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

[1] Departamento de Física, Universidade de Aveiro

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

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

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

[1] Institute of Physics Polish Academy of Sciences, 32/46 Lotników Al., 02-668 Warszawa, Poland
[2] Center for Mat. Processing, Univ. of Tennessee, Knoxville, TN 37996-2350, USA.

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

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

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

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

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

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

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

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

Optical doping of AlN by Er implantation

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

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

[1] Departamento de Física, Universidade de Aveiro

Advanced magnetic systems for devices

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

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

[1] INESC-MN, R.Alves Redol 9-1, 1000 Lisboa, Portugal.

Thermophotovoltaic materials based on GaSb

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

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

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

Advanced data analysis for IBA

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

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

[1] University of Surrey Ion Beam Centre, Guildford GU2 7XH, England.
[2] Universidad Autónoma de Madrid, Madrid, Spain.
[3] Instituto Superior de Engenharia do Porto, R António Bernardino de Almeida 431, 4200 Porto.

Characterisation of advanced materials for Nuclear Fusion reactors

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

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

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

Development and applications of ionoluminescence to study optical active defects and impurities in materials

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

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

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

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

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

[1] Departamento de Tecnología Electrónica, ETSI de Telecomunicación, Universidad Politécnica de Madrid
[2] Departamento de Física de la Materia Condensada, ETSI Industriales, Universidad de Valladolid, Spain
[3] Departamento de Física, E.P.S., Universidad Carlos III de Madrid
[4] Centro de Física Nuclear da Universidade de Lisboa