# Unit of Physics and Accelerators

# **MISSION**

- R&D of advanced materials, processes and technologies for applications to Industry, Biomedicine, Environment and Cultural Heritage using radiation techniques, in particular ion beam and ionizing radiation based techniques (gamma rays and electrons);
- Maintain and upgrade the technical infrastructures and equipment and the associated techniques and make them available to the community, through collaborations and services;
- Disseminate knowledge and know-how and promote advanced learning in the specific areas of expertise;
- Offer specialized services and consultancy, mainly targeted to solve particular needs and analytical problems;
- Development of equipment using ionizing radiation for industry and research;
- Technical assistance to the industry.

# **MAIN ACHIEVEMENTS**

- A new integrated pin-diode pre-amplifier particle detection system and the upgrade of the external ion beam line.
- Structural, compositional and optical studies of wide bandgap ternary compounds such as AlInN, MgZnO and CdZnO. (Fig. 1).
- Ion Beam analysis of new Be and divertor marker tiles as well as reciprocating probes for the Be transport experiment, before and after exposure in JET(Fig. 2).



**Fig. 2:** SE image showing microstructures observed in W-10Ta<sub>p</sub> implanted with He<sup>+</sup> and D<sup>+</sup> ions.



**Fig.1:** XRD reciprocal space map around the  $10\overline{1}5$  reciprocal lattice point of a Cd<sub>x</sub>Zn<sub>1-x</sub>O film (x=0.12) grown on MgZnO. Photographs of the visible light emission of Cd<sub>x</sub>Zn<sub>1-x</sub>O films with different CdO molar fractions.

• The study of Silver objects from different collections - "Vidigueira Treasure" from Museu Nacional de Arte Antiga and gold earrings belonging to the "Pancas Treasure", from Museu Nacional de Arqueologia - were studied to identify and quantify the major, minor and trace elements (Fig. 3).



**Fig. 3:** Left: optical photography: detail of a stain in a gold coin minted in 2011; Right: Distribution of low Z elements (Cl, K, Na) responsible for the visible stain. ( $530x530 \ \mu m2$ ).

• Three Ph.D. students started research on rare earth doping of AlxGa1-xN alloys, fuel retention on first wall materials and Al influence on the electrical and optical properties in GaInSb crystals.



**Fig. 4:**  $\beta$ - emission channeling patterns obtained from the decay of <sup>11</sup>Be implanted into a GaN single crystal. x,y axes represent angular degrees with respect to the principal directions of the crystal.

- Emission Channelling experiments with Short-Lived radioactive Isotopes (EC-SLI) at the ISOLDE GHM beamline. Emission First ever EC-SLI experiments with the short-lived <sup>11</sup>Be (14 s) isotope in GaN. (Fig. 4)
- Perturbed angular correlations to study  $^{111m}Cd/^{111}Cd$ ( $t_{1/2}$ =48 min),  $^{117}Cd/^{117}In(2.5 h)$  and  $^{111}In/^{111}Cd$ (2.8 d) in single crystals and nanowires of Ga<sub>2</sub>O<sub>3</sub>.
- Polynomial models for ionization cross-sections by proton and alpha particle impact were established for all three inner shells of atomic systems (Fig. 5).



**Fig. 5:** Comparative graph for cross-sections of K, L and M sub-shells by impact of protons in gadolinium.

• Participation in the SPIRIT project - high energy spectral mapping obtained by irradiating an agate sample with a 3.8 MeV proton beam from the Tandetron accelerator, (Fig. 6).



Fig. 6: Mapping of an agate sample using the X-Y system installed in 2011 (full operation in 2012).

- In coronary artery disease, specific markers of the inflammatory, oxidative and apoptosis processes were associated with the atherosclerotic plaque burden and its biological composition.
- In hemochromatosis patients the iron concentration in skin, reflect liver iron overload. (Fig. 7).
- The toxicity of TiO2 nanoparticles (TiO2-NP) was assessed using Daphnia magna as a model. (Fig. 9).



**Fig. 8:** Ti and Fe deposits in *Lemna fronds* (transversal section).



**Fig. 7:** Nuclear Microscopy image of human skin. Fe deposits in extracellular space around keratinocytes.

• Toxicity of nanoparticles - The elemental profiles and concentration gradients were determined in benthic organisms. Cellular and tissue wall uptake of Ti, Mn, Fe and Zn were inferred. (Fig. 8).



**Fig. 9:** *Daphnia magna* exposure to  $TiO_2$  nanoparticles: mass density image of the egg pouch delimited by the carapacae (ca) and Ti deposits in eggs (eg).

• Hybrid materials microstructure was shown to be dependent on the polymer molecular weight (Fig. 10).



Fig. 10: From Left to right: SEM micrographs of hybrids prepared with increasing PDMS molecular weight. SANS spectra from the same samples.

• New hybrid materials were prepared by gamma irradiation with addition of Ca to promote bioactivity (Fig. 11).



Fig. 11: Samples of the system PDMS-TEOS\_PrZr prepared with addition of Calcium in different solutions.

- PVA supported catalytic membranes for biodiesel production were prepared by gamma irradiation and characterized. These showed better mechanical strength than similar composition ones prepared by traditional techniques (Fig. 12).
- The irradiation effects on small fruits were evaluated as well as the potential extension of shelf-life, to improve the safety and enlarge the variety of immune-compromised patient's diet. (Fig. 13).



**Fig. 13:** Gamma irradiated sweet cherries at 5 kGy for conservation treatment assessment.



**Fig. 14:** Murine norovirus (MNV) before and after irradiation in order to measure virus infectivity response to  $\gamma$  radiation on a dried surface biofilm.



Fig. 15: Antioxidant activity vs absorbed dose.

- Developments in Nuclear Instruments and Methods including:
- modelling of radiation fields and equipment design;
- determination of nuclear data participation on n\_TOF Experiment (phase 2) at CERN;
- development and application of plasma at atmospheric pressure for scientific and industrial;
- purposes electron kinetics in He/CH<sub>4</sub>/CO<sub>2</sub> mixtures used for methane reforming in plasmas (Fig. 16).
- development of software for control and data analysis;



**Fig. 17:** RADX 100: light weight personal radiation dosemeter.



Fig. 12: SEM images of PVA supported catalytic membranes prepared with  $\gamma$ -radiation doses: a) and b) SA-5 kGy; c) SA-13 kGy; d) and e) AA-5 kGy; f) AA-13kGy.

- Work to generate data on the ionizing radiation inactivation patterns of human virus a surrogate of human norovirus the Murine norovirus in environmental matrices. (Fig. 14).
- A study of the effects of gamma radiation on real cork cooking wastewater (Fig. 15).
- Several services were performed. Namely the evaluation of the indoor concentration of airborne bacteria and fungi in several public buildings and the test of the activity of antibiotics in vitro by microbiological assay methods.



**Fig. 16:** Fraction of the energy lost by electrons in collisions spent on methane dissociation, as a function of the reduced electric field.  $He/CH_4/CO_2$  mixtures with ratios Mix1: (2:4:4), Mix2: (6:2:2); In: pure mixtures; Out: mixtures with 50% conversion for CH<sub>4</sub> and CO<sub>2</sub>.

- design of electronic instrumentation for nuclear applications; specialized services (consulting, training and technical assistance);
- marketing of Nuclear Instrumentation made in ITN (Fig. 17).

# **Groups – R&D Activities** Advanced Materials Research Group

#### TEAM

Name	Position	R&D	
Eduardo Alves	Principal Researcher	75%	
Rui Silva	Principal Researcher	100%	
Carlos Cruz	Auxiliary Researcher	80%	
Luís Alves	Auxiliary Researcher	70%	
Katharina Lorenz	Auxiliary Researcher (Ciência)	85%	
Victoria Corregidor	Auxiliary Researcher (Ciência)	100%	
Vanya Darakchieva	Auxiliary Researcher (Ciência)	10% (on leave)*	
Nuno Franco	PostDoc	100%	
Andrés Redondo-Cubero	PostDoc	100%	
Ana Cláudia	PostDoc	100%	
Marta Dias	PostDoc	100%	
Rui Martins	PostDoc	50%	
Nebiha ben Sedrine	PostDoc	50%	
Sérgio Magalhães	PhD	100%	
Maria Isabel Fialho	PhD	100%	
Norberto Catarino	PhD	100%	
Morgana Streicher	PhD	100% (start May)	
Bruno Nunes	PhD	30%	
Ângelo Costa	BI	100%	
Sérgio Miranda	BI	100% (end May)	
Chamseddine Bouhafs	BI	100% (end May)	
Jorge Rocha	TS	100%	
Filomena Baptista	ТР	100%	
* Linköning University, Sweden			

# **OBJECTIVES**

In 2012 the group explored and kept developing and applying the ion beam techniques to the study of advanced materials with high technological impact, especially in the fields of materials for fusion, wide band gap semiconductors and nanostructures for functional materials and cultural artefacts in collaboration with a long list of other groups. The objectives were as summarised below.

- 1. Supervise and operate the Ion Beam and X-ray Laboratories (IBL) guarantying the full operational status and constant upgrade of the equipment.
- 2. Research and development of ion beams based techniques to process and characterise wide band gap materials, II-VI and III-V semiconductors, superlattices and nanostructures.
- 3. Participation in the technology programme of the European Fusion Development Agreement in association with IPFN (Instituto de Plasmas e Fusão Nuclear) using ion beam techniques to study plasma surface interaction processes as well as <sup>2</sup>H retention in JET tiles. Studies of <sup>2</sup>H retention on W-based compounds and characterization of irradiated Be intermetallics and pebbles was also performed.
- 4. Promote and make available to external users the ion beam techniques to study functional materials, archaeological and cultural heritage artefacts.
  - Promote national and international collaborations and networks and apply for competitive funding programmes and projects.
  - Training and Education continued as a major commitment of the group through the supervision of M.Sc. and Ph.D. thesis and *Ciência Viva* program.

#### **MAJOR ACHIEVEMENTS**

- 1. A new integrated pin-diode pre-amplifier particle detection system and the upgrade of the external beam line were successfully accomplished namely:
  - *i*) Design a hybrid triple channel charge-sensitive low-noise preamplifier based on Hamamatsu H4083 circuit for Si PIN photodiodes detectors. Energy resolution obtained at 5.486 MeV of the <sup>241</sup>Am peak

improved from 34 keV to 24 keV. The charge gain is 0.5 V/pC, which is equivalent to 22 mV/MeV(Si). To achieve the lower noise the design of the circuit was done using high speed layout rules;

- *ii*) Execution, installation and successful operational tests of specially designed precision positioning target holder for ion beam based micro-tomography in the nuclear microprobe. The rotation stage is motorised, and steered under computer control;
- *iii*) Successful assembly and operational tests of the hardware and software for data acquisition in the analytical multi-technique IBA end-station attached to the tandem accelerator, which allows immediate data acquisition with 3 simultaneous detection channels.
- 2. Structural, compositional and optical studies of wide bandgap ternary compounds such as AlInN, MgZnO and CdZnO were performed combining ion beam analysis, X-ray techniques and photoluminescence. Major results obtained by X-ray diffraction reciprocal space maps and ion channelling reveal the composition and strain state of thin CdZnO films grown on a MgZnO buffer layers and a clear dependency of the light emission wavelength on the CdO molar fraction, *x*, is observed, figure 1.

Advances have been made in the doping by ion implantation of wide bandgap structures including non-polar a-plane GaN which shows lower implantation damage levels than conventional c-plane GaN, the rare earth doping of AlGaN alloys revealing a dependence of the rare earth incorporation site on the AlN content of the host matrix, as well as the influence of co-doping with several rare earth ions or with electrical dopants.

Finally it was shown that upon ion implantation of GaN/AlN superlattices quantum dots exhibit stronger intermixing than quantum wells under similar growth and processing conditions.



**Fig. 1:** XRD reciprocal space map around the 10<sup>1</sup> 5 reciprocal lattice point of a  $Cd_xZn_{1-x}O$  film (x=0.12) grown on MgZnO. Photographic images of the visible light emission of  $Cd_xZn_{1-x}O$  films with different CdO molar fractions x.

3. Ion Beam analysis of new Be and divertor marker tiles as well as reciprocating probes for the Be transport experiment, before and after exposure in JET was performed allowing detailed composition profiling and complete description of the tiles before exposition. Also related with JET activities the analysis and modelling of erosion and transport processes in the plasma were performed through the measurement of select tiles removed during the 2009-2010 shutdown.

New W-Ta composites produced via mechanical alloying and spark plasma sintering using pure W powder and Ta fibre (W-Ta fibre composites) for first wall materials, were implanted with He+ and D+ ion beams at different fluencies and compared with pure W and Ta plates. The results indicate that deuterium retention induces microstructural modifications leading to blistering in Ta plates and in the Ta rich regions of the W-Ta composites, presenting the TaO phase, figure 2. Additionally the results show that the D retention is higher for W than for Ta and similar for all the composites. Finally evidence was found that D retention is associated with the He enrichment in the irradiated surfaces and that D trapping in the composites is dependent on the structural type (fibres or powder).



Fig. 2: SE image showing microstructures observed in  $W-10Ta_p$  implanted with He<sup>+</sup> and D<sup>+</sup> ions.

4. Silver objects from different collections, the "Vidigueira Treasure" from Museu Nacional de Arte Antiga and gold earrings belonging to the "Pancas Treasure", from Museu Nacional de Arqueologia were studied to identify and quantify the major, minor and trace elements.

Considering the earrings of the Pancas Treasure, dated between the 5th and the 3rd centuries BC, determining the composition allowed establishing pairs of earrings, and correlating the different alloy compositions within the Pancas group to compositions of objects from the south of the Iberian Peninsula, representative of the period of oriental influence.

Also concerning studies of provenance and production techniques the composition of XVIIc. tiles (Monastery of Sta. Clara-a-Velha), and glasses (Lisbon Roman Theatre) were analysed. The results indicate recourse to glass frit as raw material for the glazes, and usage of mineral oxides of Sn, Co, Cu, Fe and Mn as colour agents for white, blue, green, yellow and purple respectively.

Finally we continued the work developed over the last year aiming at creating a composition database for coins (in order to find representative composition for each coin according with the date and place where the coins were minted), figure 3.



**Fig. 3:** Left: optical photography: detail of a stain in a gold coin minted in 2011; Right: Distribution of low Z elements (Cl, K, Na) responsible for the visible stain. (530x530 µm2).

5. Three new Ph.D. students started the research projects on rare earth doping of Al<sub>x</sub>Ga<sub>1-x</sub>N alloys, fuel retention on first wall materials and Al influence on the electrical and optical properties in GaInSb crystals.

# **RELEVANT PAPERS**

- A. Redondo-Cubero, A. Hierro, J.-M. Chauveau, K. Lorenz, G. Tabares, N. Franco, E. Alves and E. Muñoz, "Single phase a-plane MgZnO epilayers for UV optoelectronics: substitutional behaviour of Mg at large contents", *Cryst. Eng. Comm.*, 14 1637-1640, (2012), doi: 10.1039/c2ce06315h.
- N. Catarino, E. Nogales, N. Franco, V. Darakchieva, S. M. C. Miranda, B. Méndez, E. Alves, J. G. Marques, K. Lorenz, "Enhanced dynamic annealing and optical activation of Eu implanted a-plane GaN", *Europhysics Lett.* 97, 68004 (2012), doi: 10.1209/0295-5075/97/68004.

- M. Fialho, S. Magalhães, L.C. Alves, C. Marques, R. Maalej, T. Monteiro, K. Lorenz, E. Alves, "AIN content influence on the properties of AlxGa1–xN doped with Pr ions", *Nuclear Instruments and Methods in Physics Research B* 273, 149-152, (2012), doi:10.1016/j.nimb.2011.07.062.
- R. Mateus, M. Dias, J. Lopes, J. Rocha, N. Catarino, P. Duarte, R.B. Gomes, C. Silva, H. Fernandes, V. Livramento, P.A. Carvalho, E. Alves, K. Hanada, J.B. Correia, Blistering of W-Ta composites at different irradiation energies, *Journal of Nuclear Materials*, http://dx.doi.org/10.1016/j.jnucmat.2013.01.225
- V. Corregidor, L.C. Alves, J. Cruz, "Analysis of surface stains on modern gold coins", Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, doi: 10.1016/j.nimb.2012.11.039.

### **FUNDS**

Project/Service Name	Reference	Starting date	2012
SPIRIT (4098)	227012	2009	58.643,91€
InN (4099)	PTDC/FIS/100448/2008	2009	38.207,92€
Nanomod (4100)	PTDC/CTM/100756/2008	2009	107.139,51 €
DIFUSION (4102)	PTDC/CTM/100163/2008	2009	331,55€
Tomo3D (4103)	PTDC/FIS/115089/2009	2010	9.245,98€
NanoMag (4107)	PTDC/FIS/102270/2008	2009	7.169,73€
GRICES (4155)	Convene DAAD Germany	2011	2.000,00€
WSPIRIT2012 (4175)	Conference SPIRIT	2012	800,00€
MARE (RD0172)	PTDC/FIS/116719/2010	2011	1.080,00€
DIVERSOS	Old Projects	2012	20.268,22€
		Total	244.886.82 €

# **INTERNATIONALIZATION**

- SPRITE-Supporting Postgraduate Research with Internships in industry and Training Excellence, FP7-PEOPLE-2012-ITN, *Grant agreement no: 317169*.
- Autónoma University of Madrid, Spain: Characterization of metal contacts on CdZnTe for detector applications.
- Consorzio CREO, Italy: Influence of growth parameters on CdTe nanostructures for solar cell applications.
- CAPES, Brazil: Al influence on the electrical and optical properties of GaInSb crystals grown by Czochralski method.
- Culham Center of Fusion Energy (CCFE), UK: Analysis of marker tiles from JET.
- University of Tennessee, USA: PhD project: Defects in sapphire implanted with Zr and O ions.
- Wayne State University, USA: Study of new multifunctional structures incorporating oxides (VOx and ZnO) for development of new batteries.
- Polish Academy of sciences, Institute of Physics, Poland: Ion beam studies of ZnMgO/ZnO bilayers grown by MBE.
- University of Jena, Germany: Ion beam modification of novel III-nitride hetero- and nano-structures.
- University of Bonn, Germany: PAC experiments in III-N compounds.
- University of Strathclyde, U.K.: Quantum well intermixing in InGaN/GaN quantum wells.
- CEA Grenoble, France: Rare Earth doping of GaN nanowires.
- University of Caen, France: Implantation damage formation in AlN.
- University of Cadiz, Spain: TEM analysis of implanted III-nitride superlattices.
- University Complutense of Madrid, Spain: Rare Earth doping of oxide nanowires and crystals.
- Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland: High pressure high temperature annealing of III-nitrides.

- Humboldt University of Berlin, Germany: Growth of ZnCdO thin films.
- KAUST University, Saudi Arabia: Characterisation of InGaN thin films.
- National Institute for Materials Science, Tsukuba, Japan: Growth of Ga<sub>2</sub>O<sub>3</sub> bulk crystals.
- Instituto de Ciencia de Materiales de Madrid (CSIC), Madrid, Spain: Nanopattern formation in semiconductor surfaces.
- Instituto de Sistemas Optoelectrónicos y Microtecnología, Polytechnic University of Madrid, Spain: Characterization of emerging oxide-based materials for UV photonics.

# **Nuclear Methods and Instrumentation Group**

# TEAM

Name	Category	R&D
Isabel Gonçalves	Auxiliary Researcher	100%
João Manteigas	Auxiliary Researcher	100%
José Neves	Auxiliary Researcher	100%
Nuno Pinhão	Auxiliary Researcher	100%
Nuno Inácio	Graduated Technician	30%
Tiago Jesus	Assistant Technician	20%
André Janeco	PhD Student IST	100%
Carlos Carrapiço	PhD Student IST	100%
Raúl Sarmento	PhD Student IST	100%

# **OBJECTIVES**

The strategy of the group involves activities in the following lines: modelling of radiation fields, calculation of neutron physic parameters, measurement of neutron cross-sections, modelling and applications of gas discharges, design of equipment and software for nuclear applications and data analysis, consulting and technical assistance.

#### Modelling of radiation fields, calculation of neutron physic parameters

Monte Carlo calculations have been carried in the framework of the n\_TOF Collaboration (ITN participation on the n\_TOF-Ph2 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 and application of gas discharges

The study of methane conversion using non-thermal plasmas has continued with the study of (a) the electron kinetics in CH4/CO2/He mixtures, (b) the contribution of the vibrational population and multi-step processes, and (c) the impact of dissociation products (CO, H2 and O2). Electric diagnostics were developed to measure the applied power in a RF-plasma needle for plasma medicine and surface treatment applications. A code to solve the Boltzmann equation for an electron swarm in a gas was extended. The code computes the electron velocity distribution function, transport parameters, rate coefficients for the electron-collision reactions and the power losses.

#### Instrumentation and technical assistance

The main objectives are the development of equipment for CTN Groups, manufacture of equipment for specific applications and assistance to industrial companies and scientific institutions as well as technical consulting. The technical assistance takes mainly the form of specialised consultant engineering advice, installation of nuclear gauges, including calibration maintenance, repair and recharging of gauges with imported radioactive sources. The group has started providing maintenance and repairing services of HPGe detectors.

# MAIN ACHIEVEMENTS

#### Participation on n\_TOF Experiment (phase 2) at CERN

Since 2002, the team has been actively participating in the data taking campaigns conducted by the n-TOF Collaboration and in the experimental activities at the TOF Spectrometer at CERN, such as the measurements of neutron cross sections for several applications like ADS systems and EA (Energy Amplifier) for transmutation of radioactive waste, energy and radioisotopes production, medical and industrial applications.

#### Electron kinetics He/CH4/CO2 mixtures used for methane reforming in plasmas

The use of non-thermal plasma for the direct conversation of methane into Syngas and other hydrocarbons has been a subject of research in the last years. A key element to understand the complex chemistry in these plasmas and the viability of this route is the study of the electron kinetics. The electron kinetics was studied as a function of the electric field, helium concretion and vibrational temperature. The results provide important information for optimization of the discharge.



**Fig.:** Fraction of the energy lost by electrons in collisions spent on methane dissociation, as a function of the reduced electric field. He/CH4/CO2 mixtures with ratios Mix1: (2:4:4), Mix2: (6:2:2); In: pure mixtures; Out: mixtures with 50% conversion for CH4 and CO2.

#### Development of atmospheric non-thermal plasma sources for applications in plasma medicine

Plasma medicine is an innovative and emerging field combining plasma physics, life sciences and clinical medicine using plasmas for therapeutic applications. A plasma needle is under development. The results include the project of electric diagnostic transducers for the characterization of the power transmitted to the plasma and automation of gas flow.

#### A Bolzmann code for electron swarms in polyatomic gases

The Density Gradients Approximation (DGA) to describe the electron velocity distribution in gases is a highly accurate method that overcomes the limitations of the common two-term approximation. However this method is seldom used due to the complexity of his implementation and the free availability of codes based on the latter method. A code based on DGA was extended to include the treatment of polyatomic gases and will be made available as open source.

#### Consulting, design and technical assistance

The main purposes of the project were accomplished. By request from internal groups and external customers, several electronic equipment and prototypes were designed (or upgraded) and manufactured. Additionally, substantial work related to technical maintenance, calibration and quality control of different nuclear instruments and equipment was carried out. A considerable number of consulting services in the field of engineering of radiation was provided too.

In 2012, the project achieved a total income of about € 39.739, an increase of about 90% from last year, both from Portuguese (Portucel, Soporcel, Repsol Polímeros, Cimpor and Siderurgia Nacional, etc.) and foreign clients (Kuwait, Pakistan, Sri Lanka, Angola and Ireland).

The group's activities proved conducive to patenting and in 2012 the following was granted:

Processo de Conversão de metano e um oxidante em gás de síntese e hidrocarbonetos utilizando um plasma não-térmico e o auxílio de um gás raro, N.Pinhão, A. Janeco, J. Branco, national patent nº 105078, BPI, 31 Dec. 2012.

In 2012 several projects were submitted to FCT calls. Two of these projects were approved with endowment of the total required financial resources:

- "Increasing the energy efficiency of plasma conversion of methane", PTDC/FIS-PLA/2135/2012, Total Funding: € 102.716 (2013/2014). Coordination.
- "Application of ionizing radiation for a sustained environment" (ARIAS), RECI/AAG-TEC/0400/2012, Total Funding: € 499.469 (2013/2014). Co-participation of almost all of the team members.

### **RELEVANT PAPERS**

- C.Carrapiço et al. (n\_TOF collaboration), Neutron induced capture and fission discrimination using calorimetric shape decomposition, *Nuclear Instruments and Methods A*, **704** (2012), doi: 10.1016/j.nima.
- C.Guerrero et al. (n\_TOF collaboration) Monte Carlo simulations of the n\_TOF Total Absorption Calorimeter, *Nuclear Instruments and Methods A*, 671 (2012).
- C.Massimi et al. (n\_TOF collaboration), Resonance neutron-capture cross sections of stable magnesium isotopes and their astrophysical implications, *Physical Review C*, **85**, 044615 (2012), doi: 10.1103/PhysRevC.85.044615.
- F.Gunsing et al. (the n\_TOF collaboration), Measurement of resolved resonances of 232Th(n,g) at the n-TOF facility at CERN, *Physical Review C*, **85**, 064601 (2012).
- M.Calviani et al. (n\_TOF collaboration), Neutron-induced fission cross section of 245Cm: New results from data taken at the time-of-flight facility n\_TOF, *Physical Review C*, 85, 034616 (2012), doi:10.1103/PhysRevC.85.034616.

#### **FUNDS**

Project/Service	Reference	Timeframe	2012
CERN n_TOF ph2 (4th year)	CERN/FP/109314/2009	Jan2010-Dec2010	11.917,64€
CERN n_TOF Experiments (phase 2)	CERN/FP/123602/2011	Apr2012-Mar2014	9.000,00€
ANDES (Accurate Nuclear data for	PGA 249671	May2010-Apr2013	12.000,00€
Nuclear Energy Sustainability)			
Services	ITN/CR4402+IST/CR4064	Sales 2012	28.879,25 €
		Total	61.796,89 €

# **INTERNACIONALIZATION**

- CIEMAT, Spain.
- Comenius Univ., Dept. of Experimental Physics, Bratislava, Slovakia.
- Leibniz Institute for Plasma Science and Technology, Greifswald, Germany.
- n\_TOF collaboration, a consortium of several laboratories in Europe, USA and Japan.
- Research Institute for Solid State Physics and Optics, Budapest, Hungary.

# **Ionizing Radiation Technologies Group**

# TEAM

Name	Category	R&D
Fernanda Margaça	Principal Researcher	100%
Luís Ferreira	Auxiliary Researcher	100%
Sandra Cabo Verde	Auxiliary Researcher (Ciência)	100%
Helena Marcos	Informatics Technician	100%
Pedro Santos	Post-Doc Grantee	100%
Rita Melo Galvão	Post-Doc Grantee	100%
Amílcar António	Ph.D. Student	30%
Joana Lancastre	MSc Grantee	100%
Telma Silva	MSc Grantee	100%
Marina Oliveira	MSc Student	60%
Célia Lima	MSc Student	70%

# **OBJECTIVES**

The application of Radiation Technology with quality, safety and environmental sustainability, in the framework of the on-going funded projects and/or services requested. Namely for:

1. The development of new materials, both polymeric catalytically active and hybrid prepared from mixtures of polymer and metallic alkoxides, for a wide range of applications.

R&D is carried out in hybrid materials for biomedical applications and in polymeric materials catalytically active for biodiesel production by methanolysis of used oils.

#### 2. Ionization radiation treatment of fruits and vegetables for immuno-compromised patients.

Under the scope of the IAEA Coordinate Research Project CRP D6-RC-1163.2 "Development of Irradiated Foods for Immuno-compromised Patients and Other Potential Target Groups" work is in progress to evaluate the irradiation effects on small fruits and the potential extension of shelf-life, in order to improve the safety and enlarge the variety of immune-compromised patient diet.

3. Survival and Inactivation Patterns of Viral Threat Agents in the Environment: Assessment of Ionizing Radiation as Decontamination Tool.

Environmental virology is an emergent field due to the importance of food- and water-transmitted viruses. Ionizing radiation is being used more frequently as a means of disinfection to eliminate viruses.

- 4. Application of Ionizing Radiation on the Cork Wastewater Treatment
- 5. Kinetic Study of Biorecalcitrant Compounds Degradation by Pulse Radiolysis

Pulse radiolysis is a technique to study the mechanistic details of the degradation of biorecalcitrant compounds present in industrial and municipal discharges (*e.g.* pharmaceuticals), induced by free radicals formed upon radiolysis of aerated water. To implement this technique a project is in progress to adapt the existing LINAC.

- 6. Characterization and conservation of cultural heritage: ionizing radiation in artwork.
- 7. Services requested by national industries.

# **MAIN ACHIEVEMENTS**

- 1. R&D in hybrid materials progressed as to a) the dependence of the microstructure on the polymer molecular weight studied in the system PDMS TEOS PrZr; b) the influence of the PrZr content in the porosity and size of the oxide regions present in the materials prepared with fixed polymer weight; c) the preparation of hybrid materials with addition of Calcium, adding Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> solid compound or in solution.
- 2. Polymeric catalytically active materials were prepared by synthesis under gamma irradiation and PVA supported catalytic membranes for biodiesel production was characterized. These are effective catalysts in the esterification reaction of lauric acid to methyl laureate but the catalytic activity depends on the crosslinking agent and the radiation dose. Best catalytic results were obtained with PVA-Succinic acid membranes. The increase of dose from 5 to 13 kGy led to a slight increase of catalytic activity. Prepared

PVA membranes showed better mechanical strength than similar composition ones prepared by traditional techniques.

- 3. Food irradiation is a food safety tool. The irradiation effects on small fruits were evaluated as well as the potential extension of shelf-life, to improve the safety and enlarge the variety of immune-compromised patients diet. Fresh cherries and blackberries were irradiated at sub-lethal several doses (<1.5 kGy). The results showed a limited microbial inactivation for those doses, due to the preponderance of fungi as natural contaminants of these produces. The effect of higher irradiation doses on fruits will be investigated.
- 4. Environmental virology is an emergent field due to the importance of food- and water-transmitted viruses. Ionizing radiation is used as an effective means of disinfection. However, investigation of gamma irradiation to eliminate viruses is limited. Work was performed to generate data on the ionizing radiation inactivation patterns of human virus in environmental matrices. A surrogate of human norovirus (do not grow on cell culture), the Murine norovirus (MNV) was propagated using RAW 264.7 and the viral stock yield was estimated by plaque assay, that is the gold-standard method to measure virus infectivity. In the applied conditions the MNV presented exponential inactivation kinetics and a D-value of 3.7 kGy. Ongoing inactivation studies are in progress with the virus in suspension.
- 5. A study of the effects of gamma radiation on real cork cooking wastewater was performed. The effects were assessed by the antioxidant activity rate, the phenolic compounds concentration and organic matter content. It was found that gamma radiation increases antioxidant activity of cork cooking water, the amount of phenolic compounds and, at the same time, decreases the oxidizable organic matter. This is very important as the treatment increases the added-value compounds (antioxidants) in the wastewater while decreasing other organic matter leading to a valuable solution as a raw material for other industries. A PhD and a MSc thesis were concluded.
- 6. The pulse radiolysis is a powerful technique to study the mechanistic details of the degradation of biorecalcitrant compounds present in industrial (*e.g.* phenolic acids) and municipal discharges (*e.g.* pharmaceuticals), induced by free radicals formed upon radiolysis of aerated water (hydroxyl radical, hydrogen atom, superoxide anion radical and hydrated electron). To implement this technique a project is in progress to adapt the existing IST/ITN LINAC. Details were discussed with Dr Z. Zimeck , an expert of IAEA and the most suitable technical option was chosen.
- 7. Art biodeterioration asks for new approaches in restoration, preservation, conservation and decontamination areas. Under RADIART project the green deterioration marks present in the ceramic tiles of the panel "The Great View of Lisbon" was analysed. The results showed the absence of microbial colonization. A new sampling to the ceramic tile panel was made to evaluate the persistence of the microbial population. The results indicate that the superficial contamination could be related with the environmental conditions.



Fig. 1: Detail of the green deterioration marks present in the ceramic tiles from the panel "The Great View of Lisbon".

- 8. There is a growing interest in indoor air quality for a better quality environment both at home and at work as many people spend at least 80% of their time indoors. The aim of the service requested by EFACEC is to evaluate the indoor concentration of airborne bacteria and fungi in several public buildings. The concentrations were determined by impaction using the MAS-100 portable air sampler and microbial culture media.
- 9. The activity of antibiotics could be tested in vitro by microbiological assay methods. Based on a previous methodological validation done in 2010 to implement the method in the Quality Control system of Iberfar, the industry requested the determination of the potency of Neomycin Sulfate for a batch of the Nodryl product using the microbiological agar diffusion assay for inter-comparison purposes.

# **RELEVANT PAPERS**

- Rita Lourenço Paiva de Melo Galvão, PhD Thesis, *Application of Ionizing Radiation to Persistent Organic Pollutants Decomposition*, Faculdade de Ciências, Universidade de Lisboa, 14 Dec. 2012
- Lancastre J.J.H., Fernandes N., Margaça F.M.A., Miranda Salvado I.M., Ferreira L.M., Falcão A.N., Casimiro M.H., Study of PDMS conformation in PDMS-based hybrid materials prepared by gamma irradiation, *Radiation Physics and Chemistry*, 81, 1336-1340 (2012), doi:10.1016/j.radphyschem.2012.02.016.
- Nunes, N. Mesquita, S. Cabo Verde, M. J. Trigo, A. Ferreira, M. M. Carolino, A. Portugal, M. L. Botelho, Gamma radiation effects on physical properties of parchment documents: Assessment of Dmax, *Radiation*. *Physics and Chemistry*, 81, 1943-1946, (2012).
- Madureira J.; Melo R., Botelho M.L., Leal J.P., Fonseca I.M. (2012) Effect of ionizing radiation on antioxidant compounds present in cork wastewater, *Water Sci. Technol.*, 67(2):374-9 (2012).
- M.H. Casimiro, A.G. Silva, J.V. Pinto, A.M. Ramos, J. Vital, L.M. Ferreira, Catalytic poly(vinyl alcohol) functionalized membranes obtained by gamma irradiation, *Radiation Physics and Chemistry*, 81, 1314-1318 (2012), doi:10.1016/j.radphyschem.2012.01.036.

#### **FUNDS**

Project/Service	Reference	Timeframe	2012
Hybrid Materials for Biomedical	PTDC/CTM/101115/2008	2010-2013	14.973,38€
Applications			
Kinetic Study of Biorecalcitrant Compounds	PTDC/QUI-QUI/104229/2008	2010-2013	33.240,04 €
Degradation by Pulse Radiolysis			
Preparation of Polymeric Materials	PTDC/CTM-POL/114579/2009	2011-2014	0,00€
Catalytically Actives on Biodiesel			
Production, by Vegetable Oils Methanolysis			
Ionization radiation treatment of fruits and	IAEA Research Contract N.º 16281	2011-2013	7.000,00€
vegetables for immuno-compromised			
patients – feasibility study			
Survival and Inactivation Patterns of Viral	IAEA Research Contract N.º 17474	2012-2014	5.000,00€
Threat Agents in the Environment:			
Assessment of Ionizing Radiation as			
Decontamination Tool			
Application of Ionizing Radiation on the	IAEA Research Contract N.º 16513	2010-2012	4.500,00€
Cork Wastewater Treatment			
CHESTNUTSRAD - Tratamento Alterna-	Service to	2010 - 2013	2.175,06€
tivo para a Conservação da Castanha	QREN 13198/2010		
Decontamination of Lidocaine and Lactose	Service requested by ATRAL	Feb 2012	*826,91€
Determination of Neomycin Sulfate for	Service requested by IBERFAR	October 2012	246,00€
Nodryl product.			
Microbiological analysis for Indoor Air	Service requested by EFACEC	Nov-Dec 2012	1.931,80€
Quality in the scope of the Energy			
Certification for Buildings.			
Total			69.893,19€

\* This work was performed by the TRI staff but the revenue was incorrectly allocated to the project CR7702.

# **INTERNATIONALIZATION**

- NEUTRON AND MUON FACILITIES NMI3-II Access Program of the EC Scientific visit to Budapest Neutron Centre, Hungary, held in July 22-26, of 2 members of the group (FM, JL), as users of the local neutron source, funded in the framework of the current refereed proposal procedures.
- IAEA TECHNICAL COOPERATION PROJECT RER/8/015, Regional Workshop on use of Nuclear Technology for Cultural Heritage Characterization, Dating and Preservation, "Enhancing the Characterization, Preservation and Protection of Cultural Heritage Artefacts", Belgrade, Serbia, 4-6 September 2012, participation of 1 member of the group (TS).

- IAEA CRP Project no. 1359, 2<sup>nd</sup> Research Coordination Meeting on "Radiation Treatment of Wastewater for Reuse with Particular Focus on Wastewaters Containing Organic Pollutants", Jeongeup, Republic of Korea, 29 October-2 November 2012, participation of 1 member of the group (RM).
- IAEA TC Project RER/0/034 REGIONAL TRAINING COURSE on Radiation Technology for Cultural Heritage Preservation, Sacavém, Portugal, Nov 5-9 (2012) – Responsibility for Themes I (*Determination of Dmin - Inactivation of microorganisms/higienisation/preservation on tiles and cellulosic samples*), II (Determination Dmax - Impact of ionizing in materials measurement of mechanical properties and color on tiles and cellulosic samples) and III (*Routine dosimetry with amber Perspex*) of the Course and for the experimental training sessions of the participants. Several members of the group contributed to this course (LF, TS, SCV, PS, JL, HM).

# **CONTRACTS**

- Microbiological analysis for Indoor Air Quality of Lincon Electric Palmela. Report to EFACEC. December 2012, pp. 1-2.
- Microbiological analysis for Indoor Air Quality of FCP. Report to EFACEC. November 2012, pp. 1-2.
- Microbiological analysis for Indoor Air Quality of Centro Clínico Ambulatório. Report to EFACEC. November 2012, pp. 1-2.
- Microbiological analysis for Indoor Air Quality of SAMS. Report to EFACEC. October 2012, pp. 1-3.

# MATERIALS CHARACTERIZATION WITH NUCLEAR RADIOACTIVE TECHNIQUES GROUP

#### TEAM

Name	Category	R&D
João Guilherme Martins Correia	Principal Researcher	100%
Ulrich Wahl	Principal Researcher with habilitation	90%
Katharina Lorenz	Auxiliary Researcher (Ciência)	15%
Marcelo Baptista Barbosa	BI CERN-FP-116320-2010	100% up to 31-03-2012
Eric Boone	BIC CERN-FP-116320-2010	100% up to 30-04-2012
Enc bosne	BIC CERN-FP-123585-2011	100% from 20-08-2012
Ângelo Costa	BI CERN-FP-123585-2011	100% from 01-11-2012

# **OBJECTIVES**

"Materials Characterization with Nuclear Radioactive Techniques" uses the decay particles emitted by radioactive nuclei to perform electronic, magnetic and lattice site characterization of materials and soft-matter. Radioactive isotopes have nuclear properties which allow overcoming the limitations of stable isotopes / elements since they can be detected and used by a multitude of nuclear techniques, down to ~10E9 lower concentrations than standard non-radioactive techniques. Such applications rely on the production of a large variety of isotopes of different elements with high purity and intensity, available only at international laboratories such as ISOLDE.

SCIENTIFIC OBJECTIVES of this line of research are organized within proposals approved by the INTC (ISOLDE and n-TOF Scientific Committee) in two major lines of research and using the Portuguese experimental infrastructure at ISOLDE: Emission Channeling and Perturbed Angular Correlations, which study the lattice site of radioactive probes and the charge distributions and magnetic fields around them on an atomic scale.

Approved scientific proposals:

- IS453 Emission channeling lattice location experiments with short-lived isotopes. Spokesperson: U. Wahl CTN, Contact Person J. G. Correia CTN (JGC).
- IS481 The role of In in III-nitride ternary semiconductors. Spokesperson: K. Lorenz CTN, Contact person JGC.
- IS487 Study of local correlations in magnetic and multiferroic materials. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.
- IS515 Radioactive probe studies of coordination modes of heavy metal ions from natural waters to functionalized magnetic nanoparticles. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.
- EDUCATIONAL & TRAINING OBJECTIVES are embedded into the execution of the scientific R&D objectives, since our working program is fully oriented at obtaining Diploma, MSc and PhD theses.
- MAINTENANCE and MISSION costs are fully supported by project-based applications.



 $\beta$ - emission channeling patterns obtained from the decay of <sup>11</sup>Be implanted into a GaN single crystal. x,y axes represent angular degrees with respect to the principal directions of the crystal.

# MAIN ACHIEVEMENTS

IS453 - In 2012 we performed Emission Channeling experiments with Short-Lived radioactive Isotopes (EC-SLI) at our on-line setup at the ISOLDE GHM beamline using <sup>27</sup>Mg ( $t_{1/2}$ =9.4 min), <sup>61</sup>Co(1.6 h), <sup>57</sup>Mn(85 s) and <sup>56</sup>Mn(2.6 h) implanted into semiconductors such as GaMnN, GaMnAs, Si, SiC and AlN. <sup>59</sup>Fe (44.5 d) was implanted into p<sup>+</sup>-Si and GaFeN, for experiments to be performed during 2013. We further report on first ever EC-SLI experiments with the short-lived <sup>11</sup>Be(14 s) isotope in GaN. Due to its light mass, the lattice sites of Be as a dopant in semiconductors are not accessible by any other method. These experiments were possible due to the highly pure laser ionized Be beams at ISOLDE and, from our side, due to the R&D improvement of the data acquisition system actually reaching more than 5.5 kHz count rate on a self-triggered 22x22 channel pad detector.

- IS481 Perturbed angular correlations (PAC) have been used to study <sup>111m</sup>Cd/<sup>111</sup>Cd ( $t_{1/2}$ =48 min), <sup>117</sup>Cd/<sup>117</sup>In(2.5 h) and <sup>111</sup>In/<sup>111</sup>Cd (2.8 d) in single crystals and nanowires of the transparent conductive oxide Ga<sub>2</sub>O<sub>3</sub>. Density Functional Theory (DFT) simulations of charge distributions around the Cd probe have reproduced the PAC results, showing that Cd occupies <u>only</u> octahedral Ga-sites, in a defect free environment after high temperature annealing. The feasibility of doping by ion-implantation, creating p-type centres at a reasonable concentration, is under study.
- IS515 (cleaning waters using magnetic nanoparticles) *and* LOI132 (studying graphene interactions and properties with radioactive adatoms) both apply similar procedures of sample preparation, requiring the collection of the radioactive probes on ice, when using <sup>199m</sup>Hg/<sup>199</sup>Hg (42 m). Afterwards the radioactive ice is melted and eventually diluted on specific preparations for further tuning of pH and temperature. Specific liquid preparations carrying the <sup>199m</sup>Hg are then used to wet the magnetic nanoparticles or the graphene surfaces while studying, e.g., catalysis processes. Clear results have shown Hg atoms binding at different sites at the dithiocarbamate vector on magnetic nanoparticles and at the graphene surface, as a function of sample preparation and measurement conditions. To understand the observed phenomena first principle calculations of atomistic models reproducing the experimental data using cluster models and DFT methods are performed.

### **MAIN R&D RESULTS**

- Successful mounting, tests and commissioning of a Small Implantation Chamber for radioactive isotopes (SIC) designed, built and funded by our projects and ISOLDE. This chamber fits on-line at the GHM-GPS area in between the ISOLDE beam line and our EC-SLI setup, being dedicated to collect long-lived isotopes to be measured off-line.
- Successful testing of new fast VATAGP7 Si pad detectors (1 mm thick), to be commissioned during 2013/14. High performance fast readout and improved energy resolution.
- Successful readout debugging and tests of actual VATAGP3 pad on-line detector. Actually we can achieve more than 5.5 kHz and the readout limitation is still the controlling PC.
- Successful mounting, tests and first use in experiments of a small heating element needed for the high precision new Panmure goniometer in use at the EC-SLI setup. We achieved 900°C annealing temperature.
- Successful first use of TIMEPIX detectors for alpha and H particles in emission channelling or RBS/C experiments. The experimental part of this work has been done at CTN and the results have been presented at the November MEDIPIX meeting.

# **RELEVANT PAPERS**

- S. Decoster, U. Wahl, S. Cottenier, J. G. Correia, T. Mendonca, L. M. Amorim, L. M. C. Pereira, and A. Vantomme: "Lattice position and thermal stability of diluted As in Ge", Journal of Applied Physics 111, 053528 (2012). doi: 10.1063/1.3692761.
- L. M. C. Pereira, U. Wahl, J. G. Correia, S. Decoster, L. M. Amorim, M. R. da Silva, and J. P. Araújo, A. Vantomme: "Evidence of N substitution by Mn in GaN", Physical Review B, 86, 195202 (2012). doi: 10.1103/PhysRevB.86.195202.
- L. M. C. Pereira, U. Wahl, S. Decoster, J. G. Correia, L. M. Amorim, M. R. da Silva, J. P. Araujo, A. Vantomme; "Stability and diffusion of interstitial and substitutional Mn in GaAs of different doping types", Physical Review B, 86, 125206 (2012). doi: 10.1103/PhysRevB.86.125206.

- J. N. Gonçalves, A. Stroppa, J. G. Correia, T. Butz, S. Picozzi, A. S. Fenta, V. S. Amaral; "Ab initio study of the relation between electric polarization and electric field gradients in ferroelectrics", Physical Review B, 86, 035145 (2012). doi:10.1103/PhysRevB.86.035145.
- G. N. P. Oliveira, A. M. Pereira, A. M. L. Lopes, J. S. Amaral, A. M. dos Santos, Y. Ren, T. M. Mendonc, C. T. Sousa, V. S. Amaral, J. G. Correia and J. P. Araújo; "Dynamic off-centering of Cr3+ ions and shortrange magneto-electric clusters in CdCr2S4", Physical Review B, 86, 224418 (2012). doi/10.1103/PhysRevB.86.224418.

### **FUNDS**

Project/Service	Reference	Timeframe	2012
Perturbed Angular Correlations and Electron	CERN-FP-109272-2009	from 01-01-2010	18 200 12 €
Channelling Experiments at ISOLDE	CR4244	to 31-12-2010	18.200,12 C
Perturbed Angular Correlations and Electron			
Channelling Experiments at ISOLDE - applied	CERN-FP-116320-2010	from 01-02-2011	05 214 25 E
materials research with nuclear techniques,	CR4251	to 31-05-2012	95.514,25 C
training and development.			
Perturbed Angular Correlations and Electron			
Channelling Experiments at ISOLDE - applied	CERN-FP-123585-2011	from 01-06-2012	36 750 00 €
materials research with nuclear techniques,	RD0187	to 31-05-2014	30,730.00 €
training and development.			
		Total	150.264.37 €

# **INTERNATIONALIZATION**

Strong Internationalization is key to our activities. The production of a wide range of exotic radioisotopes is only possible at large-scale facilities such as CERN/ISOLDE, where during the last 20 years a Portuguese experimental infrastructure for Materials Science with radioactive isotopes has been built, fruit of the collaboration of several Portuguese and foreign universities and institutes. Making use of the beams provided by ISOLDE, this infrastructure allows studying materials with techniques that are not available elsewhere in the world, providing unique information at the atomic scale. Performing research at ISOLDE requires a scientific project, which must be first, defended at the INTC Scientific Committee that will evaluate the quality and feasibility of the research, the added value for student training and sharing of efforts and synergies among the different participants. Under Portuguese leadership there are today 4 INTC approved proposals (mentioned at "Objectivos"): IS453, IS481, IS487, IS515 and two letters of intent LOI87 *New insights in Metal-Oxide junctions for nano-electronic applications* and LOI132 *Radioactive Local Probing and Doping on Graphene*, altogether accounting for ~5% of the beam time attributed at ISOLDE Within the framework of our experiments more than 20 institutes from 10 countries collaborate, contributing with people, samples, characterization, and maintenance:

- Portugal: IST/ITN, U Lisbon, U Porto, U Aveiro, UTAD Vila Real, ISEL Lisbon,
- Belgium: KU Leuven
- Germany: U Bonn, U Saarland, U Göttingen, Max Planck Institute Stuttgart, FZR Rossendorf
- Denmark: U Copenhagen
- France: U Paris Sud
- South Africa: U Kwazulu Natal/Durban
- Japan: CERC Tsukuba, U Tokyo
- South Korea: Sungkyunkwan University
- Russia: Kurchatov Institute Moscow
- Chile: U Talca
- Since 5 years we also collaborate with the MEDIPIX collaboration, which provides us with highly, segmented position sensitive Si detectors, aimed for high-resolution EC experiments.

# **BIOMEDICAL STUDIES GROUP**

# TEAM

Name	Category	R&D
Teresa Pinheiro	Auxiliary Researcher	100%
Luís C. Alves	Auxiliary Researcher	30%
Rita Godinho	Post-Doc Researcher	100%
Catarina Ramos	MSc. Fellowship	100%
Rute Pinheiro	Assistant Technician	70%

# **OBJECTIVES**

The main objective of the group is to carry out transversal research, bridging know-how in applied Physics, Biochemistry and Biology, with clinical medicine and toxicology.

This objective is being carried out in two main scientific research areas:

- The study of new biomarkers of exposure and disease, which may contribute to the identification of at-risk individuals and patients;
- The toxicity of natural occurring and synthetic nanoparticles using aquatic organisms as models

# MAIN ACHIEVEMENTS

Major research areas focused:

#### 1) Clinical research

In coronary artery disease, specific markers of the inflammatory, oxidative and apoptosis processes (Fig. 1) were associated with the atherosclerotic plaque burden and its biological composition. Results will help identifying and treating at-risk patients before a heart attack occurs or plaque progresses to cause debilitating chest pain.

In hemochromatosis patients the iron concentration in skin (Fig. 2), a readily accessible tissue, reflect liver iron overload. This may enable better-informed decisions on when to initiate, change or stop therapy.





Fig. 2. Nuclear Microscopy image of human skin. Fe deposits in the extracellular space around keratinocytes



#### 2) Interaction between air pollution and health

Pb concentration in exhaled breath condensate proved to reflect the level of exposure in industrial environment.

#### 3) Toxicity of nanoparticles

The elemental profiles and concentration gradients were determined in benthic and aquatic organisms. Cellular and tissue wall uptake of Ti, Mn, Fe and Zn were inferred (Fig. 3).

The toxicity of TiO<sub>2</sub> nanoparticles (TiO<sub>2</sub>-NP) was assessed using *Daphnia magna* as a model. All tissues and organs, including eggs (Fig. 4), of *Daphnia* exposed to TiO<sub>2</sub>-NP showed Ti accumulation, which seems to be concentration-dependent and associated to changes in protein expression profile. Therefore, ingested TiO<sub>2</sub>-NP has consequences in the physiology of these organisms.

Fig. 4. Daphnia magna exposure to  $TiO_2$  nanoparticles: mass density image of the egg pouch delimited by the carapacae (ca) and Ti deposits in eggs (eg).



These research projects involve a variety of techniques, such as, proton microscopy, inductively coupled plasma mass spectrometry, flow cytometry, biochemical methods, magnetic resonance imaging, and radiofrequency-based techniques.

Research activities carried out are an end product of intense and interactive collaborative work among researchers in Biology, Biochemistry, Chemistry, Cardiology, Pneumology, Dermatology, and Environmental Sciences.

# **RELEVANT PAPERS**

- P. Napoleão, M. Selas, C. Freixo, M. Mota Carmo, A.M. Viegas-Crespo, R. Cruz Ferreira, T. Pinheiro. T lymphocytes alterations are associated with oxidized LDL, troponin T, white blood cells and C-reactive protein during acute myocardial infarction. Clinical Hemorheology and Microcirculation (2012), online, DOI:10.3233/CH-121665 (IF 3.398).
- M.D. Ynsa, R. Minquin, R. Rajendran, T. Pinheiro, F. Watt, Consequences of fat diet in the distribution of minerals within pancreatic tissues of rats and rabbits. Microscopy and Microanalysis, 18,1060–1066 (2012), DOI:10.1017/S1431927612001547 (IF 3.007).
- M.A. Barreiros, T. Pinheiro, P.M. Felix, C. Franco, M. Santos, F. Araújo, M.C. Freitas, S.M. Almeida. Exhaled Breath Condensate as a biomonitor for metal exposure: A new analytical challenge. J. Radional Nucl Chem. (2012), online, DOI:10.1007/s10967-012-2366-x (IF 1.520).
- A.V. Silva, S. M. Almeida, M. C. Freitas, A. M. Marques, A. I. Silva, C. A. Ramos, T. Pinheiro, INAA and PIXE characterization of heavy metals and rare earth elements emissions from phosphorite handling in harbours, J. Radioanal. Nucl. Chem., 294, 277–281 (2012), DOI:10.1007/s10967-011-1524-x (IF 1.520).
- S. M. Almeida, A. V. Silva, M. C. Freitas, A. M. Marques, C. A. Ramos, A. I. Silva, T. Pinheiro, Characterization of dust material emitted during harbour activities by k0-INAA and PIXE, J. Radioanal. Nucl. Chem. 291, 77–82 (2012), DOI:10.1007/s10967-011-1279-4 (IF 1.520).

#### FUNDS

Project/Service	Reference	Timeframe	2012
The relationship of circulating biomarkers	FCT/PIC/IC/82734/2007	Mar2009-Dec2012	28.129,15€
of apoptosis and endothelial function with			
the plaque composition using VH IVUS			
Inflammation markers in acute coronary	Liga dos Amigos do Hospital	Jan2012-Dec2012	*25.000,00€
syndromes	de Santa Marta (LAHSM-		
	CAD)		
PM <sub>fugitive</sub>	PTDC/AAC-	Jun 2010-Jun 2013	**8.400,00€
	AMB/098825/2008		
Study of NPs interaction with cells, using	Spain Government, Ministério	Mar2011-Mar2014	Travelling and
methodologies based on IBA (Ion Beam	para a Ciência e Innovación		stipends
Analysis) techniques			
NanoTox Integrated evaluation of	PTDC/CTM/099446/2008	Jan2011-Dec2013	Collaboration
nanomaterials			
		Total	36.529,15 €

\* funds managed by LAHSM.

\*\* equipment acquisition – transferred to 2013.

# **INTERNATIONALIZATION**

Biomedical applications of ion beams:

- Scientific collaboration with CMAM, Centre for Microanalysis of Materials of the Universidad Autónoma de Madrid, Spain
- Scientific advising CENBG/Université de Bordeaux, France

Medical imaging processing – cooperation with Volcano Corporation, USA, for the analysis of radiofrequency data obtained with intravascular ultrasound technique.

# ELEMENTAL CHARACTERIZATION AND SPECIATION WITH ION BEAMS GROUP

### TEAM

Name	Category	R&D
Miguel A. Reis	Auxiliary Researcher	100%
P. Cristina Chaves	Post-doc researcher	100%
Ana Taborda	Research Grantee	100%
Rute Pinheiro	Assistant Technician	30%

#### **OBJECTIVES**

- Enhancing of the participation in the Geant4 Collaboration.
  - o Achieved.
- Establishment of an expansion database based of the IAEA available EADL.
  - o Not achieved.
- Making operational the computational codes under development.
  - Various codes were concluded but some components are still under development or at the last stage of development before release.
- Making operational analytical quantitative capacity on the HRHE-PIXE line.
  - Experimental calibration was achieved but quantification capacities are still dependent on software which is operational but not yet fully developed, human interface being still underdeveloped.
- Presenting results at EXRS 2012.
  - Achieved (see Main Achievements)
- Preparing and submitting projects at the following calls:
  - ERC Synergy Grant: submitted in January.
  - FCT call 2012 for projects in all research fields: submitted a Project for Reinforcement of Competence in Geological Samples Analysis.
- Acquiring specific capacities to analyse geological samples efficiently.
  - Geological samples mapping capacity was installed but the software efficiency is not yet at the best level.
- Reactivating the atmospheric monitoring systems of LCEA.
  - No funding was available to fulfil this objective.

#### **MAIN ACHIEVEMENTS**

In the frame of the PhD of Ana Taborda and also included in the work for the Geant4 Collaboration, polynomial models for ionization cross-sections by proton and alpha particle impact, were established for all three inner shell of atomic systems. In the figure aside from this description of the work we present a comparative graph for cross-sections of K, L and M sub-shells by impact of protons in gadolinium. The polynomial models, extended to cover the energy range between 0.1 and 100 MeV are presently included in the Geant4 software package. The new results leading to



this global model were presented at the EXRS 2012 Conference and are already accepted for publication in 2013 in X-ray Spectrometry.

Within the participation in the SPIRIT project (SPIRIT EU GA 227012-CP-CSA-Infra) and included in the scope of the post-doctoral work of P. Cristina Chaves (SFRH/BPD/76733/2011), a mapping of an agate sample was carried out using the X-Y system installed in late 2011 and put in full operation in 2012. In the figure below, we present the high energy spectral mapping obtained by irradiating the sample with a 3.8 MeV proton beam from the 3MV Tandetron accelerator. The figure corresponds to a 9 x 9 mm<sup>2</sup> area and the qualitative differences in the medium elements content are clearly identified. In PIXE 2013, this results and an equivalent analysis of a chromite will be presented, both as poster as well as oral communication.



#### **RELEVANT PAPERS**

- M. A. Reis, J. Campbell, Particle Induced X-ray Emission, in Characterization of Materials, 2nd Edition, Ed. Elton N. Kaufmann, John Wiley & Suns, 2012 doi: 10.1002/0471266965.com094.pub2
- P.C. Chaves, A. Taborda, M.A. Reis, CdTe detector efficiency calibration using thick targets of pure and stable compounds, Nuclear Instruments and Methods in Physics Research B 273 (2012) 245–249 doi:10.1016/j.nimb.2011.07.086

#### **FUNDS**

Project/Service	Reference	Timeframe	2012
SPIRIT EU	GA 227012-CP-CSA-Infra	01/01 to 31/03	*4.485,00€
BPD C. Chaves	SFRH/BPD/76733/2011	01/04 to 31/12	*13.455,00€
BD Ana Taborda	SFRH/BD/43379/2008	01/01 to 30/09	**8.505,00€
		Total	26 445 00 €

\*Post-doc contract and fellowship of P. Cristina Chaves.

\*\* PhD fellowship of Ana Taborda.

#### **INTERNATIONALIZATION**

• Participation in the Geant4 Collaboration.

# **Researchers – Scientific Activities**

(ordered by category and name)

# NAME: Ulrich Wahl

**CATEGORY:** Principal Researcher **ID NUMBER:** 5480

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Project participation: Perturbed Angular Correlations and Electron Channelling Experiments at ISOLDE - applied materials research with nuclear techniques, training and development ECT-CERN-EP-116320-2010 and ECT-CERN-EP-	40%
	123585-2011	
2	Supervision of students	50%
3	Project participation: SPIRIT (Support of Public and Industrial Research Using Ion	10%
	Beam Technology) FP7 contract Nr. 227012)	
Total		100%

# WORK SUMMARY

Nº	Work Summary and Main Achievements
1	An integral part of the mentioned two FCT projects is the use of radioactive probes at the ISOLDE/CERN facility for lattice location experiments in semiconductors. Besides the scientific leadership for this type of experiments as spokesperson of the respective CERN experiment IS453 <b>"Emission channelling lattice location experiments with short-lived isotopes</b> ", my task is the active participation in beam times, the simulation of experimental data by means of manybeam calculations, data analysis for specific samples, and the training and supervision of students. In 2012 IS453 participated in three ISOLDE beam times using radioactive isotopes of Be, Mg and Mn, respectively. Due to the restrictions on missions imposed by IST as consequence of the reorganization of ITN and the implementation of general austerity budget rules, however, I was only able to participate in the last of these three beam times, using Mn isotopes. Among the results achieved are the first use of short-lived <sup>11</sup> Be ( $t_{1/2}=14$ s) for emission channelling in GaN and lattice location experiments with <sup>27</sup> Mg in AlN pre-implanted with 10 <sup>15</sup> cm <sup>12</sup> stable <sup>26</sup> Mg, and <sup>56</sup> Mn (2.6h) in GaMnN, GaMnAs, 3C-SiC, 6H-SiC, <sup>57</sup> Mn (1.7min) in n-Si, and <sup>61</sup> Co(1.6h) in n+-Si. Also in 2012 a number of papers were published on previous experiments.
2	I am currently co-supervisor of the following theses:
	<b>Lígia Amorim: PhD Thesis on</b> "Lattice location studies of implanted Mg in the III-nitride semiconductors GaN, AlN and InN", Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, Belgium, since Jan 2010.
	<b>Daniel Silva, PhD thesis on "</b> Lattice location of transition metals in Si by means of high-resolution emission channeling", Faculdade de Ciências da Universidade do Porto, since Jan. 2011.
	Valérie Augustyns: Master's thesis on "Lattice location of Mn and Ni in Ge", Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, Belgium, and Erasmus student at IST Lisboa, since Sept 2012.
	Ângelo Costa: PhD thesis on "Ion implantation doping of SiC", Instituto Superior Técnico, Universidade Técnica de Lisboa, since Nov 2012.
	All theses make use of the emission channelling technique for lattice location of implanted radioactive probes, using the ISOLDE facility at CERN.
	As co-supervisor I am responsible for the scientific training of these students (including introduction into the experimental methods, performing of experiments, data analysis, scientific interpretation, writing and publication of manuscripts) and will also oversee the writing of the thesis and participate in the jury.

3	One of ITN's task within the <b>SPIRIT project</b> was to test the application of position-sensitive detectors for RBS/C experiments. The TimePix detector used for that purpose (developed by the CERN-Medipix collaboration) consists of a $1.5 \square 1.5 \text{ cm}^2$ Si wafer, with $256 \square 256$ pixels, pixel size $55 \square \text{m}$ .
	The detector was mounted on the small scattering chamber of the Van De Graaff accelerator of IST/ITN at a distance of 193 mm from the sample position. Energy resolutions around 56 keV were achieved both for backscattered 2 MeV alpha particles and protons. Using a beam spot of 0.5 mm diameter, an angular resolution of $\sigma$ =0.1° could be established by means of comparing experimental channelling patterns from a Si crystal to simulated patterns using the Monte Carlo code FLUX.
	Following the testing phase, in 2012 first experiments with the TimePix studied a number of virgin single crystals, e.g. Si, $SrTiO_3$ and 6H-SiC, but also thin films of AlInN deposited on GaN buffer layers on sapphire. Comparison of the 2-dim. channelling patterns to results obtained with conventional RBS/C showed that the use of the TimePix represents an interesting alternative for the study of such samples, in particular due to considerably simpler sample orientation.

# **PAPERS**

- S. Decoster, U. Wahl, S. Cottenier, J.G. Correia, T. Mendonça, L.M. Amorim, L.M.C. Pereira, A. Vantomme, Lattice position and thermal stability of diluted As in Ge, *Journal of Applied Physics* 111, 053528/1-7 (2012 doi:10.1063/1.3692761.
- J.G. Correia, K. Johnston, U. Wahl, Nuclear radioactive techniques applied to materials research, *Radiochimica Acta* 100, 127-137 (2012), doi: 10.1524/ract.2011.1873.
- R.P. Borges, B. Ribeiro, A.R.G. Costa, C. Silva, R.C. da Silva, G. Evans, A.P. Gonçalves, M.M. Cruz, M. Godinho, U. Wahl, Erratum to: Magnetic and transport properties of transition-metal implanted ZnO single crystals, *European Physical Journal* B 85, 91 (2012), doi: 10.1140/epjb/e2012-30089-y.
- P. Miranda, U. Wahl, N. Catarino, K. Lorenz, J.G. Correia, E. Alves, Damage formation and recovery in Fe implanted 6H–SiC, *Nuclear Instruments and Methods in Physics Research* B 286, 89-92 (2012), doi: 10.1016/j.nimb.2011.10.072.
- L.M.C. Pereira, U. Wahl, S. Decoster, J.G. Correia, M.R. da Silva, A. Vantomme, J.P. Araújo, Stability and diffusion of interstitial and substitutional Mn in GaAs of different doping types, *Physical Review* B 86, 125206/1-8 (2012), doi: 10.1103/PhysRevB.86.125206.
- L.M.C. Pereira, U. Wahl, S. Decoster, J.G. Correia, M.R. da Silva, A. Vantomme, J.P. Araújo, Evidence of N substitution by Mn in wurtzite GaN, *Physical Review* B 86, 195202/1-4 (2012), doi: 10.1103/PhysRevB.86.195202.

# **COMMNICATIONS**

- Position-sensitive detectors for RBS channelling experiments, <u>U. Wahl</u>, J.G. Correia, P. Miranda, N. Catarino, E. Bosne, M.R. Da Silva, L. Amorim, E. Alves, Joint Research Activity Meeting of the SPIRIT (Support of Public and Industrial Research using Ion Beam Technology) EU FP7 Collaborative Project, Leuven, Belgium, March 5-6 (2012), oral.
- Lattice location of Ni in Si by means of on-line emission channelling, D.J. Silva, <u>U. Wahl</u>, J.G. Correia, L.M.C. Pereira, L. Amorim, E. Bosne, M. Ribeiro da Silva, S. Decoster, J.P. Araújo, 2012 Spring Meeting of the European Materials Research Society (E-MRS), Symposium A "Advanced silicon materials research for electronic and photovoltaic applications III", Nice, France, May 14-18(2012), oral.
- Lattice location of transition metals in dilute magnetic semiconductors, L.M.C. Pereira, U. Wahl, S. Decoster, J.G. Correia, L.M. Amorim, J.P. Araújo, K. Temst, A. Vantomme, *General Scientific Meeting 2012 of the Belgian Physical Society (BPS), Brussels, Belgium, May 30 (2012)*, oral.
- Emission Channelling experiments in solid state physics, <u>U. Wahl</u>, 2nd ARIEL Science Workshop, TRIUMF, Vancouver, Canada, July 10-11 (2012), invited talk.

- Direct measurement of the Mg lattice site location in group III-Nitrides, L.M. Amorim, <u>U. Wahl</u>, S. Decoster, L.M.C. Pereira, J.G. Correia, D.J. Silva, K. Temst, A. Vantomme, 4th International Symposium on Growth of III-Nitrides, St. Petersburg, Russia, July 16-19 (2012), oral.
- Position-sensitive detectors in ion beam analysis, <u>U. Wahl</u>, 3rd SPIRIT (Support of Public and Industrial Research using Ion Beam Technology) Workshop on "Ion Beams as a Tool for Nanotechnology", Lisbon, Portugal, July 18-20 (2012), oral.
- Lattice location study of implanted As in Ge, S. Decoster, <u>U. Wahl</u>, S. Cottenier, J.G. Correia, T. Mendonça, L.M. Amorim, L.M.C. Pereira, A. Vantomme, 18th International Conference on Ion Beam Modification of Materials (IBMM), Qingdao, China, Sept 2-7 (2012), poster.
- Lattice sites of implanted transition metals in dilute magnetic semiconductors, L.M.C. Pereira, <u>U. Wahl</u>, S. Decoster, J.G. Correia, L.M. Amorim, M.R. da Silva, J.P. Araújo, A. Vantomme, 18th International Conference on Ion Beam Modification of Materials (IBMM), Qingdao, China, Sept 2-7 (2012), poster.
- Localização de impurezas em silicio atraves da técnica "Emission channelling", D.J. Silva, <u>U. Wahl</u>, J.G. Correia, J.P. Araújo, *Física 2012, 18th National Conference of the Portuguese Physical Society (SPF), Aveiro, Portugal, Sept 6-8 (2012)*, oral.
- Localização de impurezas na rede cristalina de semiconductores nitretos, L.M. Amorim, <u>U. Wahl</u>, J.G. Correia, K. Temst, A. Vantomme, *Física 2012, 18th National Conference of the Portuguese Physical Society (SPF), Aveiro, Portugal, Sept 6-8 (2012)*, oral.
- Use of position-sensitive pixel detectors for ion beam analysis, E. Bosne, <u>U. Wahl</u>, J.G. Correia, P. Miranda, E. Alves, *Física 2012, 18th National Conference of the Portuguese Physical Society (SPF), Aveiro, Portugal, Sept 6-8 (2012)*, poster.
- Emission channeling studies of the lattice location of transition metals in dilute magnetic semiconductors, L.M.C. Pereira, <u>U. Wahl</u>, S. Decoster, J.G. Correia, L.M. Amorim, J.P. Araújo, A. Vantomme, 4th Joint International Conference on Hyperfine Interactions and International Symposium on Nuclear Quadrupole Interactions, Beijing, China, Sept 10-14 (2012), invited talk.
- Fluence dependence of the atomic configuration of 57Fe in ion-implanted ZnO, H.P. Gunnlaugsson, G. Langouche, K. Johnston, R. Mantovan, H. Masenda, T.E. Mølholt, L. Pereira, K. Bharuth-Ram, H.P. Gíslason, D. Naidoo, S. Ólafsson, <u>U. Wahl</u>, G. Weyer, 4th Joint International Conference on Hyperfine Interactions and International Symposium on Nuclear Quadrupole Interactions, Beijing, China, Sept 10-14 (2012), poster contribution.
- Lattice location of the transition metals Fe and Ni in Si by means of emission channelling, D.J. Silva, <u>U.</u> <u>Wahl</u>, J.G. Correia, L.M.C. Pereira, L. Amorim, E. Bosne, M. Ribeiro da Silva J.P. Araújo, EURISOL Town Meeting 2012, Lisbon, Portugal, Oct 17-19 (2012), poster.
- The testing of Timepix detectors for position-sensitive detection of charged-particles, E.D. Bosne, <u>U.</u> <u>Wahl</u>, J.G. Correia, P. Miranda, L. Amorim, M. Ribeiro da Silva, EURISOL Town Meeting 2012, Lisbon, Portugal, Oct 17-19 (2012), poster.
- Study of a Timepix+FitPix detection system for applications in RBS/C for materials analysis using MeV He and H beams, E. Bosne, V. Amaral, <u>U. Wahl</u>, J.G. Correia, Open Meeting of the Medipix collaboration, CERN, Geneva, Switzerland, Nov 28 (2012), oral.
- Lattice location of transition metals in dilute magnetic semiconductors using EC-SLI (IS453), L.M.C. Pereira, <u>U. Wahl</u>, J.G. Correia, S. Decoster, L.M. Amorim, J.P. Araújo, K. Temst, A. Vantomme, 2012 ISOLDE Workshop and Users Meeting, CERN, Geneva, Switzerland, Dec 17-19 (2012), oral.

# **EDUCATION – THESES SUPERVISION**

• Opponent, PhD Thesis, *Paramagnetism in ion-implanted oxides*, Torben Esmann Mølholt, University of Iceland, Reykjavik, 2 Nov 2012.

# **PROJECTS**

• FCT project application EXCL/FIS-NAN/0213/2012 "PROCESS-ION: Ion beam processing of advanced materials and nanostructures", evaluated as "outstanding" but not eligible for funding.

# **COLLABORATIONS**

• Lígia Amorim, Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, Belgium, scientific visits to IST/ITN 25-29 June 2012, 1-12 Aug 2012, data analysis of emission channelling experiments and discussion of common manuscripts.

# **NAME: Eduardo Jorge da Costa Alves CATEGORY:** Principal Researcher

**ID NUMBER:** 25357

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Management of European Projects	25%
2	Administration Activities	15%
3	Management of FCT Projects	15%
4	Scientific Supervision	15%
5	Academic and Scientific Activities	15%
6	Coordination and Management of the Ion Beam and x-Ray Laboratory (IBL)	10%
7	Management of FITN group from CFNUL	5%
Total		100%

# WORK SUMMARY

N°	Summary and Main Achievements
1	Leader of IST participation on the elaboration of the SPRITE* proposal submitted and funded by FP7- Initial Training Network (ITN).
	Early Stage Researcher (ESR) will be hired in 2013 as a PhD student of IST.
	Member of the management board of SPIRIT* project funded by FP7- Infrastructures.
	Coordination of the Portuguese participation: Development and upgrade of IBA Software and new experimental procedures to minimize analysing beam effects on targets.
	Principal Researcher of the EFDA JET Technology Workprogramme* tasks.
	Analysis of different kind of tiles and test samples from the plasma facing wall of JET chamber was realized to assess fuel retention and deposition/erosion processes.
	Principal Researcher of EFDA Fusion for Energy (F4E) Programme* projects.
	Study of chemical reactivity of Be pebbles and composites irradiated in HIDOBE project exposed to oxygen reach ambient. Oxidation is weakly affected by the irradiation.
	(*) See projects and publications indicator.
	• Vogal of the Installation Commission of IST/ITN (since April).
2	Coordination of UFA report for 2011 and IBL work plan for 2012.
2	Principal researcher of several FCT projects* running at the Ion Beam Laboratory (IBL).
3	• High resolution depth profiling of light elements in multifunctional coatings and transparent conductive oxides (TCO).
	• Lattice site and implantation damage in nitrides implanted with rare-earths.
	• Formation of regular lattices of voids and Ge quantum dots in amorphous alumina matrix and
	multilayers.
	<ul> <li>Interface roughness and mixing in GeSi/Al2O3 multilayers.</li> </ul>
	Noble metal nanoparticles formation in oxide matrices.
	• Stopping powers of light ions in Si, GaN and TiO2.
	(*) See projects and publications indicator.
4	• Supervisor of two post doc projects: Irradiation studies of tungsten based materials for fusion
4	Applications (project contract: F4E-2009-GRT-030-Action3)

	<ul> <li>Supervisor of two PhD students: Production and irradiation studies of tungsten alloys based materials for fusion environment (SFRH/BD/88533/2012) and Study of the influence of Al content on optical activity and lattice site location of rare earth implanted Al<sub>x</sub>Ga<sub>1-x</sub>N (SFRH/BD/78740/2011).</li> <li>Co-supervisor of a PhD thesis, Functionalization by ion implantation of Si: influence on tribomechanical and wettability properties at micro and nanoscales, (SFRH/BD/68513/2010).</li> </ul>
5	<ul> <li>Teaching: Coordinator Professor (20%) at Escola Superior de Tecnologia de Lisboa, Instituto Politécnico de Lisboa.</li> <li>Seminars: In the scope of the Materials PhD programme of University of Aveiro and Master</li> </ul>
	<ul> <li>Thesis of IST and University of Aveiro seminars were presented.</li> <li>Reviewer: As a regular referee of Elsevier Journals and American Institute of Physics in the areas of Physics and Material Science several manuscripts were reviewed. In addition 10 proposals for EMIR and CMAM were also assessed.</li> </ul>
	<ul> <li>Scientific collaborations with the following Institutions were established:</li> <li>University of Tennessee: Co-implantation of Zr and O in sapphire (Al2O3) to study defect formation (PhD project).</li> </ul>
	<ul> <li>University Wayne: Ion beam studies of new multifunctional structures incorporating oxides for development of batteries.</li> </ul>
	• Universidad Autónoma de Madrid: Development of double layer contacts for CdZnTe semiconductors.
	<ul> <li>Polish Academy of Sciences: Ion beam studies of ZnMgO/ZnO multilayers grown by MBE.</li> <li>CIMAP-GANIL, Caen: Implantation of Ge in Si to study the influence of stopping power on</li> </ul>
	<ul> <li>damage.</li> <li>Outreach: As Radiações e os Materiais: Interações Proveitosas. <i>País Positivo</i>, Sol, 21st December 2012.</li> </ul>
6	Coordination of the development and maintenance of the IBL equipment. Promotion of new research projects in the framework of the strategic plans for the short and long term activities: installation of new techniques and certification of some of the currents installed techniques.
7	Coordination and management of the Ion beam and Nuclear Techniques of Centro de Física Nuclear (CFNUL) assuring the integration of the activities at the IBL and RPI on the center policy.

# **PAPERS**

- M. Fialho, S. Magalhães, L.C. Alves, C. Marques, R. Maalej, T. Monteiro, K. Lorenz, E. Alves, AIN content influence on the properties of AlxGa1\_xN doped with Pr ions, *Nuclear Instruments and Methods in Physics Research B*, 273, 149-152 (2012), doi:10.1016/j.nimb.2011.07.062.
- J.M. Chappé, A.C. Fernandes, C. Moura, E. Alves, N.P. Barradas, N. Martin, J.P. Espinós, Analysis of multifunctional titanium oxycarbide films as a function of oxygen addition, F. Vaz, *Surface and Coatings Technology*, 206, 2525-2534 (2012), doi:10.1016/j.surfcoat.2011.11.005.
- F.H.M. Cavalcante, M.R. Gomes, A.W. Carbonari, L.F.D. Pereira, D.A. Rossetto, M.S. Costa, E. Alves, N.P. Barradas, N. Franco, L.M. Redondo, A.M.L. Lopes, J.C. Soares, Characterization of nanostructured HfO2 films using RBS and PAC, *Nuclear Instruments and Methods in Physics Research B*, 273, 195-198 (2012), doi:10.1016/j.nimb.2011.07.074.
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- P. Miranda, U. Wahl, N. Catarino, K. Lorenz, J.G. Correia, E. Alves, Damage formation and recovery in Fe implanted 6H-SiC, *Nuclear Instruments and Methods in Physics Research B: Beam Interactions With Materials And Atoms*, 286, 89-92, 2012, doi: 10.1016/j.nimb.2011.10.072.
- Q. Zheng, F.Dierre, V.Corregidor, R.Fernandez-Ruiz, J.Crocco, H.Bensalah, E. Alves, E.Dieguez, Deposition of nanometric double layers Ru/Au, Ru/Pd, and Pd/Au onto CdZnTe by the electroless method, *Journal of Crystal Growth*, 358, 89–93, 2012.

- J. Borges, N. Martin, N.P. Barradas, E. Alves, D. Eyidi, M.F. Beaufort, J.P. Riviere, F. Vaz, L. Marques, Electrical properties of AlNxOy thin films prepared by reactive magnetron sputtering, *Thin Solid Films*, 520, 6709-6717 (2012), doi:10.1016/j.tsf.2012.06.062.
- A. Kaminska, C-G. Ma, M.G. Brik, A. Kozanecki, M. Bo'ckowski, E. Alves, A. Suchocki, Electronic structure of ytterbium-implanted GaN at ambient and high pressure: experimental and crystal field studies, *Journal of Physics: Condensed Matter*, 24, 095803 (8pp) (2012), doi:10.1088/0953-8984/24/9/095803.
- N. Catarino, E. Nogales, N. Franco, V. Darakchieva, S.M.C. Miranda, B. Méndez, E. Alves, J.G. Marques, K. Lorenz, Enhanced dynamic annealing and optical activation of Eu implanted a-plane GaN, *EPL* (*Europhysics Letters*), 97 (2012), doi:10.1209/0295-5075/97/68004.
- J.P.B. Silva, S.A.S. Rodrigues, Anatoli Khodorov, J. Martín-Sánchez, M. Pereira, E. Alves, M.J.M. Gomes, Ph. Colomban, Films Deposited by Pulsed Laser Deposition, Structural and Electrical Properties of Nanostructured Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub>, *Journal of Nano Research*, Vols. 18-19, 299-306, (2012), doi:10.4028/www.scientific.net/JNanoR.18-19.299
- S. Magalhães, N.P. Barradas, E. Alves, I.M. Watson, K. Lorenz, High precision determination of the InN content of Al<sub>1-x</sub>In<sub>x</sub>N thin films by Rutherford backscattering spectrometry, *Nuclear Instruments and Methods in Physics Research B*, 273, 105-108 (2012), doi: 10.1016/j.nimb.2011.07.051.
- K. Lorenz, S. M. C., Miranda, E. Alves, I. S. Roqan, K. P. O'Donnell, KP, M. Bockowski, High pressure annealing of Europium implanted GaN, *Gallium Nitride Materials and Devices VII, Book Series: Proceedings of SPIE*, 8262, No. 82620C (2012), doi: 10.1117/12.906810.
- S. Sério, M.E. Melo Jorge, Y. Nunes, N.P. Barradas, E. Alves, F. Munnik, Incorporation of N in TiO2 films grown by DC-reactive magnetron sputtering, *Nuclear Instruments and Methods in Physics Research B* 273, 109-112 (2012), doi:10.1016/j.nimb.2011.07.052.
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- A. Redondo-Cubero, M. Brandt, F. Henneberger, E. Alves, K. Lorenz, Ion beams as a tool for the characterization of near-pseudomorphic CdZnO epilayers, *Oxide-Based Materials and Devices III, Book Series: Proceedings of SPIE*, 8263, Number: 82630U (2012), doi: 10.1117/12.908496.
- S.M. C. Miranda, P. Kessler, J. G. Correia, R. Vianden, K. Johnston, E. Alves, K. Lorenz, Ion implantation of Cd and Ag into AlN and GaN, *Physica Status Solidi* (*C*), 9, no. 3-4, 1060-1064 (2012), doi: 10.1002/pssc.201100203.
- N.F. Santos, J. Rodrigues, A.J.S. Fernandes, L.C. Alves, E. Alves, F.M. Costa, T. Monteiro, Optical properties of LFZ grown -Ga2O3:Eu3+ fibres, Applied Surface Science 258, 9157-9161 (2012), doi: 10.1016/j.apsusc.2011.07.069.
- J. Rodrigues, S.M.C. Miranda, N.F. Santos, A.J. Neves, E. Alves, K. Lorenz, T. Monteiro, Rare earth codoping nitride layers for visible light, *Materials Chemistry and Physics* 134, 716e720 (2012), doi: 10.1016/j.matchemphys.2012.03.056.
- L. Rebouta, P. Martins, S. Lanceros-Mendez, J.M. Barandiaran, J. Gutierrez, L.C. Alves, E. Alves, Room temperature magnetic response of sputter deposited TbDyFe films as a function of the deposition parameters, *Journal of Nano Research*, 18-19, 235-239, (2012), doi: 10.4028/www.scientific.net/JNanoR.18-19.235.
- Redondo-Cubero, A. Hierro, J.-M. Chauveau, K. Lorenz, G. Tabares, N. Franco, E. Alves, E. Muñoz, Single phase a-plane MgZnO epilayers for UV optoelectronics: substitutional behaviour of Mg at large contents, *CrystEngCommunity*, 14, 1637 (2012), doi:10.1039/C2CE06315H.

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- B. Savoini, M.M. Tardío, R. Ramírez, E. Alves, Surface morphology, thermal and electrical conductivity of a-Al2O3 single crystals implanted with Au and Ag ions, *Nuclear Instruments and Methods in Physics Research B* 286, 184–189, (2012), doi:10.1016/j.nimb.2011.11.036.
- M. Torrell, R. C. Adochite, L. Cunha, N. P. Barradas, E. Alves, M. F. Beaufort, J. P. Rivière, Albano Cavaleiro, S. Dosta, F. Vaz, Surface Plasmon Resonance Effect on the Optical Properties of TiO2 Doped by Noble Metals Nanoparticles, *Journal of Nano Research*, Vols. 18-19, 177-185, (2012), doi: 10.4028/www.scientific.net/JNanoR.18-19.177.
- E. Elamurugu, P. Shanmugam, G. Gonçalves, N. Franco, E. Alves, R. Martins, E. Fortunato, The electronic transport mechanism in indium molybdenum oxide thin films RF sputtered at room temperature, *EPL (Europhysics Letters)*, 97, No. 3, (2012), doi:10.1209/0295-5075/97/36002.
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- S.R. C. Pinto, M. Buljan, A. Chahboun, M. A. Roldan, S. Bernstorff, M. Varela, S. J. Pennycook, N. P. Barradas, E. Alves, S. I. Molina, M. M. D. Ramos, Tuning the properties of Ge-quantum dots superlattices in amorphous silica matrix through deposition conditions, M. J. M. J. Gomes, *Journal of Applied Physics*, 111, 074316 (2012), doi.10.1063/1.3702776.
- V. Darakchieva, K. Lorenz, M.-Y. Xie, E. Alves, W. J. Schaff, T. Yamaguchi, Y. Nanishi4, S. Ruffenach5 M. Moret, and O. Briot, Unintentional incorporation of H and related structural and free-electron properties of c- and a-plane InN, *Physics Status Solidi* (A), 209, no.1, 91–94 (2012), doi 10.1002/pssa.201100175.

# **COMMUNICATIONS**

Talks

- *Post-mortem analysis and simulation, latest results,* E. Alves, N. Catarino, N.P. Barradas, JET Task Force Technology Meeting, 11-14 December, Culham Science Centre, UK.
- *Chemical Reactivity of Irradiated Be Pebbles under Oxidizing Atmosphere*, E. Alves, N. Catarino, L.C. Alves, 7<sup>th</sup> IEA International workshop on Beryllium Technology for Fusion, Kalsrhue, 9-21 September, Germany.
- *Luminescence and structural studies of Al<sub>x</sub>Ga<sub>1-x</sub>N alloys doped with rare earth ions*, E. Alves, M. Fialho, K. Lorenz, T. Monteiro, 18th International Conference on Ion Beam Modification of Materials, Quingdao 7-12 September, China.
- *Ion Beam Techniques for nanotechnology: Overview and Fundamentals,* E. Alves 3rd Spirit Workshop on Ion Beams as a Tool for Nanotechnology, ITN, Sacavém, 18-20 July, 2012.
- *Chemical and Oxidation behavior of Be materials irradiated in HIDOBE-01 campaign*, E. Alves, L.C. Alves, Meeting Fusion for Energy (F4E), HIDOBE PIE, Petten 24 June, Nederland.

#### Seminars

- *Análise de sólidos com feixes de iões de alta energia:* Mestrado Integrado em Engeharia Física: Técnicas de caracterização de Estruturas, Universidade de Aveiro, 4 December 2012.
- *Nuclear techniques a window to knowledge:* Seminários de Inovação e Desenvolvimento Sustentável, IST, 15 November 2012
- *Rutherford backscattering and channeling:* Programa Doutoral de Ciência e Engenharia de Materiais, Técnicas avançadas de caracterização de materiais Universidade de Aveiro, 9 November 2012.

#### Posters

- *Studies on Deuterium retention in W based materials*, 28<sup>th</sup> Symposium on Fusion Technology, Liége, 24-27 Setember, Belgium 2012.
- *Tribological improvement of coining dies for the Portuguese Mint by nitrogen implantation*, 18<sup>th</sup> International Conference on Ion Beam Modification of Materials, Quingdao 7-12 Setember, China, 2012.

# **EDUCATION**

- Física Geral (4 ECTS), 1st Semester Class, degrees Radiologia, Radioterapia e Medicina Nuclear (3 week hours), Escola Superior de Tecnologia de Lisboa, Instituto Politécnico de Lisboa.
- Física Atómica e Nuclear (4 ECTS), 2nd semester class, degrees Radiologia, Radioterapia e Medicina Nuclear (3 week hours). Escola Superior de Tecnologia de Lisboa, Instituto Politécnico de Lisboa.
- Arguing Jury, PhD theses of Vitor Manuel Loureiro Figueiredo, "Development of Copper and Nickel based oxide thin films: Design and fabrication of thin-film transistors", Universidade Nova de Lisboa, 17th December 2012.

# **PARTICIPATION IN PROJECTS**

- *Heavy Ions for Nuclear Techniques-HINT*, RECI/FIS-NUC/0248/2012, Evaluated Outstanding.
- SPRITE-Supporting Postgraduate Research with Internships in industry and Training Excellence, FP7-PEOPLE-2012-ITN, Grant agreement no.: 317169, IST Coordinator.
- *Material transport and erosion/deposition*, EFDA JET Technology Workprogramme2012, JW12-FT-3.71, ITN Coordinator.
- Analysis of carbon-13 deposition near gas injection region from C27, EFDA JET Technology Workprogramme2011, JW11-FT-3.65, ITN Coordinator.
- Perturbed Angular Correlations and Electron Channelling Experiments at ISOLDE applied materials research with nuclear techniques, training and development. CERN/FP/123585/2011, Prime contractor IST, researcher (15%).

- *Material transport and erosion/deposition in the JET torus*, EFDA JET Technology Workprogramme2011, JW11-FT-3.68. ITN Coordinator.
- *Post Irradiation Examination of Be materials irradiated in HIDOBE-01 campaign*, Fusion for Energy, Programme contract, F4E-2009-GRT-030-Action3 (PNS-TBM). ITN Coordinator.
- Screening of an alternative production route/capacity for Be pebbles, Fusion for Energy Programme contract, F4E-2009-GRT-030- Action2 (PNS-TBM). ITN Coordinator.
- SPIRIT- Support of Public and Industrial Research Using Ion Beam Technology FP7- Infrastructures-2008-1, Grant agreement No 227012-CP-CSA-Intra (2009-2012): ITN Coordinator.
- *Neutrino mass direct determination: Portuguese contribution to MARE*, PTDC/FIS/116719/2010, Prime Contractor: U. Lisboa (M.José). ITN Coordinator.
- NAFEM- Ferromagnetic nanocrystals based on doped ZnO for tunnelling magneto resistance (TMR) devices, PTDC/FIS/098943/2008, Prime Contractor: U. Minho (M. Jesus), ITN Coordinator.
- *Multifox: Nanometric Probing and Modification of Multiferroic Oxides,* PTDC/FIS/105416/2008, Prime Contractor: U. Aveiro (Vitor Amaral), ITN Coordinator.
- DiFusion Diamond dispersions in nanostructured metals: Novel materials design for fusion reactors, PTDC/CTM/100163/2008, Prime Contractor: IST (Patrícia Carvalho), ITN Coordinator.

# **CONFERENCE ORGANIZATION / COMMITTEES**

- Organizing Committee, 13th International Conference on Nuclear Microprobe technology & Applications, Lisbon 22-27 July 2012.
- Chair, 3rd Spirit Workshop on Ion Beams as a Tool for Nanotechnology, ITN, Sacavém, 18-20 July 2012.
- International committee of International Conference Series on Ion Beam Analysis, IBA.
- International committee of International Conference Series on Ion Beam Modification of Materials, IBMM.
- International committee of International Conference Series on Radiation Effects in Insulators, REI.
- Member of Advisory Editorial Board da Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms.
- Scientific Committee of Réseau National d'accélérateurs pour les Etudes des Matériaux sous Irradiation EMIR.
- Scientific Committee of Centro de Microanálisis de Materiales, Universidad Autónoma de Madrid-CMAM, Spain (www.cmam-btmanager).

#### **COLLABORATIONS**

- Anna Marie Widdowson, CCFE Culham, UK, 26-30 March.
- Joseph Paul Coad, CCFE Culham, UK, 5-8 June.
- Karur Padmanabhan Wayne State University, USA, 25 Sep- 4 Oct.
- Adrian Kozanecki, Polish Academy of sciences, Poland, 22-26 October.
- Marcin Stachowicz, Institut of Physics, Poland, 22-26 October.

NAME: Fernanda Maria Amaro Margaça CATEGORY: Principal Researcher ID NUMBER: 5346

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Coordination of UFA	20%
2	Group coordination and the merging of the two previous groups	25%
3	Project FCT-PTDC/CTM/101115/2008 Hybrid Materials	40%
4	Other Activities	15%
Total		100%

# **WORK SUMMARY**

Nº	Work Summary and Main Achievements
1	Coordination of UFA
	• Coordination of meetings with the heads of all the UFA research groups to establish priorities and decide which acquisitions and maintenance to do.
	• With the collaboration of those groups the following was performed: a) a detailed description was made concerning the maintenance actions required in the facilities of the unit and b) the needs of the groups in what concerns technical staff to support laboratory work. In relation to the former, a guided visit was done to the facilities where reparation was needed and a budged was received. This one was sent to CI. As concerns b) a document was prepared to ask FCT for 4 Research Technician Grants which was sent to IST/ITN CI.
	• The process to acquire 2 multifunctional equipment was resumed as well as the respective maintenance contracts. A similar process was resumed as concerns 10 air conditioned equipment and supervision of their installation in laboratories/rooms in UFA.
	• Coordination of the UFA contribution to the ITN Annual Report 2011.
	Coordination of UFA Annual Report 2011.
	• Revision of the edition of the URSN contribution to the ITN Annual Report 2011.
2	Group coordination and the merging of the two previous groups
	In early 2012 two groups: Condensed Matter Physics and Radiation Technologies: Processes and Products decided to merge into one group named Ionizing Radiation Technologies, TRI. The main drive for this merge was the coming retirement of one group's head, together with the recognition that both groups use the same technologies and that their union would promote its desired development. Since I would be the head of the newly formed TRI group, I started to get acquainted with the situation of the other group as refers to a) projects in progress, b) facilities in what concerns installation and running conditions and c) staff conditions.
	Since February, regular joint meetings of the two groups were held where the above mentioned issues were dealt and progress was planned. It was decided that several group members would apply to the FCT announcement of call for proposals and that the heads of the previous groups would elaborate a proposal to apply for a project of consolidation of research skills and resources, aiming to consolidate the TRI group. Thus project "Application of Ionizing Radiation for a Sustainable Environment" was submitted and approved for funding.
3	Project FCT-PTDC/CTM/101115/2008 Hybrid Materials for biomedical applications
	IST/ITN coordination of the research activities performed in CTN in the framework of this project.
	In the year of 2012 progress has been achieved in what concerns a) the dependence of the microstructure in the polymer molecular weight. Research was carried out in the system 20 wt% PDMS - 73 wt% TEOS - 7 wt% PrZr; b) the influence of PrZr content in the porosity and size of the oxide regions present in the hybrid materials prepared with fixed polymer weigth (Mw PDMS = 43500 g/mol); c) preparation of hybrid materials with Calcium in the system (20 wt% PDMS - 79

	wt%TEOS - 1 wt% PrZr, adding: x Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> (x=1, 3, 5, 10 wt%) solid compound or x Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> (x=1, 3, 10 wt%) in solution.
	In the framework of this project a visit was made to the Budapest Neutron Centre, Hungary, to perform measurements using the local small angle neutron scattering instrument and to discuss results with Prof. Lazlo Almasy. Results were published in two papers and presented in the 10th meeting of the Ionizing Radiation and Polymers Symposium, IRaP'2012, held 14th-19th October, 2012, in Cracow, Poland.
4	Other activities
	Supervision of M Sc Joana Lancastre
	• Member of Scientific Committee of IST/ITN – participation in weekly meetings and collaboration in the development of its activities.
	• Participation in the elaboration of the following proposals to the FCT call for Scientific Research and Technological Development Projects – 2012, in which I was not the responsible researcher:
	• Application of Ionizing Radiation for a Sustainable Environment (ARIAS), Consolidation of research skills and resources project. The project was recommended for funding.
	• <i>Enhancement of biopolymers by ionizing radiation processing (BioP-Rad)</i> , Research project. The evaluation was rated Outstanding but the project was not recommended for funding.
	• Member of the IST/ITN Restructuration Committee - participation in its regular meetings.
	• Collaboration in the edition of the IST/ITN 2011 booklet.

# PAPERS

- J.J.H. Lancastre, N. Fernandes, F.M.A. Margaça, I.M. Miranda Salvado, L.M. Ferreira, A.N. Falcão and M.H. Casimiro, Study of PDMS conformation in PDMS-based hybrid materials prepared by gamma irradiation, *Radiation Physics and Chemistry* **81** (2012) 1336-1340. DOI: 10.1016/j.radphyschem.2012.02.016
- A.G.B. Castro, J.C. Almeida, I.M. Miranda Salvado, F.M.A. Margaça and M.H. Vaz Fernandes, A novel hybrid material with calcium and strontium release capability, *Materials Letters* **88** (2012) 12-15. Doi: 10.1016/j.matlet.2012.08.022

# COMMUNICATIONS

• On the Insights of the Hybrid Materials Microstructure at Nanoscale: A SANS Study, J.J.H. Lancastre, N. Fernandes, F.M.A. Margaça, I.M. Miranda Salvado, L.M. Ferreira, A.N. Falcão, M.H. Casimiro, IRaP'2012 - 10th Meeting of the Ionizing Radiation and Polymers Symposium, Cracow, Poland, Oct 14-19 (2012), Oral.

# **EDUCATION / THESES SUPERVISION**

• Arguing member in jury of PhD Thesis, *Application of Ionizing Radiation to Persistent Organic Pollutants Decomposition*, by Rita Lourenço Paiva de Melo Galvão, Faculdade de Ciências, Universidade de Lisboa, 14 December 2012

# PROJECTS

- *Hybrid Materials for biomedical applications, contract ref.* FCT-PTDC/CTM/101115/2008 (2010-2013), Total budget: 125.000 €, ITN budget: 51.072 €. Prime Contractor: Univ. de Aveiro (I.M.M. Salvado), ITN Coordinator: F.M.A. Margaça, currently in progress.
- *Hybrid Materials for Heterogeneous Catalysys (CATHY)*, submitted to FCT call for Scientific Research and Technological Development Projects 2012. The evaluation was rated Outstanding but the project was not recommended for funding.

# **COLLABORATIONS**

- I.M. Salvado, Dept. Glass and Ceramics Eng., CICECO, University of Aveiro, Portugal, twice/month visit, Collaboration research on hybrid materials for biomedical applications.
- M.H.Casimiro, REQUIMTE, CQFB, Dep. Química, Fac. de Ciências e Tecnologia, Univ. Nova de Lisboa, weekly visit, Collaboration in research of new polymeric materials and their practical use.
- Lazlo Almasy, Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, POB 49, 1525 Budapest, Hungary, Collaboration in neutron scattering experiments in hybrid materials
- Anikó Meiszterics, Neutron Spectroscopy Department, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Science, Budapest, Hungary, collaboration in neutron scattering experiments in hybrid materials.

# NOME: João Guilherme Martins Correia CATEGORIA: Principal Researcher NÚMERO MECANOGRÁFICO: 5451

### **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Project management	10%
2	SCIENTIFIC Work	20%
3	R&D Work	20%
4	Students and training	50%
Total		100%

# WORK SUMMARY

N°	Work Summary and Main Achievements
1	<b>1.1 Coordination of the work, report and funding management of project FCT-CERN-FP-123585-2011</b> supporting the Portuguese experimental infrastructure at ISOLDE. Maintenance, R&D and attendance of researchers and students, while executing our approved research proposals at the INTC (ISOLDE scientific committee), are mainly supported by this project.
	1.2 Approved scientific proposals (IS) and Letter-of-intent (LOI):
	IS453 Emission channelling lattice location experiments with short-lived isotopes. Spokesperson: U. Wahl CTN, Contact Person J. G. Correia CTN (JGC).
	IS481 The role of In in III-nitride ternary semiconductors. Spokesperson: K. Lorenz CTN, Contact person JGC.
	IS487 Study of local correlations in magnetic and multiferroic materials. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.
	LOI87 New insights in Metal-Oxide junctions for nano-electronic applications. Spokesperson: A.L. Lopes CFNUL, Contact person: JGC.
	IS515 Radioactive probe studies of coordination modes of heavy metal ions from natural waters to functionalized magnetic nanoparticles. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.
	LOI132 Radioactive Local Probing and Doping on Graphene. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.
	1.3 R&D
	Development of beta & alpha position and energy sensitive, Si detectors (timepix- and VATAGPx types) and of UHV equipment setups for on-line experiments using short lived isotopes.
2	Scientific Main Results 2012 - Analysis is being done and publications are regularly achieved. Details can be seen at the original proposals and publications list.
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	IS453 - First ever done emission-channelling (EC-SLI) experiment with the short-lived 11Be(13.8s) isotope on GaN. There is no other way to learn about Be lattice sites on materials when Be is present in diluted realistic / technological concentrations. More EC-SLI experiments were done using <sup>27</sup> Mg (9.4m), <sup>61</sup> Co(1.6h), <sup>57</sup> Mn(85.4s), <sup>56</sup> Mn(2.6h) on semiconductors GaAs:Mn, Si and AlN. <sup>59</sup> Fe (44.5d) was implanted on p+-Si and GaN, for experiments to be carried during 2013.
	IS481 - Perturbed angular correlations (PAC) has been used to study with <sup>111m</sup> Cd/ <sup>111</sup> Cd ( $T_{1/2} = 48m$ ), <sup>117</sup> Cd/ <sup>117</sup> In( $T_{1/2} = 2.5h$ ) and <sup>111</sup> In/ <sup>111</sup> Cd ( $T_{1/2} = 2.8d$ ), the relevant single crystals and nanowires of the transparent conductive oxide Ga <sub>2</sub> O <sub>3</sub> . Cd occupying octahedral Ga-sites, on a lattice fully recovered, was observed after high annealing temperatures, thus demonstrating the potential of doping by ion-implantation.
	IS515 <i>and</i> LOI132 have similar procedure preparations when using <sup>199m</sup> Hg/ <sup>199</sup> Hg (42m) PAC probes. Clear results show Hg binding at different sites at the magnetic nanoparticles and at the graphen surface, as a function of sample preparation and measurement conditions, under study with DFT methods.
3	R&D Main Results
	- Successfully mounting, commissioning, tests andcurrent running of the small implantation chamber of radioactive isotopes (SIC) designed and built by our projects and ISOLDE funds. This chamber fits on-line at the GHM-GPS area in between the ISOLDE beam line and our EC-SLI setup, being dedicated to collect long-lived isotopes to be measured off-line.
	- Successfully testing of new fast VATAGP7 pad Si (1mm) detectors, to be commissioned during 2013/14. High performance fast readout and improved energy resolution.
	- Successfully readout debugging and tests. Actually we can achieve more than 5.5 kHz and the readout limitation is still the controlling PC.
	-Successfully mounting and commissioning, tests and true runs of a very small – fully developed by us – heating element needed for the high precision new Panmure goniometer in use at the EC-SLI setup. We achieved 900°C annealing temperatures.
	- Successfully proof-of-use of timepix detectors aiming alpha and He/H particles on emission channelling and RBS/C experiments. The experimental part of this work has been done at ITN and the results have been presented at the November Medipix meeting.
4	Students and training
	Training and thesis – are the aim and the way – to perform the scientific work at our experimental infrastructure. Students come from different environments and universities. They are supported via: current projects, home institutions, or FCT grants. For students, less covered elsewhere, European funding (FP7-ENSAR-262010) covers partial expenses during beam times.
	In 2012, directed related to our projects and proposals, we had 6 PhD students (2 FCT-grant, 1 IKS- Leuven, 3 project funded) and 3 MSc students (project funded). Two undergraduate students (IKS- Leuven Erasmus student at IST and an IST summer student at ISOLDE) are / have been working with us.
	Work performed at ISOLDE – JGMC PhD co-supervisor of:
	<ul> <li>Ângelo Costa: "Ion implantation doping of SiC", IST, Universidade Técnica de Lisboa, since Nov 2012.</li> </ul>
	• Abel Fenta: "Hyperfine Techniques Studies of surfaces and interfaces using isolated ad-atom radioactive probes", Universidade de Aveiro/CICECO, since Nov 2012.
	• Marcelo Barbosa: "Atomistic view of the functionalization of wide gap semiconductor nanowires – <i>defects recombination rates and excited states</i> ", Universidade do Porto/IFIMUP, since Jan 2012.
	• Pos-Doc co-responsible of: João Gonçalves: "Study of hyperfine properties of multiferroic

materials and low dimensional structures (graphene and other carbon layered and nanostructred materials), CICECO and ISOLDE, since Mar 2012.

#### PAPERS

- J.G. Correia, K. Johnston and U. Wahl: "Nuclear radioactive techniques applied to materials research", Radiochimica Acta 100, 127-137 (2012), doi: 10.1524/ract.2011.1873.
- S. Decoster, U. Wahl, S. Cottenier, J. G. Correia, T. Mendonca, L. M. Amorim, L. M. C. Pereira, and A. Vantomme: "Lattice position and thermal stability of diluted As in Ge", *Journal of Applied Physics* 111, 053528 (2012), doi: 10.1063/1.3692761.
- L. M. C. Pereira, U. Wahl, J. G. Correia, S. Decoster, L. M. Amorim, M. R. da Silva, and J. P. Araújo, A. Vantomme: "Evidence of N substitution by Mn in GaN", *Physical Review B*, 86, 195202 (2012), <u>doi:</u> 10.1103/PhysRevB.86.195202.
- L. M. C. Pereira, U. Wahl, S. Decoster, J. G. Correia, L. M. Amorim, M. R. da Silva, J. P. Araujo, A. Vantomme; "Stability and diffusion of interstitial and substitutional Mn in GaAs of different doping types", *Physical Review B*, 86, 125206 (2012). doi: 10.1103/PhysRevB.86.125206.
- P. Miranda, U. Wahl, N. Catarino, K. Lorenz, J.G. Correia, E. Alves, Damage formation and recovery in Fe implanted 6H–SiC, *Nuclear Instruments and Methods in Physics Research* B 286, 89-92 (2012), doi: 10.1016/j.nimb.2011.10.072.
- J. N. Gonçalves, A. Stroppa, J. G. Correia, T. Butz, S. Picozzi, A. S. Fenta, V. S. Amaral; "Ab initio study of the relation between electric polarization and electric field gradients in ferroelectrics", *Physical Review B*, 86, 035145 (2012), doi:10.1103/PhysRevB.86.035145.
- G. N. P. Oliveira, A. M. Pereira, A. M. L. Lopes, J. S. Amaral, A. M. dos Santos, Y. Ren, T. M. Mendonc, C. T. Sousa, V. S. Amaral, J. G. Correia and J. P. Araújo; "Dynamic off-centering of Cr3+ ions and short-range magneto-electric clusters in CdCr2S4", *Physical Review B*, 86, 224418 (2012), doi/10.1103/PhysRevB.86.224418.
- S. M. C. Miranda, P. Kessler, J. G. Correia, R. Vianden, K. Johnston, E. Alves and K. Lorenz; "Ion implantation of Cd and Ag into AlN and GaN", *Physica. Status Solidi C*, 9, No. 3–4, 1060–1064 (2012), doi: 10.1002/pssc.201100203.
- P. Kessler, K. Lorenz, S. M. C. Miranda, R. Simon, J. G. Correia, K. Johnston, R. Vianden and the ISOLDE collaboration; "Cd doping of AlN via ion implantation studied with perturbed angular correlation", *Physica. Status Solidi C*, 9, No. 3–4, 1032–1035 (2012), doi: 10.1002/pssc.201100207.

#### **COMMUNICATIONS**

#### Invited Talks

- Applications of radioactive ion beams at EURISOL, new tools, new ideas, new people, <u>J. G. Correia</u>, *Eurisol Town meeting, Instituto Superior Técnico, Lisboa, Portugal, Oct 15-19 (2012), invited talk.*
- Five Years of Applications of EXOCTIC radioactive ion beams at ISOLDE, J. G. Correia, The 16th IUPAP International Conference on Electromagnetic Isotope Separators and Techniques Related to Their Applications (EMIS2012) Matsue, Japan, Dec 2 7 (2012), invited talk.
- Emission channeling studies on the lattice location of transition metals in dilute magnetic semiconductors, L. M. C. Pereira, U. Wahl, S. Decoster, <u>J. G. Correia</u>, L. M. Amorim, J. P. Araújo, K Temst, and A. Vantomme, 4th Joint Meeting of the 16th International Conference on Hyperfine Interactions and the 20th international Symposium on Nuclear Quadrupole Interactions (HFI/NQI 2012), Beijing, China, Sep 10-14 (2012), invited talk.
- Thin films, nano-structures and ion implantation a microscopic-world viewed at atomic scale by exotic nuclear methods, M. Barbosa, J. N. Gonçalves, A. Redondo-Cubero, S. M. C. Miranda, R. Simon, P. Kessler, M. Brandt, F. Henneberger, E. Nogales, B. Méndez, K. Johnston, E. Alves, R. Vianden, J. P. Araújo, K. Lorenz, J. G. Correia, EMRS Fall Meeting 2012, Symposium L, University of Technology, Warsaw, Poland, Sep 17-21 (2012) ), invited talk.

#### Talks

- Position-sensitive detectors for RBS channelling experiments, U. Wahl, J.G. Correia, P. Miranda, N. Catarino, E. Bosne, M.R. Da Silva, L. Amorim, E. Alves, Joint Research Activity Meeting of the SPIRIT (Support of Public and Industrial Research using Ion Beam Technology) EU FP7 Collaborative Project, Leuven, Belgium, March 5-6 (2012), oral.
- Lattice location of Ni in Si by means of on-line emission channelling, D.J. Silva, <u>U. Wahl</u>, J.G. Correia, L.M.C. Pereira, L. Amorim, E. Bosne, M. Ribeiro da Silva, S. Decoster, J.P. Araújo, 2012 Spring Meeting of the European Materials Research Society (E-MRS), Symposium A "Advanced silicon materials research for electronic and photovoltaic applications III", Nice, France, May 14-18(2012), oral.
- Lattice location of transition metals in dilute magnetic semiconductors, L.M.C. Pereira, U. Wahl, S. Decoster, J.G. Correia, L.M. Amorim, J.P. Araújo, K. Temst, A. Vantomme, *General Scientific Meeting 2012 of the Belgian Physical Society (BPS), Brussels, Belgium, May 30 (2012)*, oral.
- Lattice location of transition metals in dilute magnetic semiconductors using EC-SLI (IS453), L. M. C. Pereira, U. Wahl, S. Decoster, J. G. Correia, L. M. Amorim, J. P. Araújo, K. Temst, and A. Vantomme ISOLDE workshop and users meeting 2012, Geneva, Switzerland, Dec 17-19 (2012), oral.
- Direct measurement of the Mg lattice site location in group III-Nitrides, L.M. Amorim, U. Wahl, S. Decoster, L.M.C. Pereira, J. G. Correia, D.J. Silva, K. Temst, and A. Vantomme, 4th International Symposium on Growth of III-Nitrides, St. Petersburg Russia, July 16-19 (2012), oral.
- Study of a Timepix+FitPix detection system for applications in RBS/C materials analysis using MeV He and H beams, E. D. Bosne, U. Whal, J. G. Correia, V. Amaral, Medipix2 open meeting, CERN, Geneva, Switzerland, Nov 28 (2012), oral.
- Localização de impurezas na rede cristalina de nitretos semicondutores, L. M. Amorim, U. Wahl, J. G. Correia, K. Temmest, A. Vantomme, 18<sup>a</sup> Conferência Nacional de Física, Aveiro, Portugal, Set 6-8 (2012), oral.
- Localização de metais de transição em silício através da técnica emission channeling, D. J. Silva, U. Wahl, J. G. Correia, J. P. Araújo, 18<sup>a</sup> Conferência Nacional de Física, Aveiro, Portugal, Set 6-8 (2012), oral.

#### Posters

- Lattice location of Ni in Si by means of on-line emission channelling, D. J. Silva, U. Wahl, J. G. Correia, L. M. C. Pereira, L. M. Amorim, E. Bosne, M. M. Ribeiro da Silva, S. Decoster, J. P. Araújo *E-MRS 2012* Spring Meeting, Strasbourg, France, May 15-17 (2012), poster.
- Lattice sites of implanted transition metals in dilute magnetic semiconductors, L. M. C. Pereira, U. Wahl, S. Decoster, J. G. Correia, L. M. Amorim, J. P. Araújo, K Temst, and A. Vantomme, 18th International Conference on Ion Beam Modifications of Materials (IBMM2012), Qingdao, China, Sep 10-14 (2012), poster.
- Ab-initio computation of electric field gradients and magnetic hyperfine fields as local property probes in multiferroics, J. N. Gonçalves, A. S. Fenta, A. Stroppa, J. G. Correia, S. Picozzi, V. S. Amaral, Psi-k Research Conference on Computational Oxide Spintronics, Cranage Hall, Manchester, United Kingdom, May 6-10 (2012), poster.
- Ab-initio calculation and study of hyperfine properties of layered ferroelectrics doped with magnetic ions, A. S. Fenta, J. N. Gonçalves, A. Stroppa, <u>J. G. Correia</u>, S. Picozzi, and V. S. Amaral, *Psi-k Research Conference on Computational Oxide Spintronics, Cranage Hall, Manchester, United Kingdom, May 6-10* (2012), poster.
- Ab-initio calculation and study of hyperfine properties of layered ferroelectrics doped with magnetic ions, A. S. Fenta, J. N. Gonçalves, A. Stroppa, J. G. Correia, S. Picozzi, and V. S. Amaral, Joint Symposium ISAF/ECAPD/PFM, University of Aveiro, Portugal, July 9-13 (2012), poster.
- Ab-initio computation of electric field gradients and magnetic hyperfine fields as local property probes in multiferroics, J. N. Gonçalves, A. S. Fenta, A. Stroppa, <u>J. G. Correia</u>, S. Picozzi, V. S. Amaral, Joint Symposium ISAF/ECAPD/PFM, University of Aveiro, Portugal, July 9-13 (2012), poster.

- Lattice location study of implanted As in Ge, S. Decoster, U. Wahl, S. Cottenier, J.G. Correia, T. Mendonça, L.M. Amorim, L.M.C. Pereira, A. Vantomme, 18th International Conference on Ion Beam Modification of Materials (IBMM), Qingdao, China, Sept 2-7 (2012), poster.
- Ab-initio study of the relation between electric polarization and electric field gradients in ferroelectrics, J. N. Gonçalves, A. Stroppa, J. G. Correia, T. Butz, S. Picozzi, A. S. Fenta, V. S. Amaral, Eurisol Town meeting, Instituto Superior Técnico, Lisboa, Portugal, Oct 15-19 October (2012), poster.
- Nuclear radioactive techniques applied to study add-atoms on surfaces, A. S. Fenta, <u>J. G. Correia</u>, A. Gottberg, K. Johnston, Y. Kadi, V. S. Amaral, J. N. Gonçalves, *Eurisol Town meeting, Instituto Superior Técnico, Lisbon, Portugal, Oct 15-19 October (2012)*, poster.
- The testing of Timepix detectors for position-sensitive detection of charged-particles, E. D. Bosne, U. Wahl, J. G. Correia, P. Miranda, L. M. Amorim, M.R. da Silva, Eurisol Town meeting, Instituto Superior Técnico, Lisboa, Portugal, Oct 15-19 October (2012), poster.
- CdCr2S4: Randomly oriented dipoles arising from Cr3+ dynamic off-centering, G. N.P. Oliveira, A.M. Pereira, A.M.L. Lopes, J.S. Amaral, A.M. dos Santos, T.M. Mendonça, C. T. Sousa, Y. Ren, V. S. Amaral J. G. Correia, J. P. Araújo, Eurisol Town meeting, Instituto Superior Técnico, Lisbon, Portugal, Oct 15-19 October (2012), poster.
- Lattice location of the transition metals Fe and Ni in Si by means of emission channeling from implanted radioactive isotopes, D. J. Silva, U. Wahl, J. G. Correia, L.M.C. Pereira, L. Amorim, E. Bosne, M. Ribeiro da Silva and J.P. Araújo, Eurisol Town meeting, Instituto Superior Técnico, Lisbon, Portugal, Oct 15-19 October (2012), poster.
- The study of thin films and nanostructures at atomic scale using exotic nuclear methods, M. Barbosa, J. N. Gonçalves, A. Redondo-Cubero, S. M. C. Miranda, R. Simon, P. Kessler, M. Brandt, F. Henneberger, E. Nogales, B. Méndez, K. Johnston, E. Alves, R. Vianden, J. P. Araujo, K. Lorenz, <u>J. G. Correia</u>, Eurisol Town meeting, Instituto Superior Técnico, Lisbon, Portugal, Oct 15-19 October (2012), poster.
- que se aprende ao simular à escala atómica em compostos multiferróicos?, A. S. Fenta, J. N. Gonçalves, V. S. Amaral, J. G. Correia, A. Stroppa, S. Picozzi, Física 2012, 18<sup>a</sup> Conferência Nacional de Física, University of Aveiro, Aveiro, Portugal, Sep 6-8 (2012), poster.
- Use of position-sensitive pixel detectors for ion beam analysis, E. D. Bosne, U.Wahl, J. G. Correia, V.S. Amaral, A. A. C. S.Lourenço, P. Miranda and E. Alves, Física 2012, 18<sup>a</sup> Conferência Nacional de Física, University of Aveiro, Aveiro, Portugal, Sep 6-8 (2012), poster.

#### **EDUCATION – THESES SUPERVISION**

- Co-supervisor (J. G. Correia), PhD Thesis, Advanced nanoscopic studies in magneto-electric manganites and high TC superconductors by Tânia Manuela de Melo Mendonça, Faculdade de Ciências, Universidade do Porto, 17<sup>th</sup> February 2012.
- Opponent (J. G. Correia), PhD Thesis, *Nuclear Techniques Using Radioactive Beams for Biophysical Studies* by Monika Kinga Stachura, Faculty of Science, Department of Chemistry, University of Copenhagen, 14<sup>th</sup> December 2012.
- Opponent (J. G. Correia), M. Sc. Thesis, *Effect of Calcium Oxide Microstructure on the Diffusion of Isotopes* by João Pedro Fernandes Ramos, Dep. Química, Universidade de Aveiro, 14<sup>th</sup> February 2012.
- Opponent (J. G. Correia), M. Sc. Thesis, *Neutronic performance and elements of radiological protection and safety of CERN's HIE-ISOLDE Radioactive Ion Beam production facility* by Ricardo Manuel dos Santos Augusto, IST, Universidade Técnica de Lisboa, 19<sup>th</sup> October 2012.

#### **PROJECTS**

• Perturbed Angular Correlations and Electron Channelling Experiments at ISOLDE - applied materials research with nuclear techniques, training and development, FCT-CERN-FP-116320-2010, €120,000 (from the 1st January 2011 up to the 31st March 2012), Leading Institution ITN, Coordinator: J.G. Correia (60%).

• Perturbed Angular Correlations and Electron Channelling Experiments at ISOLDE - applied materials research with nuclear techniques, training and development, FCT-CERN-FP-123585-2011, €245000 (from the 1st July 2012 up to the 31st May 2014). Leading Institution CTN/IST-ID, Coordinator: J.G. Correia (60%).

## **CONFERENCE ORGANIZATION / COMMITTES**

• J.G. Correia, member of the Nuclear Quadrupole Interactions (NQI) Conference International Advisory Committee, since 2005.

# NAME: Rui Manuel Coelho da Silva

**CATEGORY:** Principal Researcher **ID NUMBER:** 25383

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	PTDC/FIS /102270/2008	20%
	Nanostructured magnetic nitrides	
2	PTDC/CTM-MET/112831/2009	15%
	Fault-tolerant anticorrosion coatings for magnesium alloys	
3	PTDC/FIS /115089/2009	30%
	Depth-selective Ion Microprobe Tomography-Tomo3D	
4	QREN/COMPETE AdI/23274/2012	15%
	Nobly Decorated Crystal-NobleDec	
5	Medieval Portuguese tiles: materials, production techniques and provenance study	10%
	(co-supervision of SFRH/BD/73007/2010)	
6	Data acquisition and interface control	10%
Total		100%

N°	Summary and Main Achievements
1	Aiming at developing embedded magnetic nitrides of Fe, Co and Ni, single crystals of these metals were implanted at room temperature with 50 keV N+ ions to fluences of $5 \times 1017$ cm $\Box 2$ , under $10^{\circ}$ incidence to avoid channelling effects. The presence of nitride phases was investigated by XRD, and also with CEMS in the case of Fe. The structural and composition modifications were followed by RBS and RBS/C, and the nitrogen depth profiles and implanted fluences investigated with the $14N(p,p)14N$ elastic reaction.
	The results show that Fe2N, Co2N and Ni2N could be identified in the as-implanted state, Co2N forming in <i>m</i> -cobalt but not in <i>c</i> -cobalt, Fe2N forming for all crystal orientations. These results contrast with findings of previous work with similarly implanted polycrystalline plates where Ni3N was found instead and no CoxN phases appeared at all. Parallel work using the reactive sputtering technique with Co, showed that controlling the amount of nitrogen in the plasma forming media, yield films containing the near-Co4N and Co3N phases.
2	Aiming at developing fault-tolerant anticorrosion coatings for magnesium alloys, samples of ZE41 Mg-based aeronautic grade alloy were analysed with proton beams with energies in the range 1.35 MeV to 2 MeV and with 2 MeV 4He ion beams, by RBS, ERD and PIXE. Anodized and PEO polymer coated samples were also analysed. A total of 105 RBS and NRA spectra were collected, for 35 measurements, plus 22 ERD and RBS spectra for H characterization. The results obtained show that: <i>i</i> ) there is F and H in all surface modified samples, anodized and PEO coated; <i>ii</i> ) a MgO/Mg(OH)2 layer with thickness of ~0.1 µm or less developed upon anodization; <i>iii</i> ) F sits at the surface, while H extends through the anodized region; <i>iv</i> ) on the contrary, in PEO coated samples F most probably spreads across several $\Box$ m, eventually across the entire coatings. These results were communicated to and shared with the research partners IST, UA and EADS.

3	Aiming at developing and endowing IST/ITN with the capability of performing tomographic reconstruction from PIXE and STIM-T map sets obtained with the ion microprobe from sub-millimetre samples, the following tasks were completed successfully:
	- Generation of STIM-T map sets from SiC microcomposite fibre materials for demonstration of practical feasibility;
	- Implementation of concept, commitment to LIP precision mechanical workshop, assembly, installation and test of a $4+1$ degrees of freedom positioning stage for precise alignment of samples with the rotation axis. The 4 degrees of freedom of the setup goniometer have micrometre precision. The motorized rotation stage allow a minimum step of $0.45^{\circ}$ rotation under computer control;
	- Implementation of an alignment procedure using a micro-TV camera coupled to a binocular magnifier, allowing nearly precession-free rotation
	- Implementation of pre-processing and reconstruction software <i>TomoAlign</i> and back filtered projection-based <i>Tomo3D</i> to digitally correct experimental alignment inaccuracies and reduce tomogram stability artefacts;
	- Development of a new algorithm for removal of background noise and spectral spikes;
	- Test of a gas flow ionization chamber developed at LIP for use with on-axis STIM-T.
4	Aiming at contributing to solve problems of adhesion, durability, consistency and reproducibility of decorative paintings with the noble metals Au and Pt in high added value crystal glasses, a collection of Pb-crystal glass samples with Au decorative films in different stages of manufacturing, from the first paint applications to the final heat treatments, were analysed by PIXE and RBS, and the results compared with mea-surements by SEM-EDS, FTIR and Raman spectroscopies. Substrate Pb-crystal glass samples were also characterised. The compositions found agree with those expected from the batch compositions used by the glass-maker.
	The average thickness per painting layer, its characteristic spread and contents in Au and Ag metals were obtained. These are generally consistent with the application information provided by the manufacturers of the Au paints. However interlayers were identified between successive application layers which composition and/or density depart from adjacent layers and are consistent with Ag-Au sulphides/oxides.
	RBS and PIXE analyses of areas showing degradation of the decorative paint showed a change in thickness but not conclusive differences in elemental composition, the issue remaining open.
5	Aiming at contributing to solve the question of whether there was local production of decorative tiles in Portugal, in the historic period from late XIVc. to early XVIc., samples from a collection of Hispano-Moresque tiles unearthef during archaeological excavations of the Monastery of Santa Clara-a-Velha, were analysed by PIXE and RBS. The results were cross-compared with results obtained by XRF, SEM-EDS and Raman spectroscopy.
	Homogeneous glazes with high lead contents (37-54 wt.%) were found suggesting usage of glass frit. Oxides of tin, cobalt, copper, iron and manganese were identified as colour agents in white, blue, green, yellow and purple glazes respectively. Mineral bustamite was found in purple glazes, and wollastonite and quartz in several glaze-ceramic interfaces. Cassiterite was identified for every colour, although tin was only identified in white and blue glazes.
	Cobalt was found in association with Fe, Ni and Cu but no As was detected, in consistency with Co ore material imported from Saxony before 1520. However a positive identification of its source was not yet achieved. The composition results are consistent with those reported in the literature for Mudéjar ceramics, and show considerable similarity between the glazes of "cuerda-seca" and "arista" tiles, sugges-ting usage of similar recipes.
6	Computer codes of general use in IBA experiment control and automatic data acqui-sition, and for spectral data conversion were continuously improved and expanded in specific capacities, namely:
	- GonMTRS32 code used for automatic experiments and data acquisition by RBS, PIXE and RBS/channelling was made much more robust, by reworking the code and adding checks and protections (crash/malfunction rate reduced to near zero); was en-dowed with new and improved

graphics interface featuring enhanced handling of the angular scan plots display; added acquisition control and data storage options; added experimental control of a new setup (dedicated for JET materials characterization by IBA);

- CvDataX code for spectral data format conversion was enhanced by allowing for new input and output formats (added formats).

An update of the user interface Genie2k (CANBERRA©) for MCA boards control/data acquisition, was installed, configured and tested, and its interaction with GonMTRS32 code tested.

Experimental software SerialMTRS developed for testing control of stepping motors via COTS (*Commercial Off The Shelf*) control drive and power units, aiming at duplicating the IBA experimental control setup GUIs in use with the VG accelerator, for use with the tandem accelerator.

#### PAPERS

- R.P. Borges, B. Ribeiro, A.R.G. Costa, C. Silva, R.C. da Silva, G. Evans, A.P. Gonçalves, M.M. Cruz, M. Godinho, U. Wahl, Erratum: Magnetic and transport properties of transition-metal implanted ZnO single crystals, European Journal of Physics B, 85-3 (2012) 85: 91. doi:10.1140/epjb/e2012-30089-y.
- B. Berini, A. Fouchet, E. Popova, J. Scola, Y. Dumont, N. Franco, R.M.C. da Silva, N. Keller, High temperature phase transitions and critical exponents of Samarium orthoferrite determined by in situ optical ellipsometry, Journal of Applied Physics 111, 053923 (2012). doi:10.1063/1.3692088.
- B. Ribeiro, R.P. Borges, R.C. da Silva, N. Franco, P. Ferreira, E. Alves, B. Berini, A. Fouchet, N. Keller, M. Godinho, Structural and magnetic properties of thin films of BaFeO3-d deposited by pulsed injection metal-organic chemical vapour deposition, Journal of Applied Physics, 111, 113923 (2012). doi:10.1063/1.4729269.
- A.C. Marques, D. Beaseley, L.C. Alves, R.C. da Silva, Selected pre-processing methods to STIM-T projections, *in* Computational modelling of objects represented in images, Fundamentals, Methods and Applications III, Di Giamberardino *et al.*, Eds., CRC Press, pp.377-382 (2012). ISBN 978-0-415-62134-2, doi: 10.1201/b12753-70.
- S. Routa, N. Popovicia, S. Daluia, M.L. Paramês, R.C. da Silva, A.J. Silvestre, O. Conde, Phase growth control in low temperature PLD Co: TiO2 films by pressure, Current Applied Physics, X(2012)1-7. doi:10.1016/j.cap.2012.11.005.

#### **COMMUNICATIONS**

- Structural and magnetic properties of pseudocubic BaFeO<sub>3-δ</sub> thin films produced by PI-MOCVD, B. Ribeiro, R.P. Borges, R.C. da Silva, N. Franco, P. Ferreira, E. Alves, M. Godinho, SCTE2012 18th International Conference on Solid Compounds of Transition Elements, Lisboa, Portugal, 31 Mar.-05 Apr., 2012. Talk (by B. Ribeiro).
- Architectural tiles in the Monastery of Santa Clara-a-Velha in Coimbra, Portugal: study of the production techniques, S. Coentro, R. Trindade, A. Candeias, J. Mirão, L. Cerqueira, R. Silva, V. Muralha, Global Pottery 1st International Congress on Historical Archaelogy & Archaeometry for Societies in Contact, Barcelona, Spain, 7-9 May, 2012. Talk (by S. Coentro).
- μ-Raman analysis of Hispano-Moresque historical tiles, Susana Coentro, Luís Cerqueira, Rui M.C. Silva, Vânia S.F. Muralha, ChemCH-2012: 2nd International Congress Chemistry for Cultural Heritage, Istanbul, Turkey, 9-12 Jul., 2012. Talk (by S. Coentro).
- *Iron, nickel and cobalt nitrides produced by* N+ *ion implantation,* A.R.G. Costa, R.C. da Silva, L.P. Ferreira, Margarida Pires, N. Franco, M. Godinho, M.M. Cruz, JEMS 2012 Joint European Magnetic Symposia, Parma, Italy, 09-14 Sep., 2012. Talk (by A. Costa).
- Chemical characterisation of Hispano-Moresque tiles from the Monastery of Santa Clara-a-Velha in Coimbra, Portugal, Susana Coentro, Rui A.A. Trindade, António Candeias, José Mirão, Luís Cerqueira, Rui M.C. Silva, Vânia S.F. Muralha, Azulejar-2012, Aveiro, Portugal, 10-12 Oct., 2012. Talk (by S. Coentro).

- Magnetoelectric coupling in BaTiO3/Fe, R.P. Borges, B. Ribeiro, N. Sobolev, R.C. da Silva, C. Magén, M.M. Cruz, M. Godinho, SCTE2012 – 18th International Conference on Solid Compounds of Transition Elements, Lisbon, Portugal, 31 Mar.-05 Apr., 2012. Poster.
- Formation of transition metal nitrides by N+ ion implantation, A.R.G. Costa, R.C. da Silva, L.P. Ferreira, N. Franco, M. Godinho, M.M. Cruz, SCTE2012 18th International Conference on Solid Compounds of Transition Elements, Lisboa, Portugal, 31 Mar.-05 Apr., 2012. Poster.
- Characterization of Co/N thin films deposited by reactive sputtering, C. Silva, A. Vovk, R.C. da Silva, P. Štrichovanec, P.A. Algarabel, A.P. Gonçalves, R.P. Borges, M. Godinho, M.M. Cruz, SCTE2012 18th International Conference on Solid Compounds of Transition Elements, Lisbon, Portugal, 31 Mar.-05 Apr. 2012. Poster.
- Analysis of Hispano-Moresque architectural tiles by μ-Raman spectroscopy, S. Coentro, R. Silva, V. Muralha, Global Pottery 1st International Congress on Historical Archaelogy & Archaeometry for Societies in Contact, Barcelona, Spain, 7-9 May, 2012. Poster.
- Study of Hispano-Moresque tiles from the Monastery of Santa Clara-a-Velha in Coimbra, Portugal, using μ-PIXE, Susana Coentro, Rui A.A. Trindade, Vânia S.F. Muralha, Luís Cerqueira, Rui M.C. Silva, 13th International Conference on Nuclear Microprobe Technology & Applications, Lisbon, Portugal, 22 27 Jul., 2012. Poster.
- New gas detector setup for on-axis STIM tomography experiments, A.C. Marques, M.M.F.R. Fraga, P. Fonte, D.G. Beasley, L.C. Alves, R.C. da Silva, 13th International Conference on Nuclear Microprobe Technology & Applications, Lisbon, Portugal, 22 27 Jul., 2012. Poster.
- Selected pre-processing methods to STIM-T projections, A.C. Marques, D.G. Beaseley, L.C. Alves, R.C. da Silva, CompImage2012, Computational Modelling of Objects Presented in Images: Fundamentals, Methods and Applications, Rome, Italy, Sep 5-7, 2012. Poster.
- Study of substrate induced anisotropy in Co-N thin films, C. Silva, A.Vovk, R.C. da Silva, P.Štrichovanec, P.A. Algarabel, A.P. Gonçalves, R.P. Borges, M. Godinho, M.M. Cruz, JEMS 2012 Joint European Magnetic Symposia, Parma, Italy, 09-14 Sep., 2012. Poster.
- Lectures in Ion Beam Analysis, the RBS technique: lecture in the framework of one semester course on *Methods of Inspection and Analysis*, for the 8th semester of Conservation and Restoration curricular plan, Faculty of Sciences and Technology, Universidade Nova de Lisboa, 27 Nov., 2012.
- Lectures in Ion Beam Analysis, the PIXE technique: lecture in the framework of one semester course on *Methods of Inspection and Analysis*, for the 8th semester of Conservation and Restoration curricular plan, Faculty of Sciences and Technology, Universidade Nova de Lisboa, 03 Dec., 2012.
- Ion Beam Techniques: fundamentals, SPIRIT Intensive Course on Ion Beams as a Tool for Nanotechnology, IST/CTN, Sacavém, Portugal, 18 Jul., 2012.

#### **EDUCATION / THESES SUPERVISION**

- Co-supervisor of post-doctoral work of D.Sc. Ana Cláudia Santana Marques, 3D Microprobe: Tomography by PIXE, RBS and STIM (SFRH/BPD/65817/2009).
- Co-supervisor of doctoral work of M.Sc. Susana Xavier Coentro, *Medieval Portuguese tiles: materials, production techniques and provenance study* (SFRH/BD/73007/2010).
- Invited Professor, *Nuclear Physics*. Theoretical lectures and laboratory practice on nuclear physics at introductory level: one semester course for the 7th semester of the Physical Engineering and Biomedical Engineering curricular plans, Faculty of Sciences and Technology, Universidade Nova de Lisboa.
- Welcome and introductory talks about the mission and the on-going technical and scientific work at IST/ITN, for regular scheduled visitors students from high schools and universities (responsibility shared with colleague research officers António Falcão and Nuno Barradas).

#### PROJECTS

• *Nanostructured magnetic nitrides*-Nanomag. Grant PTDC/FIS /102270/2008. Leading Institution: FFCUL. IST/ITN Coordinator: R.C. Silva (20%). IST/ITN budget (overall): 41875 €.

- Fault-tolerant anticorrosion coatings for magnesium alloys-Fatomag. Grant PTDC/CTM-MET/112831/2009. Leading Institution: IST. IST/ITN Coordinator: R.C. Silva (15%). IST/ITN budget (overall): 19932 €.
- Depth-selective Ion Microprobe Tomography-Tomo3D. Grant PTDC/FIS /115089/2009. Leading Institution: IST/ITN. PI: A.C. Marques (FCT post-doctoral fellow, 100%). IST/ITN Coordinator: R.C. Silva (30%). Budget (overall): 92322 €.
- *Nobly Decorated Crystal*-NobleDec. Grant AdI/23274/2012, QREN programme COMPETE. Leading Institution: VAA-Vista Alegre/Atlantis. IST/ITN Coordinator: R.C. Silva (20%). IST/ITN budget (overall): 102000 €.

## **CONFERENCE ORGANIZATION / COMITTEES**

- Member of the Organising Committee, of the 13th International Conference on Nuclear Microprobe Technological Applications (ICNMTA), Lisboa, Portugal, 22-27 July, 2012.
- Member of the refereeing, revising and editorial board for the proceedings of the 13th *International Conference on Nuclear Microprobe Technological Applications* (ICNMTA), Lisboa, Portugal, 22-27 July, 2012.

## **COLLABORATIONS**

- M. Fraga, P. Fonte, R.F. Marques and LIP-Coimbra, Laboratório de Instrumentação e Física Experimental de Partículas, Coimbra, Portugal. Development and performance tests of prototype gas detector for on-axis STIM tomography.
- M. Ventura, A.J. Parola, A. Ruivo, A.P. Matos, VICARTE, Centro para o Vidro a Cerâmica e a Arte, Univ. Nova de Lisboa, Monte da Caparica, Portugal. Study of new colouration processes in glasses.
- M. Ventura, *et al.*, REQUIMTE, Dep. Chemistry, Faculty of Sciences and Technology, Univ. Nova de Lisboa, Monte da Caparica, Portugal. Induction and study of photochromic and luminescence behaviour in hackmanite by thermal reduction.

# **NAME: Carlos Manuel Marques da Cruz**

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 25356

#### **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Staff Engineer (Chief Engineering of the Instrumentation and Accelerators of the Ion	70%
	Beam Laboratory)	
2	Participation of ITN on n_TOF experiments (phase 2) at CERN	10%
3	EMRP Project: IND04 MetroMetal	15%
	EMRP Project: JRP- i13 MetroNORM	
4	Ionizing Radiation Tecnologes (TRI)	5%
Total		100%

Nº	Work Summary and Main Achievements
1	1.1 - Responsibilities for inspecting, testing and troubleshooting electronic systems, performing advanced engineering tasks in order to achieve higher reliability and availability of the equipments;
	Designing and fabricating electronic, mechanical and software interfaces for data acquisition, AMS technique;
	Calibration, testing, debugging hardware modules, reworking, modifying and inspecting highly complex electronic/electrical instrumentation and automation systems required for research inside and outside IST/ITN, namely FCTUL (Ortec and XRF analyzer equipment);

	Technical advice, reviews, studies and analyses in support of other groups technical projects;
	Finished the automation of the vertical axis for the vacuum chamber used in materials studies of the <i>JET experiment</i> . A step motor was mechanical and electrically adapted and connected to existent control equipment.
	Documenting projects and communicating project progress to the user community.
	<i>1.2 - SPIRIT Project:</i> Development and processing of advanced materials with ion beams – Specific equipment (design of CSP preamplifiers based on Hamamatsu H4083 and Amptek A250 chips):
	Circuit design, PCB fabrication, assembling and tests of nuclear preamplifiers with the purpose of replacing old Ortec and Canberra preamps;
	In circuit designing attention was paid to the layout details, in order to reduce the effect of leakage and stray capacitance;
	The complete assembly and one S-3590-09 detector were housed for tests inside a vacuum chamber with an 241Am triple source and included in a standard nuclear instrumentation chain;
	Performed tests revealed excellent results during operation up to 80V detector bias voltage. The electrical noise from the H4083 was estimated at 550 electrons/FWHM. The charge gain was 0.5V/pC, which is equivalent to 22mV/MeV(Si);
	In case of H4083 a triple channel preamplifier was designed using SMD technology fitting within a 2-layer PCB size of 50x50 mm.
	The other designed circuit was based on a hybrid state-of-the-art chip - The A250. This chip can be used with a wide range of detectors having capacitance from less than one, to several thousand pF and it can be incorporated into any system where charge amplification is required.
	We are waiting the best opportunity to make effective tests with this assembly.
2	This project is the continuation of the involvement of ITN in the activities of the n_TOF Collaboration. In the past we have made circuits for the TAC (Total Absorption Calorimeter) that is inside the n_TOF experimental area. The TAC is a segmented $4\pi$ array made of 40 BaF2 crystals forming a spherical shell of 20 cm and 50 cm inner and outer diameters respectively, and is used for measuring capture reactions of small mass and radioactive samples.
	We are expected to collaborate in the project for optimization of particle detection systems after the construction of a 2nd Experimental Area (EAR-2), vertically located 20 m on top of the n_TOF spallation target with its enhanced capabilities for measurements of neutron-induced reactions.
3	EMRP Project: IND04 MetroMetal: Ionising radiation metrology for the metallurgical industry.
	Data collection on systems and methods used for monitoring cast stell, scrap, slags and fume dusts. Studies for the sample chamber and optimal detector type were evaluated by the group.
	EMRP Project: JRP- i13 MetroNORM: Metrology for processing materials with high natural radioactivity.
	This project has been approved and will start in March 2013 addressing several scientific and technical objectives.
4	Zwick Universal Mechanical Testing Machine (Zwick 1435).
	Carver Laboratory Hydraulic Press (Model C).
	Technical advice and supervision of a fellow in the functional up-grade of the control system and digital data acquisition.
	Recovery of the Programmable Temperature Control System (mechanical stress tests and preparation of samples for tensile tests).
	Recovery put into operation and calibration of the complete system of radiation protection instrumentation monitors of the <i>UTR facility</i> (BERTHOLD).

# TALKS

• Evidence of Structural Order Recovery in LDPE Based Copolymers Prepared by Gamma Radiation, L.M. Ferreira, J.P. Leal, M.H. Casimiro, C. Cruz, J.J.H. Lancastre, A.N. Falcão, IRaP'2012 - 10th Meeting of the Ionizing Radiation and Polymers Symposium, Cracow, Poland, Oct 14-19 (2012), Oral.

# NAME: Isabel Maria Ferro Pereira Gonçalves

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 25361

# **RESEARCH ACTIVITIES**

Nº	Activity Description	R&D
1	Participation of ITN on n_TOF experiments (phase 2) at CERN	50%
2	Cooperation with CERN: Optimization studies of the ISOLDE targets and design of	30%
	HIE-ISOLDE	
3	ANDES (Accurate Nuclear Data for nuclear Energy Sustainability)	20%
Total		100

Nº	Work Summary and Main Achievements
1	A complete and precise knowledge of cross sections for neutron induced processes is required for multiple applications such as the design of ADS and EA systems for the transmutation of nuclear waste and energy production, radioisotope production for medical and industrial applications and Astrophysics, Nuclear Physics and Nuclear Technology.
	The n_TOF Collaboration has been carrying out experimental campaigns at the neutron time of flight spectrometer at CERN, using the CERN/PS accelerator complex. In this facility, a proton pulse of 7•10**12 protons of 20 GeV impinges on a lead target every 2.4 seconds. After collimation, a neutron flux of the order of 10**5 neutrons/cm**2/pulse is available to perform cross section measurements in the detectors station located 185 m downstream. ITN team is involved in collaboration with INFN-Bari and CEA-Saclay in the analysis of the data recorded during 2004 and from 2009, as well as the feasibility studies associated to the construction of the second experimental area. In this way we concluded the analysis of the data on neutron capture on U-233, taken using the BaF2 calorimeter, and data taken during 2009 and 2010 using the BaF2 calorimeter and the C6D6 detectors for the neutron capture cross-sections of Fe and Ni isotopes.
2	The production of Radioactive Ion Beams (RIBs) is of great importance for scientific studies in the fields of Nuclear Physics and Astrophysics, for Materials Science studies and also for Medicine.
	One of the most important installations worldwide for the production of Radioactive Ion Beams (RIB), using the ISOL (Isotope Separation On-Line) method is the ISOLDE facility at CERN, where more than 1000 radioactive isotopes have been produced. These isotopes are currently produced at ISOLDE following the bombardment of various primary targets with a pulsed proton beam of energy 1.4 GeV and intensity 2 $\mu$ A. Most of these isotopes can be accelerated in the REX-ISOLDE facility to energies up to 2.8 MeV/u.
	In this project, the ITN group aims at the continuation of the on-going collaboration with CERN in the optimization of the target systems at ISOLDE – computational activities as well as of design and tests of prototypes, and in Radiological Protection and Shielding studies of the future facility HIE-ISOLDE ("upgrade" of the existing installation for higher proton beam energy and intensity) – computational activities of shielding design and experimental validation through measurements.
3	The participation of the ITN team consisted on the determination of the capture neutron cross sections for 238U and 241Am and the fission cross sections for 240Pu and 242Pu, using the TOF spectrometer at CERN.

## **PAPERS**

- Silvia Barros; Eduardo Gallego; Alfredo Lorente; Isabel F. Goncalves; Pedro Vaz; Hector Rene Vega-Carrillo, Dosimetric Assessment And Characterisation Of The Neutron Field Around A Howitzer Container Using A Bonner Sphere Spectrometer, Monte Carlo Simulations And The Nsdann And Nsduaz Unfolding Codes, *Radiation Protection Dosimetry (2012)*, doi: 10.1093/rpd/ncs246.
- F. Gunsing et al. (the n\_TOF collaboration), Measurement of resolved resonances of 232Th(n,g) at the n-TOF facility at CERN, *Physical Review C*, **85**, 064601 (2012).
- C.Massimi et al. (n\_TOF collaboration), Resonance neutron-capture cross sections of stable magnesium isotopes and their astrophysical implications, *Physical Review C*, **85**, 044615 (2012), doi: 10.1103/PhysRevC.85.044615.
- M.Calviani et al. (n\_tof collaboration), Neutron-induced fission cross section of 245Cm: New results from data taken at the time-of-flight facility n\_TOF, *Physical Review C*, **85**, 034616 (2012), doi:10.1103/PhysRevC.85.034616.
- C. Guerrero et al. (n\_TOF collaboration), Simultaneous measurements of neutron-induced capture and fission reactions at CERN, *European Physical Journal A*, 48, 1 (2012).
- C. Guerrero et al. (n\_TOF collaboration), Measurement and resonance analysis of the <sup>237</sup>Np neutron capture cross section, *Physical Review C*, **85**, 044616 (2012), doi:10.1103/PhysRevC.85.044616.
- C. Guerrero et al. (n\_TOF collaboration) Monte Carlo simulations of the n\_TOF Total Absorption Calorimeter, *Nuclear Instruments and Methods A*, 671 (2012).
- C. Guerrero et al. (n\_TOF collaboration), Simultaneous measurements of neutron-induced capture and fission at CERN, *The European Physical Journal A*, **48** (2012) 29.
- C. Carrapiço et al. (n\_TOF collaboration), Neutron induced capture and fission discrimination using calorimetric shape decomposition, *NIM A, Vol 704*, doi: 10.1016/j.nima.2012

#### **EDUCATION**

- I. Gonçalves, Supervisor of the Ph. D. Thesis, *Nuclear Technology, Dosimetry and Radiological Protection Aspects of Accelerator Driven Systems (ADS) and Radioactive Ion Beam (RIB) facilities*, by Yuriy Romanets, Instituto Superior Técnico, Universidade Técnica de Lisboa, 2012
- Gonçalves, Supervisor of the Ph. D. Thesis, *Measurements of the 233U neutron capture cross section at the n\_TOF facility at CERN*, by Carlos Alberto de Almeida Carrapiço, Instituto Superior Técnico, Universidade Técnica de Lisboa, 12 December 2012
- Gonçalves, Supervisor of Ph.D. Thesis, *Measurements of Fission Cross Sections of Actinides and of Neutron Capture Cross Sections of Fe and Ni Isotopes Using the n\_TOF Spetrometer at CERN*, by Raul Cambraia Lopes Sarmento Pereira, Instituto Superior Técnico, Universidade Técnica de Lisboa, 18 December 2012
- I. Gonçalves, Member of the jury, Ph.D. of Yuriy Romanets, Instituto Superior Técnico, Universidade Técnica de Lisboa, 2012.
- Gonçalves, Member of the jury, Ph.D. of Carlos Alberto de Almeida Carrapiço, Instituto Superior Técnico, Universidade Técnica de Lisboa, 12 December 2012.
- Gonçalves, Member of the jury, Ph.D. of Raul Cambraia Lopes Sarmento Pereira, Instituto Superior Técnico, Universidade Técnica de Lisboa, 18 December 2012.

# **PROJECTS**

- *CERN/FP/123602/2011*, Participation of ITN on n\_TOF experiments (phase 2) no CERN, Coordinator: Isabel Gonçalves (50%). (Funding 60000€, 2 years)
- *ANDES*, (Accurate Nuclear Data for nuclear Energy Sustainability), Euraton Seventh Framework Programme Grant agreement 249671. Leading Institution: CIEMAT, Madrid, Spain. IST/ITN Coordinator: Isabel Gonçalves (20%).

• *CHANDA*, (Solving Challenges In Nuclear Data For The Safety Of European Nuclear Facilities), Proposal for FP7-Fission-2013. Leading Institution: CIEMAT, Madrid, Spain. IST/ITN Coordinator: Isabel Gonçalves (10%).

## NAME: João António Borges Manteigas

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 25362

#### **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Management	35%
2	Technical Services to External Clients	55%
3	Technical Services to IST/ITN Units	10%
Total		100%

#### WORK SUMMARY

Nº	Work Summary and Main Achievements
1	Coordinator of the "Nuclear Methods and Instrumentation" group:
	• Line of activity: development of methods, techniques and instrumentation using ionizing radiation for applications in industry and research.
	Coordination of the subgroup "Nuclear Instrumentation – Services":
	• Line of activity: Supply of equipment brand IST/ITN and specialized services, including technical assistance and consultancy.
	Coordinator of the Activities Plan for 2012;
	Collaboration in the preparation of the:
	• Activity Report of the do ITN 2011 (flyer);
	• Activity Report of the ITN/UFA 2011;
	• Progress Report of ITN/UFA (QUAR 2011);
	Collaboration in the submission to the FCT projects:
	• "ARIAS - Application of Ionizing Radiation for a Sustainable Environment" (RECI/AAG-TEC/0400/2012 – approved, 499.469,00€, starting date: 01-01-2013);
	• "Increasing the energy efficiency of plasma conversion of methane" (PTDC/FIS- PLA/2135/2012 – approved, 102.716,00 €, starting date: 01-01-2013).
2	Quality control of the manufacturing process of small series of equipment, brand IST/ITN.
	Consulting, design, installation, repair and maintenance of nuclear equipment for enterprises;
	Sale of equipment brand IST/ITN to domestic and foreign customers:
	• Total invoice: 38.284,80 € (please see annex)2/3
3	Maintenance and recovery of HpGe Detectors;
	Maintenance of electronic equipment:
	• Total invoice: 1.454,00 € (please see annex).

#### **PUBLICATIONS**

#### **Internal Reports / Services**

• J.B. Manteigas, J. Neves, N. Pinhão, Technical Assistance in the Field of Engineering Applications of Radiation and Radioisotopes, UFA/ITN, 2011.

• J.B. Manteigas, I. Gonçalves, J. Neves, N. Pinhão, Progress Report "Nuclear Instruments and Methods" vs QUAR/UFA 2011.

# NOME: José Luís de Sousa Neves

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 5368

#### **R&D ACTIVITIES**

Nº	Activity Description	R&D
	Consulting, Design & Technical Assistance in the Field of Engineering Applications of	55%
1	Radiation and Radioisotopes	
	Collaboration with different ITN research groups in preparatory tasks in order to	15%
2	submit several scientific projects to FCT	
3	Participation of ITN in the n_TOF (Phase 2) experiment at CERN	15%
4	Study and design of different prototypes of AC, DC and RF "High Voltage Power	15%
	Generators"; Measurements of voltage-current characteristics of a plasma needle	
Total		100%

Nº	Work Summary and Main Achievements
1	The main purposes of the project are the design and manufacture of electronic equipment, consulting in the field of engineering applications and technical assistance. By request from internal groups and external customers, several electronic equipment and prototypes were designed (or upgraded) and manufactured. In addition, substantial work related to technical maintenance, calibration and quality control of different nuclear instruments and equipment was carried out.
	Examples:
	• "RADX100" (Pocket Radiation Dosimeter) – up to 12 new such equipment are produced and quite a lot of maintenance and calibrations actions were carried out in particular for the Portuguese Navy
	• "Triple Power Supply/Readout System" (equipment designed to control 3 El-Flow® Advanced Mass Flow Meter/Controller from Bronkhorst <sup>®</sup> High-Tech B.V., Holland, in-situ and remotely) – upgraded
	• "RPI Maquette" (Maqueta do Reactor Português de Investigação) - a new Power Controller Board was designed using CAD software and a USB controller was implemented
	2012 Total Income: €39.739,00
2	A lot of scientific projects were submitted to FCT in 2012; two of them are approved with endowment of the total required financial resources:
	(i) "Increasing the energy efficiency of plasma conversion of methane", PTDC/FIS- PLA/2135/2012, <b>Total Funding:</b> €102.716,00 (starting 2013-01-01) – I am involved in the experimental work which require the construction of a DBD reactor for high temperature studies and the modification of existing High Voltage Power Supplies in order to increase the frequency range and feedback control of applied voltage.
	(ii) "Application of Ionizing Radiation for a Sustainable Environment ", (Project ARIAS), RECI/AAG-TEC/0400/2012, Total Funding: €499.469,00 (starting 2013-01-01) – Mostly this project means a very large Resource Consolidation, so, we have done some searching and preparing work directed to the elaboration of tenders needed to the acquisition of several complex and expensive Laboratory Equipment as well as a large Automation System.
3	The n_TOF (Phase 2) project is the continuation of ITN involvement in the activities of the n_TOF experiment at CERN.

	The n_TOF experiment is a consortium of 40 laboratories in European countries, U.S.A., Japan and Russia that aims at performing high precision cross-sections measurements of the neutron induced reactions of great relevance for innovative technological applications like transmutation of nuclear waste and energy production, radioisotope production for medical and industrial applications and several topics in Nuclear Physics and Astrophysics
	Essentially, the n_TOF instrument is a pulsed neutron source coupled to a 200 m flight path designed to study neutron-nucleus interactions for neutron kinetic energies ranging from a few meV to several GeV. The neutron kinetic energy is determined by time-of-flight, hence the name n_TOF.
	My collaboration was connected to the optimization of Voltage Dividers of the $4\pi$ Total Absorption Calorimeter, TAC, a set of 48 scintillation crystals coupled to photomultiplier tubes and included as well some technical advising tasks.
	CERN/FP/123602/2011, Total Budget: €30.000,00
4	I have studied, designed and tested some prototypes of AC, DC and RF "High Voltage Power Generators" for applications related with non-thermal plasmas produced by a dielectric barrier discharge (DBD).
	Furthermore, in order to measure the small RF power absorbed by samples under investigation (organic materials and living tissues), I also begin the development of a measurement system of voltage–current characteristics of a plasma needle, working with low-temperature RF discharge at 13.56 MHz. For these purposes I have designed a set of small derivative probes (inductive and capacitive). Now we need to improve the calibration of this measurement system.

#### **REPORTS / SERVICES**

- J. Manteigas, J. Neves, N. Pinhão, Technical Assistance in the Field of Engineering Applications of Radiation and Radioisotopes, UFA/IST, 2011.
- J. Manteigas, I. Gonçalves, J. Neves, N. Pinhão, Nuclear Instruments and Methods, Progress Report vs QUAR/UFA", 2011.

# NAME: Luís Manuel Cerqueira Lopes Alves

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 25454

## **R&D ACTIVITY**

N°	Activity Description	R&D
1	Research	75%
2	Experimental development	25%
Total		100%

N°	Work Summary and Main Achievements
1	Research has been carried out through National and European projects funding and collaborations:
	Advanced materials for nuclear fusion reactors
	Study of Be pebbles both for trace elements determination and for establishing the oxide surface layer formation and extent of previously long neutron irradiated pebbles after annealing at different temperatures and atmospheres, as a function of time.
	Optoelectronics materials
	Complementary study of optoelectronic materials (such as yttria stabilized zirconia doped
	with Pr, $Mn^{2+}$ activated ZnGa <sub>2</sub> O <sub>4</sub> fibres, GaN nanowires) using ionluminescence for
	determining their behaviour in harsh environmental conditions and establish their

	luminescence behaviour as a function of beam particle fluency.
	<i>Decorated industrial glasses (Atlantis)</i> Study of gold decorated glasses, determining crystal glass composition, gold layer composition, thickness extent and uniformity using PIXE and RBS. Gold "oxidation" observed in some bottles is being investigated also using complementary techniques as FTIR and RAMAN spectroscopy aiming determining the cause of alteration and propose preventing methods.
	Cultural heritage
	a) Metal objects
	Collaboration with three main institutions for materials characterization:
	Museu National de Arte Antiga – characterization of Indo-Portuguese Silver Jewellery, with the analysis of several pieces comprising the "Vidigueira Treasure";
	Museu Nacional de Arqueologia – material composition and similarity study of gold pieces of the "Pancas Treasure";
	Imprensa Nacional Casa da Moeda – investigation of defects of recently minted commemorative gold coins, contributing to the establishment of a better quality control in its manufacture.
	b) Ancient ceramics and glasses
	Raw material and colour pigments composition of XVII century tiles (Monastery of Sta Clara-a-Velha), and glasses from the Lisbon Roman Theatre aiming establishing production techniques and provenance.
2	Development of an experimental system for tomography of thin samples using PIXE and STIM techniques with micrometre spatial resolution is being carried out. A precision rotation stage has been designed, built, installed and tested mainly using the STIM technique on a test sample composed of a thin SiC fibre coated with alumina with particles detected by a Si Pin diode. Aiming at reducing the problems inherent to the beam radiation damage of Si Pin diodes and then the long-run quality of the obtained images, a gas detector prototype has been built (in collaboration with researchers from LIP, Coimbra) and tested. The obtained images from the structure of a butterfly wing using this detector prototype have been compared with the ones obtained with a Si Pin diode and the obtained results were good enough to proceed with further developments of the gas detector in what accounts to detector energy resolution improvement and attainable count rate.

#### **PAPERS**

- N.F. Santos, J. Rodrigues, A.J.S. Fernandes, L.C. Alves, E. Alves, F.M. Costa, T. Monteiro, Optical properties of LFZ grown beta-Ga2O3:Eu3+ fibres, App. Surf. Sci. 258, 23 (2012) 9157-9161, http://dx.doi.org/10.1016/j.apsusc.2011.07.06.
- L.M. Ferreira, J.P. Leal, P.A. Rodrigues, L.C. Alves, A.N. Falcão, M.H. Gil, Characterization of PE-g-HEMA films prepared by gamma irradiation through nuclear microprobe techniques, Radiation Physics and Chemistry, Vol. 81, 9, (2012) 1319–1323. <u>http://dx.doi.org/10.1016/j.radphyschem.2012.01.045</u>.
- M. Fialho, S. Magalhaes, L.C. Alves, C. Marques, R. Maalej, T. Monteiro, K. Lorenz, E. Alves, AlN content influence on the properties of AlxGa1-xN doped with Pr ions, Nucl. Instr. and Meth. B 273 (2012) 149-152. <u>http://dx.doi.org/10.1016/j.nimb.2011.07.062</u>.
- L. Rebouta, P. Martins, S. Lanceros-Mendez, J.M. Barandiaran, J. Gutierrez, L.C. Alves, E. Alves, Room temperature magnetic response of sputter deposited TbDyFe films as a function of the deposition parameters, J. Nano Research 18-19 (2012) 235-239, <a href="http://dx.doi.org/10.4028/www.scientific.net/JNanoR.18-19.235">http://dx.doi.org/10.4028/www.scientific.net/JNanoR.18-19.235</a>.
- Diana Guimaraes, Maria Luisa Carvalho, Vera Geraldes, Isabel Rocha, Luis Cerqueira Alves, Jose Paulo Santos, Lead in liver and kidney of exposed rats: aging accumulation study, Source: Journal of trace

elements in medicine and biology : organ of the Society for Minerals and Trace Elements (GMS), 26, 4 (2012) 285-90 <u>http://dx.doi.org/10.1016/j.jtemb.2012.02.006</u>.

## **COMMUNICATIONS**

- Trace elemental profiles in teeth of sperm whales from Azores, R.M. Godinho, J. Raimundo, R. Antunes C. Vale, S. Mendes, L. C. Alves, T. Pinheiro, 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- Micro-scale elemental partition in tissues of the aquatic plant Lemna minor L. exposed to highway drainage water, R.M. Godinho, J. Raimundo, C. Vale, B. Anes, P. Brito, L. C. Alves, T. Pinheiro, 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- New gas detector setup for on-axis STIM tomography experiments, A.C. Marques, M.M.F.R. Fraga, P. Fonte, D.G. Beasley, L.C. Alves, R.C. da Silva, 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- Fast Simulation of Proton Induced X-Ray Emission Tomography Using CUDA, D.G. Beasley, A.C. Marques, L.C. Alves, R.C. da Silva, 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- *Microprobe analysis, iono- and photo- luminescence of Mn2+ activated ZnGa2O4 fibres,* N.F. Santos, A.J.S. Fernandes, L.C. Alves, N.A. Sobolev, E. Alves, K. Lorenz, F.M. Costa, T. Monteiro, *13th International Conference on Nuclear Microprobe Technology and Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- A comparative study of photo- cathodo- and iono- luminescence of GaN nanowires implanted with rare earth ions, J. Rodrigues, S.M.C. Miranda, M. Peres, E. Nogales, L.C. Alves, E. Alves, G. Tourbot, B. Daudin, B. Méndez, K. Lorenz, T. Monteiro, *13th International Conference on Nuclear Microprobe Technology and Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Oral Presentation (J. Rodrigues).
- The influence of photon excitation and proton irradiation on the luminescence properties of yttria stabilized zirconia doped with praseodymium ions, M.R.N. Soares, L.C. Alves, E. Alves, K. Lorenz, F. M. Costa, T. Monteiro, , 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- Effect of rapid thermal annealing on the composition of Au/Ti/Al/Ti ohmic contacts for GaN-based microdevices, A. Redondo-Cubero, M.D. Ynsa, M.F. Romero, L.C. Alves, E. Muñoz, , 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Oral Presentation (A. Redondo-Cubero).
- *CdTe nano-structures for photovoltaic devices*, V. Corregidor, L.C. Alves, N. Franco, M.A. Barreiros, N. V. Sochinskii, E. Alves, *13th International Conference on Nuclear Microprobe Technology and Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- Analysis of surface stains on modern gold coins, V. Corregidor, L.C. Alves, J.Cruz, , 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Oral Presentation, (V. Corregidor).
- The Earrings of Pancas Treasure: analytical study by X-ray based techniques a first approach, I. Tissot, M. Tissot, M. Manso, L.C. Alves, M.A. Barreiros, T. Marcelo, M. L. Carvalho, V. Corregidor, M. F. Guerra, 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation,
- Study of Hispano-Moresque tiles from the Monastery of Santa Clara-a-Velha in Coimbra, Portugal, using μ-PIXE, S. Coentro, R. Trindade, L.C. Alves, V. Muralha, R.C. da Silva, , 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation,
- Study of Fossilized Eggshells from the Late Jurassic Dinosaur Clutch of Porto das Barcas (Lourinhã formation, Portugal), R.M.S. Martins, R. Araújo, R. Castanhinha, O. Mateus, L.C. Alves, F. Beckmann,

N. Schell, *13th International Conference on Nuclear Microprobe Technology and Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.

- Towards the understanding of the intentionally induced yellow luminescence in GaN nanowires, J. Rodrigues, S.M.C Miranda, A.J.S Fernandes, E. Nogales, L.C. Alves, E. Alves, G. Tourbot, T. Auzelle, B. Daudin, B. Méndez, T. Trindade, K. Lorenz, F.M. Costa, T. Monteiro, *Fall Meeting of the European Materials Research Society (E-MRS), Symposium J: Rare earth doped semiconductors and nanostructures for photonics*, September 17-21 (2012), Warsaw, Poland, Poster Presentation.
- On the influence of silica type on the structural integrity of dense La<sub>9.33</sub>Sr2Ge<sub>4</sub>O<sub>26</sub> electrolytes for SOFCs, C. Alves, T. Marcelo, F.A.C. Oliveira, L. C. Alves, J. Mascarenhas, B. Trindade, Fall Meeting of the European Materials Research Society (E-MRS), symposium F: Nanoceramics and Ceramic based Nanocomposites September 17-21 (2012), Warsaw, Poland, Poster Presentation.
- *Microwave Hybrid Sintering of La<sub>9.33</sub>Si*<sub>2</sub>*Ge*<sub>4</sub>*O*<sub>26</sub> *for SOFC electrolytes*, C. Alves, M. Santos, T. Marcelo, J. Mascarenhas, L.C. Alves, B. Trindade, F.A. Costa Oliveira, 6<sup>th</sup> *International Meeting on Developments in Materials, Processes and Applications of Emerging Techniques*, 2-4 July 2012, Alvor, Portugal, Poster Presentation.
- Combination of IBA techniques to study art-historical objects using a microprobe, V. Corregidor, C.P. Marques, R.C. Silva, P.A. Rodrigues, M. Vilarigues, T. Silva, S. Cabo Verde, M.L. Botelho, M.I. Prudêncio, S. Coentro, V. Muralha, E. Alves, L.C. Alves, 2nd Luminescence in Archaeology International Symposium, 5-7 September 2012, Lisbon, Portugal, Poster presentation.
- Luminescence signals and emissions from grains of quartz prepared from Portuguese granite and pegmatite, C.I. Burbidge. M. Martini, M. Fasoli, G. Cardoso, L.C. Alves, I. Villa, 2nd Luminescence in Archaeology International Symposium, 5-7 September 2012, Lisbon, Portugal, Poster presentation.
- *Irradiation defects produced in IBIL analysis of sapphire*, C. Marques, L.C. Alves, R.C. Silva, E. Alves, *2nd Luminescence in Archaeology International Symposium*, 5-7 September 2012, Lisbon, Portugal. Poster presentation.
- External Ion Beam Analysis of "Tesouro da Vidigueira" Collection", V. Corregidor, L.C. Alves, A. Candeias, L. Penalva, B. Maduro, 2nd International Workshop on Physical & Chemical Analytical Techniques in Cultural Heritage, 4-5 June 2012, Lisboa, Portugal. Oral presentation (V. Corregidor).
- Tribological improvement of coinage dies for the Portuguese Mint by nitrogen implantation, J. Cruz, V. Corregidor, B. Nunes, E. Alves, L.C. Alves, R. Colaço, P. Alexandrino, P. Leitão, 18th International Conference on Ion Beam Modifications of Materials (IBMM2012), 2-7 September, 2012, Qingdao, China. Poster presentation.
- *MeV Ion Beam Microscopy: a Tool for Materials Characterization*, L.C. Alves, V. Corregidor, T. Pinheiro, L. Ferreira, *SPMicros2012 Microscopy: A tool for the advancement of science*, September 24-25, 2012, Lisbon, Portugal. Oral presentation.
- Investigation of elemental distribution in cat femoral head by nuclear microprobe and SEM for Paget disease of bone studies, C. Santos, M. Fonseca, V. Corregidor, L. C. Alves, H. Luis, M. Capelão, J. C. Branco, P. A. Carvalho, A. P. Jesus, SPMicros2012 Microscopy: A tool for the advancement of science, September 24-25, 2012, Lisbon, Portugal. Poster presentation.
- Analysis of a gold solidus of roman emperor Valentinian I, J. Cruz, V. Corregidor, L.C. Alves, P.A. Carvalho, M.A. Stanojev Pereira, M. Fonseca, *SPMicros2012 Microscopy: A tool for the advancement of science*, September 24-25, 2012, Lisbon, Portugal. Poster presentation.
- Architectural tiles in the Monastery of Santa Clara-a-Velha in Coimbra, Portugal: study of the production techniques, S. Coentro, R. Trindade, A. Candeias, J. Mirão, L. Cerqueira, R. Silva, V. Muralha, Global Pottery 1st International Congress on Historical Archaeology & Archaeometry for Societies in Contact, Barcelona, Spain, 7-9 May 2012. Oral presentation (S. Coentro).
- μ-Raman analysis of Hispano-Moresque historical tiles, Susana Coentro, Luís Cerqueira, Rui M.C. Silva, Vânia S.F. Muralha, *ChemCH-2012: 2nd International Congress Chemistry for Cultural Heritage*, Istambul, Turkey, 9-12 Jul. 2012. Oral presentation (S. Coentro).

- Chemical characterisation of Hispano-Moresque tiles from the Monastery of Santa Clara-a-Velha in Coimbra, Portugal, Susana Coentro, Rui A.A. Trindade, António Candeias, José Mirão, Luís Cerqueira, Rui M.C. Silva, Vânia S.F. Muralha, Azulejar-2012, Aveiro, Portugal, 10-12 Oct. 2012. Oral presentation (S. Coentro).
- Analysis of Hispano-Moresque architectural tiles by μ-Raman spectroscopy, S. Coentro, R. Silva, V. Muralha, Global Pottery 1st International Congress on Historical Archaeology & Archaeometry for Societies in Contact, Barcelona, Spain, 7-9 May 2012. Poster presentation.
- Selected pre-processing methods to STIM-T projections, A.C. Marques, D.G. Beasley, L.C. Alves, R.C. da Silva, CompImage2012, Computational Modelling of Objects Presented in Images: Fundamentals, Methods and Applications, Rome, Italy, Sep 5-7 (2012). Poster.

# **EDUCATION**

- Co-supervisor of post-doctoral work of D.Sc. Ana Cláudia Santana Marques, *3D Microprobe: Tomography by PIXE, RBS and STIM* (SFRH/BPD/65817/2009).
- Member of Jury Ph.D. Thesis in Conservation Science, Pedro Manuel Francisco Valério, *Archaeometallurgical study of pre and protohistoric production remains and artefacts from Southern Portugal*, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, 2012.
- Hands-on: Microbeam studies of microdomains, 3rd SPIRIT Workshop on Ion Beams as a Tool for Nanotechnology, IST/CTN, Sacavém, Portugal, 18 Jul. 2012

# **PROJECTS**

- DiFusion Diamond dispersions in nanostructured metals: Novel materials design for fusion reactors, PTDC/CTM/100163/2008 Leading Institution: IST/UTL, Portugal. IST/ITN team member: L.C. Alves (10%).
- *Nanostructured magnetic nitrides-Nanomag.* PTDC/FIS /102270/2008. Leading Institution: FFCUL, Portugal. IST/ITN team member: L.C. Alves (5%).
- *Depth-selective Ion Microprobe Tomography*-Tomo3D. PTDC/FIS/115089/2009. Leading Institution: IST/ITN. PI: A.C. Marques (FCT post-doctoral fellow, 100%). IST/ITN team member: L.C. Alves (25%).
- *Nobly Decorated Crystal*-NobleDec. Grant AdI/23274/2012, QREN programme COMPETE. Leading Institution: VAA-Vista Alegre/Atlantis. IST/ITN team member: L.C. Alves (20%).
- *Fusion Energy Material Science (FEMaS)*, Euratom Seventh Framework Programme for Nuclear Research and Training, Grant agreement No 224752-CA. Leading Institution: Max-Planck Institut für Plasmaphysik, Garching, Germany. IST/ITN team member: L.C. Alves (10%).
- Support of Public and Industrial Research Using Ion Beam Technology (SPIRIT), Seventh Framework Programme: Capacities Specific Programme Research Infrastructures, Grant agreement No 227012-CP-CSA-Intra (2009/03/01), Leading Institution: Forschungszentrum,Dresden-Rossendorf, Germany. IST/ITN team member L.C. Alves (10%).

# **CONFERENCE ORGANIZATION / COMMITTEES**

• Organising committee of the 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisbon, Portugal, 22-27 July, 2012.

# **COLLABORATIONS**

- Alexandra Barreiros, LNEG, Lisbon (Ion beam microanalysis, collaboration)
- Maria Dolores Ynsa, CMAM Centro de Micro-Análisis de Materiales, Universidad Autonoma de Madrid, Madrid, Spain (Ion beam microanalysis, collaboration)
- M. Fraga, P. Fonte, R.F. Marques and LIP-Coimbra, Laboratório de Instrumentação e Física Experimental de Partículas, Coimbra, Portugal. Development and performance tests of prototype gas detector for on-axis STIM tomography

- Luisa Penalva, Belmira Maduro, António Candeias Museu Nacional de Arte Antiga, Portugal. (Ion beam microanalysis, collaboration)
- Márcia Vilarigues, Solange Muralha, Susana Coentro, Mathilda Larson, Inês Coutinho Dept. of Conservation and Restoration from FCT-UNL (Ion beam microanalysis, collaboration).
- Isabel Tissot Museu de Arqueologia, Portugal (Ion beam microanalysis, collaboration).
- Filomena Guerra Centre de Recherche et de Restauration des Musées de France (Ion beam microanalysis, collaboration).

#### NAME: Luís Miguel Mota Ferreira CATEGORY: Auxiliary Researcher ID NUMBER:

#### **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Project Biomedical Hybrids	25%
	Hybrid Materials for Biomedical Applications (PTDC/CTM/101115/2008)	
2	Project Biodiesel	15%
	Preparation of Polymeric Materials Catalytically Actives on Biodiesel Production, by	
	Vegetable Oils Methanolysis	
	(PTDC/CTM-POL/114579/2009)	
3	PHEMA-IL composites	5%
4	Laboratory of Macromolecular Materials	20%
5	Molecular simulation	5%
6	Scientific co-orientation	12%
7	Technical and scientific orientation	12%
8	IAEA TC Project RER/0/034 - Regional Training Course on Radiation Technology	1%
	for Cultural Heritage Preservation.	
9	Other activities	5%
Total		100%

Nº	Work Summary and Main Achievements
1	Project Biomedical Hybrids
	Synthesis and characterization of hybrid (MH) glass-polymer systems produced by gamma irradiation of the precursors (PDMS, TEOS, PrZr)
	Study of:
	(i) Influence of the polymer molecular weight (range 4200 g/mol – 43500 g/mol) on the microstructure of the MH, specifically the size and fractal dimension of the oxide regions in systems 20 wt% PDMS - 73 wt% TEOS - 7 wt% PrZr;
	(ii) Characterization of the effect of increasing catalyst content in size and porosity of the oxide microscopic domains.
	Using (Mw PDMS = 43500 g/mol), systems:
	33 wt% PDMS - $(67-x)$ TEOs - $x$ PrZr (x = 1, 2, 3 e 5 wt%)
	(25-x)PDMS - 75TEOS - xPrZr (x= 1.4, 2.9, 4.3 wt%)
	(50-x)PDMS - 50TEOS - xPrZr (x= 1.4, 2.9, 4.3, 5.7 wt%
	(iii) Microstructural changes in MH prepared from precursors in weight percent composition (20wt%PDMS - 79wt%TEOS - 1wt% PrZr) followed by the addition of Ca (both solid and in solution).

	x Ca3(PO4)2 (x=1, 3, 5, 10 wt%) solid
	x Ca3(PO4)2 (x=1, 3, 10 wt%) dissolved
	All samples prepared (from sol-gel and gamma irradiation techniques) have been analysed by thermal analysis (DSC and TGA) at our laboratory.
	Overall results: two articles published, two articles submitted for publication and two communications.
	(Results were presented in the 10th meeting of the Ionizing Radiation and Polymers Symposium, IRaP'2012, Cracow, Poland, Oct 14-19, 2012).
2	Project Biodiesel
	Synthesis by gamma irradiation and characterization of PVA supported catalytic membranes for biodiesel production by methanolysis of used oils.
	PVA was successfully cross-linked with succinic and adipic acid, confirming that gamma irradiation is an effective method for anchoring a catalytic resin on cross-linked PVA. These supported resin membranes have shown to be effective catalysts in the esterification reaction of lauric acid to methyl laureate.
	However, their catalytic activity is dependent on the crosslinking agent and on gamma radiation dose of preparation.
	Best catalytic results were obtained with PVA-Succinic acid membranes. The increase of dose from 5 to 13 kGy leads to a slight increase of membrane's catalytic activity.
	PVA membranes
	Prepared samples were also characterized relatively to their thermal and mechanical stability and degree of functionalization.
	Samples showed better mechanical strength when compared with similar composition membranes prepared by traditional techniques.
	Overall results: two articles published, four articles submitted for publication and four communications.
	(Results were presented in:
	- 10th Meeting of the Ionizing Radiation and Polymers Symposium, IRaP'2012, Cracow, Poland, October 14-19, 2012
	- EUROMEMBRANE 2012, London, United Kingdom, Sept 23-27, 2012.
	- Symposium in Honour of Ramôa Ribeiro. Catalysis: From the active site to the process, Lisbon, Portugal, Oct 8-9, 2012).
3	PHEMA-IL composites
	A novel porous polymer-ionic liquid composite with poly(2-hydroxyethyl methacrylate) (PHEMA) and 1-butyl-3-methylimidazolium hexafluorophosphate (BMIPF6) has been synthesized by gamma irradiation without heat or chemical initiators. The products can be reversibly converted into organogels.
	The composites obtained are potential candidates for electrochemical applications.
	The developed gamma irradiation technique, currently under optimization process, can be a simple and versatile alternative way to obtain these materials.
	Overall results: one article published.
4	Laboratory of Macromolecular Materials
	Technical responsibility, maintenance, management and upgrade of the macromolecular materials laboratories.
	Main achievements:

	- Functional up-grade of the control system and digital data acquisition for the Zwick Universal Mechanical Testing Machine (Zwick 1435).
	- Recovery of the programmable temperature control system of the hydraulic press used for mechanical stress tests and preparation of samples for tensile tests (Carver Laboratory Hydraulic Press – Model C).
5	Molecular simulation
	Configuration of a workstation for molecular mechanics and dynamic simulation studies of macromolecular materials. Software tests and preliminary studies.
	This work was done in the framework of the Biomedical's Project. Results obtained, even preliminary, allowed already clarifying some issues related with the molecular conformations of the hybrid materials associated with mechanical weaknesses observed when bioactive agents (e.g., calcium) are introduced in the composition of the hybrid material. Studies are on-going in the direction to clarify the differences in molecular organization between the materials prepared by sol-gel technique and by gamma irradiation.
	Results analysis was done in straight collaboration with Dr. João Paulo Leal from UCQR, IST/ITN. Nuno Miguel da Silva Fernandes MSc., collaborated in this task by our orientation as fellow of the project during three months.
6	Scientific co-orientation
	Scientific co-orientation, jointly with Dr. Fernanda Margaça, of the fellow Joana Jacóme Henriques de Lancastre MSc., within the Project Biomedical Hybrids.
	Scientific orientation in the field of irradiation techniques for hybrid materials preparation and their characterization by thermal, FTIR and mechanical analysis.
7	Technical and scientific orientation
	Technical and Scientific orientation of the fellow Nuno Miguel da Silva Fernandes MSc., for the:
	- Development, assembling and test of the control system and digital data acquisition for the Zwick Universal Mechanical Testing Machine (Zwick 1435).
	- Recovery of the programmable temperature control system of the hydraulyc press used for mechanical stress tests and preparation of samples for tensile tests (Carver Laboratory Hydraulic Press – Model C).
	Dr. Carlos Cruz from UFA, IST/ITN collaborated in these tasks.
	- Data processing and tests of molecular mechanics simulation routines applied to hybrid materials (within the Project Biomedical Hybrids). Dr. João Paulo Leal from UCQR, IST/ITN also collaborated in this task.
8	IAEA TC Project RER/0/034 - Regional Training Course on Radiation Technology for Cultural Heritage Preservation
	Former in the Regional Training Course on Radiation Technology for Cultural Heritage Preservation - IAEA TC Project RER/0/034, Lisbon, Portugal, Nov 5-9 (2012).
	Responsible for Theme II of the Course: Impact of Ionizing Radiation in Materials (Tiles and Cellulose based materials), and for the experimental training sessions
	Evaluation of structural damages and appearance (color) degradation as a reference for Dmax determination.
	This activity had the collaboration of the fellow Joana Jacóme Henriques de Lancastre, MSc. (UFA, IST/ITN) and of Dr. Maria Helena Casimiro (REQUINTE, FCT-UNL).
9	Other activities
	Participation in the elaboration of the following proposals to the FCT call for Scientific Research and Technological Development Projects – 2012, in which I was not the proponent researcher:

Application of Ionizing Radiation for a Sustainable Environment (ARIAS), Consolidation of research skills and resources project.

Status: The project was recommended for funding.

Hybrid Materials for Heterogeneous Catalysis (CATHY),

Status: The evaluation was rated Outstanding but the project was not recommended for funding.

## PAPERS

- <u>Ferreira L.M.</u>, Leal J.P., Rodrigues P.A., Alves L.C., Falcão A.N., Gil M.H., Characterization of PE-g-HEMA films prepared by gamma irradiation through nuclear microprobe techniques, *Radiation Physics and Chemistry*, 81, 1319-1323 (2012), doi:10.1016/j.radphyschem.2012.01.045
- M.H. Casimiro, A.G. Silva, J.V. Pinto, A.M. Ramos, J. Vital, L.M. Ferreira, Catalytic poly(vinyl alcohol) functionalized membranes obtained by gamma irradiation, *Radiation Physics and Chemistry*, 81, 1314-1318 (2012), doi:10.1016/j.radphyschem.2012.01.036
- Lancastre J.J.H., Fernandes N., Margaça F.M.A., Miranda Salvado I.M., Ferreira L.M., Falcão A.N., Casimiro M.H., Study of PDMS conformation in PDMS-based hybrid materials prepared by gamma irradiation, *Radiation Physics and Chemistry*, 81, 1336-1340 (2012), doi:10.1016/j.radphyschem.2012.02.016
- R.N. dos Santos, A.G. Silva, L.M. Ferreira, M.H. Casimiro, A.M. Ramos, J. Vital, Methanolysis of soybean oil over basic polymeric catalytic membranes, *Proceedings of EUROMEMBRANE 2012; Procedia Engineering*, 44, 1607-1611 (2012), doi: 10.1016/j.proeng.2012.08.885
- M.H. Casimiro, M.C. Corvo, A.M. Ramos, E.J. Cabrita, A.M. Ramos, L.M. Ferreira, Synthesis and characterization of novel γ-induced porous PHEMA-IL composites, *Materials Chemistry and Physics*, 1-6, (2012), ), http://dx.doi.org/10.1016/j.matchemphys.2012.11.061

# **COMMUNICATIONS**

- Evidence of Structural Order Recovery in LDPE Based Copolymers Prepared by Gamma Radiation, L.M. Ferreira, J.P. Leal, M.H. Casimiro, C. Cruz, J.J.H. Lancastre, A.N. Falcão, *IRaP'2012 10th Meeting of the Ionizing Radiation and Polymers Symposium, Cracow, Poland, Oct 14-19 (2012)*, Oral.
- On the Insights of the Hybrid Materials Microstructure at Nanoscale: A SANS Study, J.J.H. Lancastre, N. Fernandes, F.M.A. Margaça, I.M. Miranda Salvado, L.M. Ferreira, A.N. Falcão, M.H. Casimiro, IRaP'2012 10th Meeting of the Ionizing Radiation and Polymers Symposium, Cracow, Poland, Oct 14-19 (2012), Oral.
- Impact of Ionizing Radiation in Materials (Tiles and Cellulose based materials); Evaluation of structural damages and appearance (color) degradation as a reference for Dmax determination, L.M. Ferreira, IAEA TC Project RER/0/034 Regional Training Course on Radiation Technology for Cultural Heritage Preservation, Lisbon, Portugal, Nov 5-9 (2012), Talk.
- PVA supported catalytic membranes for biodiesel production obtained by gamma irradiation, , M.H. Casimiro, A.G. Silva, R. Alvarez, A.M. Ramos, J. Vital, L.M. Ferreira, *IRaP'2012 10th Meeting of the Ionizing Radiation and Polymers Symposium, Cracow, Poland, Oct 14-19 (2012)*, Poster.
- Methanolysis of soybean oil over basic polymeric catalytic membranes, dos Santos, R. N., Silva, A. G., Casimiro, M. H., Ferreira, L. M., Ramos, A. M., Vital, J., Symposium in Honour of Ramôa Ribeiro. Catalysis: From the active site to the process, Lisbon, Portugal, Oct 8-9 (2012), Poster.
- Production of biodiesel by methanolysis of soybean oil over basic polymeric catalytic membranes, dos Santos, R. N., Silva, A. G., Casimiro, M. H., Ferreira, L. M., Ramos, A. M., Vital, J., EUROMEMBRANE 2012, London, United Kingdom, Sept 23-27 (2012), Poster.

# **EDUCATION / THESES SUPERVISION**

• Former in Regional Training Course on Radiation Technology for Cultural Heritage Preservation - IAEA TC Project RER/0/034, Subject: Impact of Ionizing Radiation in Materials (Tiles and Cellulose based

materials); Evaluation of structural damages and appearance (colour) degradation as a reference for Dmax determination, Lisbon, Portugal, Nov 5-9 (2012).

## **PROJECTS**

- *PTDC/CTM/101115/2008 Hybrid Materials for Biomedical Applications*. Total budget: 125.000 €, ITN budget: 51.072 €. Leading institution: Univ. Aveiro (I.M.M. Salvado), Aveiro, Portugal. IST/ITN Coordinator: F. Margaça (25%); (February/2010 to February/2013); currently in progress.
- PTDC/CTM-POL/114579/2009 Preparation of Polymeric Materials Catalytically Actives on Biodiesel Production, by Vegetable Oils Methanolysis. Total budget: 146.524 €, ITN budget: 8.160 €. Leading institution: FCT-UNL (J. Vital), Caparica, Portugal. IST/ITN Coordinator: L.M. Ferreira (15%); (February/2011 to February/2014), currently in progress.
- PTDC/CTM-POL/3000/2012 Enhancement of Biopolymers by Ionizing Radiation Processing (BioP-Rad). Leading institution: IST/ITN, Loures, Portugal. IST/ITN Coordinator: L.M. Ferreira (45%); Partners: FCT-UNL. submitted to FCT call for Scientific Research and Technological Development Projects 2012. The evaluation was rated Outstanding but the project was not recommended for funding. Situation: FCT decision was contested by the proponent investigator.

#### **COLLABORATIONS**

- M.H.Casimiro, REQUIMTE, CQFB, Dep. Química, Fac. de Ciências e Tecnologia, Univ. Nova de Lisboa, weekly visit; Collaboration in research of new polymeric materials prepared or modified by ionizing radiation and their practical use.
- I.M. Salvado, Dept. Glass and Ceramics Eng., CICECO, University of Aveiro, Portugal, twice/month visit; Collaboration research on hybrid materials for biomedical applications.

# NAME: Miguel Adrião Mateus dos Reis

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 5377

# **R&D ACTIVITIES**

Nº	Description Activity	R&D
1	SPIRIT EU GA 227012-CP-CSA-Infra	15%
2	Supervision of the PhD thesis of Ana Taborda	10%
3	HRHE-PIXE systems development and optimization	5%
4	Maintenance of the PIXE end-station of Van de Graaff	2%
5	ERC Synergy Grant project submission	5%
6	Submission to other calls	5%
7	Publications, conferences and Geant4 Collaboration	15%
8	DT2 e DT2fit codes development	18%
9	Services and support to the community	10%
10	Coordination of the Unit of Physics and Accelerators	15%
Total		100

N°	Work Summary and Main Achievements
1	In the SPIRIT project the CEEFI group is involved in the tentative of establishing a chemical
	speciation technique using PIXE. In 2012, results on the mapping of high resolution and high
	energy X-rays spectra were obtained from an agate sample. High resolution spectra have been
	reanalysed after it become evident that the previous results were not the best possible. Data from
	the SPIRIT task was base of a deep discussion regarding some spectra details within the scope of
	Ana Taborda PhD thesis. This discussion was quite fruitful in 2012, leading to the conclusion that
	coupling to outer shells, so far assumed to be a minor contribution to spectra, must indeed be taken
	into account for a correct description of the observed phenomena.

2	As mentioned in the scope of the SPIRIT task, supervision of Ana Taborda's PhD work lead to important results towards the establishing of a PIXE based speciation method. In 2012 this PhD thesis was concluded and therefore various discussions, thesis text analysis as well as detail discussions of the conclusions and their consequences for the group work were carried out. The thesis has been delivered at the University and will be defended in the beginning of 2013.
3	In the first three months of 2012, an X,Y automated positioning system installed in the HRHE- PIXE chamber in the end of 2011, was put in full operation. This allowed the mapping of an agate sample irradiated at high energy, still in the scope of the SPIRIT project, and afterwards the mapping of a geological sample from collaboration with the National Energy and Geology Laboratory (LNEG). Results from both these experiments are about to be presented at the PIXE conference to take place in Brazil from 3 to 8 of March 2013. The geological sample was studied in the scope of the Poc-Doctorate fellowship of P. Cristina Chaves, cooperation with the Centre for Atomic Physics of the University of Lisbon.
4	Maintaining operational the standard PIXE system installed as end-station of the van de Graaff accelerator requires that from time to time both the electromagnet bending field and the X-ray transmission to the active volume of the Si(Li) detector are experimentally calibrated. Overall this work took one week of effective work, which corresponds to about 2% of working time.
5	Taking into account the far reaching potential of the research activities being undertaken, a international team involving members from ITN, from the Faculty of Sciences of the University of Lisbon and from the University of Surrey, joined towards submitting a proposal to the European Research Council Synergy Grants program. The final steps towards submitting the proposal (for a global budget of close to 11 MEuros) took almost all available time in the first three weeks of the year. The project was not approved for funding but important links to international partners were strengthened.
6	Access to funding being a major issue for the future of the activities lead to the submission and participation in five projects of the FCT 2012 call.
7	
	During 2012, major steps forward were being set base on exhaustive interpretation of the merging between experimental data and theoretical <i>ab initio</i> calculations. Various developments, reanalysis and careful scrutiny of available results was needed to present two major communications, one at the European Conference on X-ray Spectrometry, in Vienna, where evidences were presented to the X-ray community showing that present day methods used in the calculations of transition energies and rates must be re-analysed, and a second one, accepted for publication in the end of the year after, contains details on how these conclusions will lead us ultimately to the chemical speciation PIXE method. Once again, long established assumptions were shown wrong and a major contribution to the advance of science was made possible, even if this had implications on the number of publications that could be submitted in 2012. Published works all correspond to activities from 2011.
	During 2012, major steps forward were being set base on exhaustive interpretation of the merging between experimental data and theoretical <i>ab initio</i> calculations. Various developments, reanalysis and careful scrutiny of available results was needed to present two major communications, one at the European Conference on X-ray Spectrometry, in Vienna, where evidences were presented to the X-ray community showing that present day methods used in the calculations of transition energies and rates must be re-analysed, and a second one, accepted for publication in the end of the year after, contains details on how these conclusions will lead us ultimately to the chemical speciation PIXE method. Once again, long established assumptions were shown wrong and a major contribution to the advance of science was made possible, even if this had implications on the number of publications that could be submitted in 2012. Published works all correspond to activities from 2011. In the context of publication and availability of results by others, it is still important to mention that polynomial approaches to the calculation of ionization cross sections by protons and alpha particles, partially established under the scope of the PhD work of Ana Taborda, were compiled and made available also in the framework of the Geant4 Collaboration for K, L and M shells.
8	During 2012, major steps forward were being set base on exhaustive interpretation of the merging between experimental data and theoretical <i>ab initio</i> calculations. Various developments, reanalysis and careful scrutiny of available results was needed to present two major communications, one at the European Conference on X-ray Spectrometry, in Vienna, where evidences were presented to the X-ray community showing that present day methods used in the calculations of transition energies and rates must be re-analysed, and a second one, accepted for publication in the end of the year after, contains details on how these conclusions will lead us ultimately to the chemical speciation PIXE method. Once again, long established assumptions were shown wrong and a major contribution to the advance of science was made possible, even if this had implications on the number of publication and availability of results by others, it is still important to mention that polynomial approaches to the calculation of ionization cross sections by protons and alpha particles, partially established under the scope of the PhD work of Ana Taborda, were compiled and made available also in the framework of the Geant4 Collaboration for K, L and M shells. First established the beginning of the decade of 1990s, the DATTPIXE software package has been used in ITN for more than 20 years now to analyse PIXE data. The developments both in operative systems and programming context (internet access and data standardization becoming a major issue for data handling codes) coupled to the developments carried out by the team recently, lead to the necessity of a major upgrade in DATTPIXE. DT2 package, which took a significant part of the working time during 2012, is the near future replacement of DATTPIXE and includes xml based data for input and output (following the standards being established in the scope of the SPIRIT project), as well as a new fitting routine able to deal with high resolution spectra and compatible to the needs of fitting spectra under a

	community, carried out during 2012. In the case of the rejection problems, some insight could be found, which showed that the proper technique to further investigate the issue was not PIXE nor any Nuclear Analytical technique, still these were invaluable to be able to reach a first set of results starting from zero information.
10	In the first three months of 2012, the activities related to the coordination of the Physics and Accelerator Unit took a major fraction of the working time. The establishing of the Action Plan for 2012 was achieved. The end of these activities in April 2012 makes that the percentage of time dedicated to it is small even though in the beginning of the year a much high fraction of time was dedicated to this task.

## **PAPERS**

- M. A. Reis, J. Campbell, Particle Induced X-ray Emission, in Characterization of Materials, 2nd Edition, Ed. Elton N. Kaufmann, John Wiley & Suns, 2012 doi: 10.1002/0471266965.com094.pub2
- P.C. Chaves, A. Taborda, M.A. Reis, CdTe detector efficiency calibration using thick targets of pure and stable compounds, Nuclear Instruments and Methods in Physics Research B 273 (2012) 245–249 doi:10.1016/j.nimb.2011.07.086

## **COMMUNICATIONS**

- *PIXE in the slow collisions regime*, Miguel A. Reis, P. Cristina Chaves, Ana Taborda, M. Luísa Carvalho and José Pires Marques, *European conference on X-ray Spectrometry, IAEA Conference Center, Vienna, Austria Jun, 18-22 (2012)*, Invited Talk.
- Polynomial approximation to universal M-shell ionisation cross-sections, Ana Taborda, P. Cristina Chaves, M. Luísa Carvalho and Miguel A. Reis., European conference on X-ray Spectrometry, IAEA Conference Centre, Vienna, Austria Jun, 18-22 (2012), Poster.

## PROJECTS

- Inner Core X-rays in Molecular and Solid State Systems Structures for Technology, Earth observation and Cultural heritage IICXMS4TEC) Seventh Framework Programme European Research Council Synergy Grant 2012, Leading Institution: IST/ITN, Corresponding Principal Investigator: Miguel A. Reis (submitted).
- Mapeamento Elementar em Geologia e Amostras de Aerossóis com Raios-X, Transições de Auger e Especiação (MEGA-ARTE), Projectos de IC&DT de Consolidação de Competências e Recursos em Investigação – Ciências Naturais e do Ambiente – 2012, RECI/GEO-FIQ/0522/2012 Leading Institution: IST/ITN, Principal Investigator: Miguel A. Reis (submitted).

# **CONFERENCE ORGANIZATION / COMMITTEES**

• President of the International Advisory Committee of the International Conference on Particle Induced Xray Emission (next Conference to be held on Brazil, 3-8 March 2013).

# **COLLABORATIONS**

- Centro de Física Atómica da Universidade de Lisboa.
- Co-orientação do Programa de Pós Doutoramento de P. Cristina Chaves sobre aplicações PIXE de alta resolução e alta energia para caracterização de amostras geológicas.
- Member of the Geant4 Collaboration.

#### NAME: Nuno Rombert Pinhão CATEGORY: Auxiliary Researcher ID NUMBER: 25379

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Methane conversion in plasmas produced by dielectric barrier discharges	25%
2	Development of a "plasma needle" for biomedical applications	15%
3	Development of software for non-thermal plasmas modelling	30%
4	Maintenance and recovery of HPGe detectors	10%
5	Science management activities	20%
Total		100%

# WORK SUMMARY

Nº	Summary of Work and Achievements
1	Syngas - a H <sub>2</sub> , CO and CO <sub>2</sub> mixture - is a key intermediate in the chemical industry and plays an
	increasing role in energy conversion. The project studies the use of non-thermal plasmas for
	production of Syngas and the direct production of high hydrocarbons from methane and an oxidant
	$(CO_2 \text{ or } O_2)$ . The influence of gas temperature, population of vibrational excited states and
	composition on the electron kinetics were studied. Formalism for the treatment of vibrational
	excited states for polyatomic gases in the electron Boltzmann equation was developed. Preliminary
	results have been published in two international conferences. A national patent request has been
	submitted.
2	Plasma Medicine is a new and fast raising field of application of non-thermal plasmas. The
	development of very low-power and low-temperature plasma sources at atmospheric pressure that
	produce oxygen and nitrogen radicals as well as UV radiation, finds application on biological
	decontamination and cleaning of surfaces. The areas of application include several medical
	disciplines and industrial processing. A prototype of a RF plasma needle and electric diagnostics for
2	the measurement of the power transferred to the samples were developed.
3	A code for solving the electron Boltzmann equation for a swarm in the hydrodynamic regime and
	compute transport parameters and rate coefficients is under development. The code is able to nandle
	any number of gases and uses a new formalism to nandle polyatomic gases and the effect of multi-
	allowing interactive use of the code
Δ	HPGe detectors are commonly used for high resolution gamma and X-ray spectrometry. The
-	maintenance of these equipment is expensive and usually requires long stop periods. However
	several maintenance operations can be performed "in home" with the available resources and
	expertise and a small laboratory had been set for this purpose. The protocol for replacement of
	sensitive components in a glove box was set and used on the recovery of detectors.
5	Science management activities include:
	1. Preparation of projects for a FCT call;
	2. Invited honorary member of the "Fórum dos Conselhos Científicos dos Laboratórios de Estado"
	and member of the organizing board of a cycle of scientific meeting on "A Ciência na Prevenção
	e Mitigação dos Riscos em Portugal";
	3. Project referee for the Research Foundation Flanders, FWO;
	4. Referee for IOP and Elsevier journals;
	5. Involvement on the preparation of the plan of Activities for 2012 for the group and several other
	documents.

# COMMUNICATIONS

- Influence of the voltage waveform of a DBD discharge on the conversion of CH<sub>4</sub> and CO<sub>2</sub>, N. R. Pinhão, A. Janeco, L. M. Redondo, H. Canacsinh, J. Branco, ESCAMPIG XXI, Viana do Castelo, Portugal, July 10-14 (2012)
- Study of the electron kinetics in He/CH4/CO2 mixtures for Syngas production, A. Janeco, N. R. Pinhão, V. Guerra, ESCAMPIG XXI, Viana do Castelo, Portugal, July 10-14 (2012)

• Effect of rare gas and product concentration on the electron kinetics of He/CH<sub>4</sub>/CO<sub>2</sub> mixtures for Syngas production, Vasco Guerra, André Janeco, Nuno Pinhão, GEC LXV, Austin, Texas, USA, 22-26 Oct (2012)

#### **PROJECTS**

• Increasing the energy efficiency of plasma conversion of methane (AEECMP), project proposal to FCT call. Leading Institution: IST/ITN, Coordinator: N. Pinhão (60%) [the project was approved]

## **CONFERENCE ORGANIZATION / COMMITTEES**

• Member of the Organizing Board of the cycle of meeting on "A Ciência na Prevenção e Mitigação dos Riscos em Portugal": 1st meeting on "Riscos Naturais", 20/09/2012, FCG, Lisbon; 2nd meeting on "Riscos do Ambiente e Qualidade do Ar", 8/11/2012, FCG, Lisbon.

## PATENTS

• PROCESSO DE CONVERSÃO DE METANO E UM OXIDANTE EM GÁS DE SÍNTESE E HIDROCARBONETOS UTILIZANDO UM PLASMA NÃO-TÉRMICO E O AUXÍLIO DE UM GÁS RARO, N. Pinhão, A. Janeco, J. Branco, National patent nº 105078, BPI, 31 Dec 2012.

# NAME: Maria Teresa Ferreira Marques Pinheiro

**CATEGORY:** Auxiliary Researcher **ID NUMBER:** 25083

#### **R&D ACTIVITIES**

Order	Activity Description	R&D
1	Research	70%
2	Teaching	30%
Total		100%

N°	Work Summary and Main Achievements
1	Major research areas focused:
	1) Clinical research
	In coronary artery disease, specific markers of the inflammatory, oxidative and apoptosis
	processes were associated with the atherosclerotic plaque burden and its biological
	composition. Results will help identifying and treating at-risk patients before a heart attack
	occurs or plaque progresses to cause debilitating chest pain.
	In hemochromatosis patients the iron concentration in skin, a readily accessible tissue, reflect
	liver iron overload. This may enable better-informed decisions on when to initiate, change or
	stop therapy.
	2) Interaction between air pollution and health
	Pb concentration in exhaled breath condensate proved to reflect the level of exposure in
	industrial environment.
	3) Toxicity of nanoparticles
	The elemental profiles and concentration gradients were determined in benthic organisms. Cellular and tissue wall uptake of Mn, Fe and Zn were inferred.
	The toxicity of TiO <sub>2</sub> nanoparticles (TiO <sub>2</sub> -NP) was assessed using Daphnia magna as a
	model. All tissues and organs, including eggs, of Daphnia exposed to TiO <sub>2</sub> -NP showed Ti
	accumulation, which seems to be concentration-dependent and associated to changes in
	protein expression profile. Therefore, ingested TiO <sub>2</sub> -NP has consequences in the physiology
	of these organisms.
	These research projects involve a variety of techniques, such as, proton microscopy,
	inductively coupled plasma mass spectrometry, flow cytometry, biochemical methods,
	magnetic resonance imaging, and radiofrequency-based techniques.
2	Professor in charge of the semestrial Biophysics course, Physics Dept., IST.

## **PAPERS**

- P. Napoleão, M. Selas, C. Freixo, M. Mota Carmo, A.M. Viegas-Crespo, R. Cruz Ferreira, T. Pinheiro. T lymphocytes alterations are associated with oxidized LDL, troponin T, white blood cells and C-reactive protein during acute myocardial infarction. Clinical Hemorheology and Microcirculation (2012), online, DOI:10.3233/CH-121665 (IF 3.398).
- M.D. Ynsa, R. Minquin, R. Rajendran, T. Pinheiro, F. Watt, Consequences of fat diet in the distribution of minerals within pancreatic tissues of rats and rabbits. Microscopy and Microanalysis, 18,1060–1066 (2012), DOI:10.1017/S1431927612001547 (IF 3.007).
- M.A. Barreiros, T. Pinheiro, P.M. Felix, C. Franco, M. Santos, F. Araújo, M.C. Freitas, S.M. Almeida. Exhaled Breath Condensate as a biomonitor for metal exposure: A new analytical challenge. J. Radional Nucl Chem. (2012), online, DOI 10.1007/s10967-012-2366-x (IF 1.520).
- V. Silva, S. M. Almeida, M. C. Freitas, A. M. Marques, A. I. Silva, C. A. Ramos, T. Pinheiro, INAA and PIXE characterization of heavy metals and rare earth elements emissions from phosphorite handling in harbours, J. Radioanal. Nucl. Chem., 294, 277–281 (2012), DOI 10.1007/s10967-011-1524-x (IF 1.520).
- S. M. Almeida, A. V. Silva, M. C. Freitas, A. M. Marques, C. A. Ramos, A. I. Silva, T. Pinheiro, Characterization of dust material emitted during harbour activities by k0-INAA and PIXE, J. Radioanal. Nucl. Chem. 291, 77–82 (2012), DOI 10.1007/s10967-011-1279-4 (IF 1.520).

## **COMMUNICATIONS**

- C. Ramos, P. Napoleão, T. Pinheiro, M. Selas, R. Cruz Ferreira, M. Mota Carmo, A.M. Viegas-Crespo. Activation of peripheral blood T lymphocytes in coronary artery disease. 80th European Atherosclerosis Society Congress (EAS 2012), Milan, Italy, 25-28 May (2012), Poster Presentation.
- C. Ramos, P. Napoleão, C. Fondinho, M. Selas, C. Freixo, A.M. Viegas-Crespo, M. Mota Carmo, T. Pinheiro, R. Cruz Ferreira, Inter-relação dos marcadores sanguíneos de função endotelial e actividade inflamatória com a composição da placa avaliada por VH IVUS. Estudo Preliminar, XXXIII Congresso Português de Cardiologia, Vilamoura, Portugal, 22-24 Abril (2012), Oral Talk.
- T. Pinheiro, Inter-relação dos marcadores sanguíneos de função endotelial e actividade inflamatória com a composição da placa avaliada por VH IVUS, in: "Doenças cardiovasculares, factores de risco e biomarcadores" seminar series, Universidade dos Açores, Centro de Investigação de Recursos Naturais, Grupo de Ciências Biomédicas, Ponta Delgada, Portugal, 28 September (2012), Invited Talk.
- T. Pinheiro, Integrated view of Cardiac Biomarkers, Symposium in: Translational Approach in Cardiovascular and Metabolic Diseases A University Perspective, Santa Marta Lisbon Summer Meeting 2012, Lisboa, Portugal, 29-30 June (2012), Invited Talk.
- R.M.Godinho, J. Raimundo, R. Antunes, C. Vale, S. Mendes, L. C. Alves, T. Pinheiro, Trace elemental profiles in teeth of sperm whales from Azores, *13th International Conference on Nuclear Microprobe Technological Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- R. M. Godinho, J. Raimundo, C. Vale, B. Anes, P. Brito, L. C. Alves, T. Pinheiro, Metal contaminants from highway drainage water were internalized by the aquatic plant Lemna minor, *13th International Conference on Nuclear Microprobe Technological Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Poster Presentation.
- T. Pinheiro, Liliana Moita, Luís Silva, E. Mendonça, A. Picado, Nuclear Microscopy as a tool in nano TiO2 Bioaccumulation Studies in aquatic species, *13th International Conference on Nuclear Microprobe Technological Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July (2012), Oral Talk.
- L.C. Alves, V. Corregidor, T. Pinheiro, L. Ferreira, MeV Ion Beam Microscopy: a Tool for Materials Characterization, *SPMicros2012 Microscopy: A tool for the advancement of science*, September 24-25, 2012, Lisbon, Portugal. Oral Talk.

# **EDUCATION**

• T. Pinheiro, Biophysics Course, Semestrial, Physics and Biomedical Engineering master degrees, Physics Department, IST.

- T. Pinheiro, Seminar "Poluição, Nanopartículas e Sistema Respiratório", Biologia Humana e Ambiente Master degree, Facudade de Ciências, Universidade de Lisboa, March 2012.
- T. Pinheiro, Ph.D. Thesis, New Biomarkers of Exposure to Metals Using Exhaled Breath Condensate (EBC), Pedro M. Félix, TUDelft, Delft University of Technology, The Netherlands, October 2012 (http://www.iospress.nl/book/new-biomarkers-of-exposure-to-metals-using-exhaled-breath-condensate-ebc/)
- T. Pinheiro, Member of Jury Ph.D. Thesis in Biology and Biochemistry, Rita Ferin Borges, Atherosclerotic Risk Factors in Asymptomatic Azorean Subjects, Universidade dos Açores, September 2012.
- T. Pinheiro, Examiner of Ph.D. Thesis in Physics: Chen Xiao, The construction and implementation of a dedicated beam line facility for ion beam imaging, University of Singapore, October 2012.
- T. Pinheiro, Examiner of M. Sc. Thesis in "Biologia Humana e Ambiente": Nuno Duro, Avaliação do metabolism do monóxido de azoto eritrocitário, Faculdade de Ciências, Universidade de Lisboa, December 2012.

# **PROJECTS**

- FCT/PIC/IC/82734/2007 (March 2009 –December 2012)- The relationship of circulating biomarkers of apoptosis and endothelial function with the plaque composition using VH IVUS. Leading Institution: IST/ITN Coordinator: T. Pinheiro (30%). Participants: CHLC/MS -Hosp. Sta Marta; CESAM-FFC/FC/UL; CESPU.
- Liga dos Amigos do Hospital de Sta Marta (2012) Inflammation markers in acute coronary syndromes. Leading Institution: Serviço de Cardiologia, Hospital de Santa Marta. Coordinator: T. Pinheiro (5%).
- PTDC/CTM/099446/2008 Avaliação integrada de Nanomateriais: Caracterização e determinação da Toxicidade Ambiental-NanoTox Integrated evaluation of nanomaterials: Characterization and Assessment of Environmental Toxicity-NanoTox. Leading Institution: LNEG. IST/ITN coordinator: T. Pinheiro (10%).
- Governo de Espanha, Ministerio para a Ciência e Innovación (2011-2014) Study of NPs interaction with cells, using methodologies based on IBA (Ion Beam Analysis) techniques. Leading Institution: CMAM. Coordinator IST/ITN: T. Pinheiro (10%). Participants: CIBA, University Singapore.
- PTDC/AAC-AMB/098825/2008 (2010-2013) PM<sub>fugitive</sub>: Mitigating the Environmental and Health Impacts of Particles from Fugitive Emissions. Leading institution: IST/ITN coordinator: S. Marta Almeida. IST/ITN participant: T. Pinheiro (15%). Participants: Instituto de Soldadura e Qualidade / SAPEC.

# **CONFERENCE ORGANIZATION / COMMITTEES**

- T. Pinheiro, Conference Chair, *13th International Conference on Nuclear Microprobe Technological Applications* (ICNMTA 2012), Lisboa, Portugal, 22-27 July, 2012 (http://www.icnmta2012.itn.pt/).
- T. Pinheiro, Symposium organization "Translational Approach in Cardiovascular and Metabolic Diseases - A University Perspective" in: Santa Marta Lisbon Summer Meeting 2012, Lisbon, 29-30 June (2012) (http://www.chlc.min-saude.pt/ ResourcesUser/CHL/Sala\_imprensa/ Summer\_Meeting\_2012.pdf)
- T. Pinheiro, Workshop Chair, Biomarcadores sanguíneos e imagiologia da placa aterosclerótica, Sacavém, 10 December 2012 (http://www.itn.pt/pt/ev/2012/Workshop-IVUS-2012-programa.pdf)
- T. Pinheiro, Member of the International Committee of the ICNMTA conference series (International Conference on Nuclear Microprobe Technology and Applications)
- T. Pinheiro, Member of the AIFIRA Platform Programme Advisory Panel, CENBG, Bordeaux, France.

#### **COLLABORATIONS**

- Alexandra Barreiros, LNEG, Lisboa (Micro-analytical techniques, collaboration)
- Ana Abreu, Hospital de Santa Marta, Faculdade de Ciências Médicas, Universidade Nova de Lisboa (Cardiology, collaboration)

- Maria Dolores Ynsa, CMAM Centro de Micro-Análisis de Materiales, Universidad Autonoma de Madrid, Madrid, Spain (Ion beam microanalysis, collaboration)
- Paulo Filipe, Clinica de Dermatologia, Faculdade de Medicina, Universidade de Lisboa (Dermatology, collaboration).
- René Santus, Département RDDM, Muséum National d'Histoire Naturelle, Paris, France (Dermatology, collaboration).

#### **NAME: Katharina Lorenz**

**CATEGORY:** Auxiliary Researcher (Ciência 2007) **ID NUMBER:** 25461

#### **R&D ACTIVITES**

Nº	Activity Description	R&D
1	Ion beam modification and neutron irradiation studies of wide bandgap	30%
	semiconductor hetero- and nanostructures PTDC/CTM/100756/2008 (coordinated by	
	K. Lorenz)	
2	Ion beam modification of novel III-nitride hetero- and nano-structures (bilateral	10%
	project FCT/DAAD) (coordinated by K. Lorenz)	
3	Electron emission Channelling and Perturbed Angular Correlations Solid State	15%
	Physics Experiments at ISOLDE CERN/FP/116320/2010 (coordinated by J.G.	
	Correia)	
4	Free-charge carrier properties and doping mechanisms of InN-based materials	10%
	PTDC/FIS/100448/2008 (coordinated by V. Darakchieva)	
5	Training: supervision of PhD students, research fellows and post-docs; classes in	20%
	international schools and laboratory classes	
6	Others: Submission of new projects, participation in academic juries, refereeing of	15%
	journal papers, evaluation of research projects	
Total		100%

Nº	Work Summary and Main Achievements
1	Doping by ion implantation and radiation effects in advanced wide bandgap semiconductor
	structures have been studied with emphasis on low dimensional structures such as the rare earth
	doping of nanowires and intermixing studies of quantum well and quantum dot superlattices.
	Structural and compositional studies of wide bandgap ternary compounds such as AlInN, ZnMgO
	and ZnCdO are performed using ion beam analysis and X-ray techniques.
2	Ion implantation and in-situ RBS/C measurements have been performed in AlGaN alloys during a
	10-day beamtime at the University of Jena. Surprisingly, very little difference has been found for
	the damage accumulation processes for alloys with different AlN content. Furthermore, the
	implantation damage of GaN grown along different crystal directions was evaluated and
	significant differences have been found for a-plane GaN in an intermediate fluence regime.
3	In the frame of this project I am spokesperson for an international collaboration at ISOLDE/CERN
	(project IS481). This year two radioactive beamtimes for <sup>111m</sup> Cd and <sup>117</sup> Ag were carried out for
	Perturbed Angular Correlation measurements of Ga <sub>2</sub> O <sub>3</sub> nanowires, powder pellets and single
	crystals.
4	My main task within this project is the measurement of unintentional hydrogen doping in III-N
	layers by Elastic Recoil Detection Analysis as well as their structural characterization by
	Rutherford Backscattering Spectrometry and Channelling. The main achievement was the
	correlation of hydrogen impurities with the free charge carrier concentration in n-type InN thin
	films grown by molecular beam epitaxy.
5	I have been supervising one PhD student (Sérgio Magalhães), one research fellow (Sérgio
	Miranda) and on post-doc (Andrés Redondo).
	I gave a theoretical lecture and a laboratory class on "Ion beam studies of nanostructures" within

	the 2rd CDIDIT Workshop on Lon Deams as a Teal for Nonstachuslassy
	the 3 <sup>rd</sup> SPIRIT workshop on ion Beams as a 1001 for Nanotechnology.
	I gave a laboratory class on RBS within the course "Técnicas Nucleares" for Master degree
	students in physical engineering of Lisbon University.
6	Four new projects were submitted of which three were recommended for funding.
	I was examiner in one PhD jury and one habilitation jury.
	I acted as referee for 8 papers.
	I evaluated one research project for the Latvian Science Council.

## **BOOK CHAPTER**

• K. Lorenz and E. Wendler, "Implantation damage formation in GaN and ZnO" Chapter in "Ion Implantation" ed. M. S. Goorsky, INTECH 2012.

## **PAPERS**

- P. Miranda, U. Wahl, N. Catarino, K. Lorenz, J.G. Correia, E. Alves, "Damage formation and recovery in Fe implanted 6H–SiC", *Nuclear Instruments and Methods in Physics Research B*, 286, 89-92, (2012), doi:10.1016/j.nimb.2011.10.072
- S. Leclerc, B. Lacroix, A. Declémy, K. Lorenz, and P. Ruterana, "Mechanisms of damage formation in Eu-implanted AlN", *J. Appl. Phys.* 112, 073525, (2012) http://dx.doi.org/10.1063/1.4758311
- N. Catarino, E. Nogales, N. Franco, V. Darakchieva, S. M. C. Miranda, B. Méndez, E. Alves, J. G. Marques, K. Lorenz, "Enhanced dynamic annealing and optical activation of Eu implanted a-plane GaN", *Europhysics Lett.* 97, 68004 (2012), doi: 10.1209/0295-5075/97/68004
- A. Redondo-Cubero, A. Hierro, J.-M. Chauveau, K. Lorenz, G. Tabares, N. Franco, E. Alves and E. Muñoz, "Single phase a-plane MgZnO epilayers for UV optoelectronics: substitutional behaviour of Mg at large contents", *Cryst. Eng. Comm.*, 14 1637-1640, (2012), doi:10.1039/c2ce06315h
- J. Rodrigues, S.M.C. Miranda, N.F. Santos, A.J. Neves, E. Alves, K. Lorenz, T. Monteiro, "Rare earth codoping nitride layers for visible light", *Materials Chemistry and Physics* 134, 716-720 (2012), doi:10.1016/j.matchemphys.2012.03.056
- S.M.C. Miranda, N. Franco, E. Alves, K. Lorenz, "Cd ion implantation in AlN", *Nuclear Instruments and Methods in Physics Research B* 289, 43-46, (2012), http://dx.doi.org/10.1016/j.nimb.2012.08.007
- M. Auf der Maur, K. Lorenz, A. Di Carlo, "Band gap engineering approaches to increase InGaN/GaN LED efficiency", *Optical and Quantum Electronics* 44, 83-88, (2012), doi:10.1007/s11082-011-9536-x
- K. P. O'Donnell, M. Auf der Maur, A. Di Carlo, K. Lorenz, "It's not easy being green: Strategies for allnitrides, all-colour solid state lighting" *Phys. Status Solidi RRL* 6, 49-52 (2012), doi:10.1002/pssr.201100206
- M. Fialho, S. Magalhães, L.C. Alves, C. Marques, R. Maalej, T. Monteiro, K. Lorenz, E. Alves, "AIN content influence on the properties of AlxGa1–xN doped with Pr ions", *Nuclear Instruments and Methods in Physics Research B* 273, 149-152, (2012), doi:10.1016/j.nimb.2011.07.062
- S. Magalhães, N.P. Barradas, E. Alves, I.M. Watson, K. Lorenz, High precision determination of the InN content of Al<sub>1-x</sub>In<sub>x</sub>N thin films by Rutherford backscattering spectrometry, *Nuclear Instruments and Methods in Physics Research B*, 273, 105-108, (2012), doi:10.1016/j.nimb.2011.07.051.
- S. M. C. Miranda, K. Lorenz, E. Alves, J.G. Correia, P. Kessler, R. Vianden, K. Johnston, "Ion implantation of Cd and Ag into AlN and GaN", *Phys. Status Solidi C*, 9, 1060-1064, (2012), doi:10.1002/pssc.201100203
- P. Kessler, K. Lorenz, S.M.C. Miranda, R. Simon, J.G. Correia, K. Johnston, R. Vianden, and the ISOLDE collaboration "Cd doping of AlN via ion implantation studied with perturbed angular correlation", *Phys. Status Solidi C*, 9, 1032 (2012), doi:10.1002/pssc.20100207
- J. Rodrigues, M. Peres, M. J. Soares, K. Lorenz, J. G. Marques, A. J. Neves, T. Monteiro "Influence of neutron irradiation and annealing on the optical properties of GaN", *Phys. Status Solidi C*, 9, 1016 (2012), doi:10.1002/pssc.201100200

- K. Lorenz, S. M. C. Miranda, E. Alves, I. S. Roqan, K. P. O'Donnell, and M. Boćkowski, "High pressure annealing of Europium implanted GaN", *Proc. of SPIE* Vol. 8262, 82620C (2012), doi:10.1117/12.906810
- A. Redondo-Cubero, M. Brandt, F. Henneberger, E. Alves and K. Lorenz, "Ion beams as a tool for the characterization of near-pseudomorphic CdZnO epilayers", *Proc. of SPIE* Vol. 8263, 82630U (2012), doi: 10.1117/12.908496
- E. Nogales, I. López, B. Méndez, J. Piqueras, K. Lorenz, E. Alves and J.A. García, "Doped gallium oxide nanowires for photonics", *Proc. of SPIE* Vol. 8263, 82630B (2012), doi:10.1117/12.907766
- Vyacheslav Kachkanov, Igor Dolbnya, Kevin O'Donnell, Katharina Lorenz, Sergio Pereira, Ian Watson, Thomas Sadler, Haoning Li, Vitaly Zubialevich, and Peter Parbrook, "Characterisation of III-nitride materials by synchrotron X-ray microdiffraction reciprocal space mapping", *Phys. Status Solidi C*, 1–5 (2012), doi:10.1002/pssc.201200596
- M. Fialho, K. Lorenz, S. Magalhães, A. Redondo-Cubero, J. Rodrigues, N.F. Santos, T. Monteiro, E. Alves, "Optical doping of AlxGa1-xN compounds by ion implantation of Tm ions", AIP Conf. Proc. IIT 1496, 63 (4 p.), (2012), doi:10.1063/1.4766490

#### **SEMINARS**

• Doping of III-nitride semiconductors with rare earth ions for light emission from IR to UV, K. Lorenz, University of Jena, Germany, 09 Nov. 2012, Invited Seminar

#### **INVITED LECTURES**

- IST/ITN Sacavém, 19. 07. 2012, Lecture within the 3<sup>rd</sup> SPIRIT Workshop on Ion Beams as a Tool for Nanotechnology: "*Ion beam studies of nanostructures*"
- IST/ITN Sacavém, 19. 07. 2012, Laboratory class within the 3<sup>rd</sup> SPIRIT Workshop on Ion Beams as a Tool for Nanotechnology: "*Hands-on session: Ion beam studies of nanostructures*"

#### **COMMUNICATIONS**

#### Invited Talks at Conferences

- Doped gallium oxide nanowires for photonics, <u>E. Nogales</u>, I. López, B. Méndez, J. Piqueras, K. Lorenz, E. Alves, J. A. García, *SPIE Photonics West*, OPTO, Oxide-based Materials and Devices III, 22-25 January 2012 in San Francisco, California United States
- Ion beams as a tool for advanced structural characterization in ZnO-based materials, <u>A. Redondo-Cubero</u>, K. Lorenz, E. Alves, R. Gago, A. Hierro, M. Vinnichenko, J.-M. Chauveau, A. Nakamura, M. Krause, J. Temmyo, E. Muñoz, M. Brandt, F. Henneberger, *SPIE Photonics West*, OPTO, Oxide-based Materials and Devices III, 22-25 January 2012 in San Francisco, California United States
- Thin films, nano-structures and ion implantation a microscopic-world viewed at atomic scale by exotic nuclear methods, <u>M. Barbosa</u>, J. N. Gonçalves, A. Redondo-Cubero, S. M. C. Miranda, R. Simon, P. Kessler, M. Brandt, F. Henneberger, E. Nogales, B. Méndez, K. Johnston, E. Alves, R. Vianden, J.P. Araujo, K. Lorenz, J. G. Correia, Fall *Meeting of the European Materials Research Society (E-MRS)*, Symposium L: Defect-induced effects in nanomaterials, September 16 21, 2011, Warsaw, Poland

#### Oral Presentations at Conferences

- Rare earth doping of III-nitrides: in situ doping vs. ion implantation, <u>K. Lorenz</u>, S. Magalhães, S. Miranda, N. Catarino, N. Franco, E. Alves, M. Peres, J. Rodrigues, T. Monteiro, I. S. Roqan, K.P. O'Donnell, E. Nogales, B. Méndez, V. Fellmann, B. Daudin, A. Nishikawa, Y. Fujiwara, *SPIE Photonics West*, OPTO, Gallium Nitride Materials and Devices VII, 23-26 January 2012 in San Francisco, California United States
- Potential of ion-induced intermixing in AlN/GaN superlattices: implantation damage build-up at low temperatures, <u>A. Redondo-Cubero</u>, K. Lorenz, E. Wendler, V. Fellmann, and B. Daudin, 19th International Conference on Ion Implantation Technology (IIT2012), 25-29 June 2012, Valladolid, Spain
- *The potential of ion beam analysis for the characterization of III-nitride nanostructures*, <u>K. Lorenz</u>, S.M.C. Miranda, A. Redondo-Cubero, S. Magalhães, L.C. Alves, N. P. Barradas, E. Alves, B. Daudin, K.

P. O'Donnell, C. Wetzel, Fall *Meeting of the European Materials Research Society (E-MRS)*, Symposium K: Highly precise characterization of materials for nano and bio technologies, September 16 – 21, 2011, Warsaw, Poland

- Towards the understanding of the intentionally induced yellow luminescence in GaN nanowires, <u>J.</u> <u>Rodrigues</u>, S.M.C. Miranda, A.J.S Fernandes, E. Nogales, L.C. Alves, E. Alves, G. Tourbot, B. Daudin, B. Méndez, K. Lorenz, F. M. Costa, T. Monteiro, *Fall Meeting of the European Materials Research Society* (*E-MRS*), Symposium L: Defect-induced effects in nanomaterials, September 16 – 21, 2011, Warsaw, Poland
- A comparative study of photo- cathodo- and iono- luminescence of GaN nanowires implanted with rare earth ions, <u>J. Rodrigues</u>, S.M.C. Miranda, M. Peres, E. Nogales, L.C. Alves, E. Alves, G. Tourbot, B. Daudin, B. Méndez, K. Lorenz, T. Monteiro, *13th International Conference on Nuclear Microprobe Technology & Applications 2012*, 22 27 July 2012, Lisbon, Portugal
- Characterization of InGaN and InAlN Epilayers by Microdiffraction X-ray Reciprocal Space Mapping, <u>V.</u> <u>Kachkanov</u>, I. P. Dolbnya, K. P. O'Donnell, K. Lorenz, S. Pereira and I. M. Watson, UKNC 2012 Conference, 4-5 January 2012, Bath, U.K.
- *Temperature-dependent luminescence hysteresis of Eu-implanted p-type GaN*, <u>K.P. O'Donnell</u>, R.W. Martin, M. Boćkowski and K. Lorenz, UKNC 2012 Conference, 4-5 January 2012, Bath, U.K.
- Luminescence Hysteresis and Identification of a Possible Charge-State-Alternation Resonance of the Mg Acceptor, <u>K.P. O'Donnell</u>, P.R. Edwards, R.W. Martin, K. Lorenz, E. Alves, V. Darakchieva, AVS 59th International Symposium & Exhibition, 28 October 2 November, 2012, Tampa, FL United States.
- Characterisation of III-nitride materials by synchrotron X-ray microdiffraction reciprocal space mapping, <u>Vyacheslav Kachkanov</u>, Igor Dolbnya, Kevin O'Donnell, Katharina Lorenz, Sergio Pereira, Ian Watson, Thomas Sadler, Haoning Li, Vitaly Zubialevich, and Peter Parbrook, 4th International Symposium on Growth of III-Nitrides, July 16-19, 2012, St. Petersburg, Russia
- Luminescence studies of AlxGa1-xN alloys doped with rare earth ions, M. Fialho, K. Lorenz, S. Magalhães, J. Rodrigues, N. F. Santos, T. Monteiro, and <u>E. Alves</u>, 18th International Conference on Ion Beam Modifications of Materials (IBMM2012), 2-7 September 2012. Qingdao, China
- Towards efficient solid state lighting using ion beam techniques, <u>A. Redondo-Cubero</u>, E. Wendler, M. Auf der Maur, A. Di Carlo, E. Alves, P.R. Edwards, K. P. O'Donnell, C. Wetzel, K. Lorenz, *International Workshop on the Modification and Analysis of Materilas for Future Energy Source*, 17-20 September 2012, Madrid, Spain.

#### Poster presentation at conferences

- Optical doping of AlxGa1-xN compounds by Ion Implantation of Tm ions, <u>M. Fialho</u>, K. Lorenz, S. Magalhães, A. Redondo-Cubero, J. Rodrigues, N. F. Santos, T. Monteiro, and E. Alves, 19th International Conference on Ion Implantation Technology (IIT2012), 25-29 June 2012, Valladolid, Spain
- Damage study of Eu implantation on non-polar and polar GaN, N. Catarino, <u>A. Redondo-Cubero</u>, E. Alves, E. Nogales, B. Méndez, and K. Lorenz, 19th International Conference on Ion Implantation Technology (IIT2012), 25-29 June 2012, Valladolid, Spain
- Disorder Induced Blue Luminescence in RF-deposited ZnO films, <u>M. Peres</u>, S. Magalhães, M.R. Soares, M.J.Soares, E. Alves, K. Lorenz, M. R. Correia, A.C. Lourenço, T. Monteiro, *Fall Meeting of the European Materials Research Society (E-MRS)*, Symposium L: Defect-induced effects in nanomaterials, September 16 – 21, 2011, Warsaw, Poland
- Microprobe analysis, iono- and photo- luminescence of manganese activated ZnGa2O4 fibres, <u>N. F. Santos</u>, A. J. S. Fernandes, L. C. Alves, N. A. Sobolev, E. Alves, K. Lorenz, F. M. Costa, T. Monteiro, 13th International Conference on Nuclear Microprobe Technology & Applications 2012, 22 27 July 2012, Lisbon, Portugal
- The influence of photon excitation and proton irradiation on the luminescence properties of yttria stabilized zirconia doped with praseodymium ions, <u>M. R. N. Soares</u>, M. J. Soares, L.C. Alves, E. Alves, K. Lorenz, F. M. Costa, T. Monteiro, 13th International Conference on Nuclear Microprobe Technology & Applications 2012, 22 27 July 2012, Lisbon, Portugal

- Temperature-dependent hysteresis, photochromism and photobleaching of the emission spectrum of europium-implanted, magnesium-doped HVPE GaN, Kevin O'Donnell, Robert Martin, Paul Edwards, Katharina Lorenz, Eduardo Alves, and Michal Bockowski, International Conference on the Physics of Semiconductors 2012, 2 July 3 August 2012, Zurich, Switzerland
- Luminescence Study of Rare Earth Implanted GeO<sub>2</sub> Nanowires, <u>Pedro Hidalgo</u>, Katharina Lorenz, Bianchi Mendez, Javier Piqueras, Eduardo Alves. *MRS Fall Meeting 2012*, Symposium FF: Semiconductor Nanowires–Optical and Electronic Characterization and Applications, 25 30 November, Boston, United States.
- Comparison of low- and room-temperature damage formation in Ar ion implanted GaN and ZnO, <u>E.</u> <u>Wendler</u>, W. Wesch, A. Yu. Azarov, N. Catarino, A. Redondo-Cubero, E. Alves, K. Lorenz, 18th International Conference on Ion Beam Modifications of Materials (IBMM2012), 2-7 September 2012. Qingdao, China

# **EDUCATION**

#### Training

• Laboratory class, Mestrado em Engenharia Física da Universidade de Lisboa, within the course "Técnicas Nucleares" 2012.

## Participation in PhD jury

• Examiner in the PhD exam of Dr. Vincent Fellmann which took place on the 13<sup>th</sup> of January 2012 at the University of Grenoble, France. Title: Croissance et caractérisations structurales e optiques d'hétérostructures de nitrures d'éléments III émettant dans l'UV.

#### Participation in habilitation jury

• Examiner in the HDR (Habilitation à Diriger des Recherches) exam of Dr. Denis Jalabert, which took place on the 1st of October 2012 at the University of Grenoble, France. Title: Analyse de nanostructures semi-conductrices par faisceau d'ions.

#### Thesis supervision

• Ongoing: PhD, Sérgio Nuno Canteiro de Magalhães, "Carateriazação e Modificação de Heteroestruturas de Nitretos do Grupo III", at University of Aveiro and IST

# **PROJECTS**

#### Running projects

- Ion beam modification and neutron irradiation studies of wide bandgap semiconductor hetero- and nanostructures, FCT PTDC/CTM/100756/2008. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz (30%).
- *Ion beam modification of novel III-nitride hetero- and nano-structures*, FCT/DAAD bilateral project. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz (10%).

#### Submitted projects

- Bandgap engineering of III-nitride quantum wells for efficient green light emitting diodes, FCT PTDC/FIS-NAN/0973/2012. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz (35%). – recommended for funding
- Functionalising wide bandgap semiconductor nanowires using ion beams: Novel materials for nano-light emitters and nano-sensors, FCT PTDC/CTM-NAN/2156/2012. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz (35%).- recommended for funding
- Ion beam modification of novel III-nitride hetero- and nano-structures, FCT/EGIDE bilateral project. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz (10%).-under evaluation (French part recommended for funding)
- Solid State Lighting Redefined by Bandgap Engineering Techniques (SORBET), European Project FP7-ICT-2011-8. Leading Institution: IST/ITN. IST/ITN Coordinator: K. Lorenz.– passed threshold but was not recommended for funding

## **CONFERENCE ORGANIZATION / COMMITTEES**

• Member of the program committee and session chairman of "Oxide-based Materials and Devices III", SPIE International Symposium on SPIE OPTO, 21-26 January 2012, San Francisco, USA

# **COLLABORATIONS**

- Prof. Dr. Pablo Esquinazi, University of Leipzig, Germany, 04 Oct.2012, seminar on defect-induced magnetism in non-magnetic oxides
- Prof. Dr. Elke Wendler, University of Jena, Germany, 01-04 Dec. 2012, research visit within bilateral project FCT/DAAD

# NAME: Sandra Isabel Silva Damas Cabo Verde

**CATEGORY:** Auxiliary Researcher (*Ciência 2008*) **ID NUMBER:** 5470

# **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	"Ionization radiation treatment of fruits and vegetables for immuno-compromised	30%
	patients – feasibility study", IAEA Research Contract No. 16281	
2	"Survival and Inactivation Patterns of Viral Threat Agents in the Environment:	25%
	Assessment of Ionizing Radiation as Decontamination Tool", IAEA Research Contract	
	No. 17474	
3	"Characterization and conservation of cultural heritage: neutrons and ionizing radiation	20%
	in artwork" – RADIART". FCT project PTDC/HIS-HEC/101756/2008	
4	"Application of Ionizing Radiation on the Cork Wastewater Treatment", IAEA	10%
	Research Contract No. 16513	
5	Microbiological analysis for Indoor Air Quality in the scope of the Energy	10%
	Certification for Buildings. Requested Service by EFACEC.	
6	Determination of Neomycin Sulfate for Nodryl product. Requested Service by Iberfar	5%
	Pharmaceutical Industry.	
Total		100%

Nº	Work Summary and Main Achievements
1	Food irradiation is a food safety tool. Under the scope of the IAEA Coordinate Research Project
	CRP D6-RC-1163.2 "Development of Irradiated Foods for Immuno-compromised Patients and
	Other Potential Target Groups" it is intended to evaluate the irradiation effects on small fruits and
	the potential extension of shelf-life, in order to improve the safety and variety of immune-
	compromised patients diet. Based on that, fresh cherries and blackberries were irradiated at a Co-
	60 source at sub-lethal several doses (<1.5 kGy). Microbiological, physico-chemical and sensorial
	parameters were assessed after irradiation and during storage time. The results point out to a
	limited microbial inactivation for the applied radiation doses, due to the preponderance of fungi
	(generally more radioresistant) as natural contaminants of these produces. Regarding the physical
	and rheological properties of the studied fruits, no changes in colour were observed, but there was
	decrease in the resistance of the pellicle fracturability with the increasing of radiation dose. The
	performed sensorial analysis indicated a similar acceptability among irradiated and non-irradiated
	fruits. The effect of higher irradiation doses on fruits will be further investigated, in an attempt to
	augment the reduction of the microbial population of blackberries without significantly decrease
	the quality of the fruits.
2	Environmental virology is an emergent field due to the importance of food- and water-transmitted
	viruses. Ionizing radiation is being used more frequently as a useful and effective means of
	disinfection. However, investigation of gamma irradiation to eliminate viruses is limited. Under
	the scope of an IAEA Research project "Survival and inactivation patterns of viral threat agents in
	the environment: assessment of ionizing radiation as decontamination tool" it is aimed to generate
	data on the ionizing radiation inactivation patterns of human virus in environmental matrices. A
	surrogate of human norovirus (do not grow on cell culture ), the Murine norovirus (MNV) was propagated using RAW 264.7 and the viral stock yield was estimated by plaque assay, that is the gold-standard method to measure virus infectivity. In an initial approach it was intended to study the inactivation of MNV on a dried surface biofilm. The virus film was exposed to several sub-lethal doses (>10 kGy) at a Co-60 source and the infectivity of the virus was assessed by the plaque assay technique. For the applied conditions the MNV presented an exponential inactivation kinetics and a D-value of 3.7 kGy. On-going inactivation studies are being performed with the virus in suspension.
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3	Art biodeterioration is one concerning issue that leads to the necessity of developing new approaches in restoration, preservation, conservation and decontamination areas. In the current phase of the RADIART project the main goal was to analyse the green deterioration marks present in the ceramic tiles from the panel "The Great View of Lisbon", in order to understand the link between the agent and pathology. It was applied an integrated microbiological and instrumental analysis methodology that included microbiological culture-based techniques, scanning electron microscopy with backscattered electron imaging (SEM-BSE) analysis and Raman spectroscopy. The results obtained point out to the absence of microbial colonization as cause of this particular alteration pattern and thus other causes should be considered for the conservative purposes. On-going studies are being performed to identify the deteriorating agent for further development of an effective restoration plan of the "Great view of Lisbon" masterpiece. Moreover, a new sampling to the ceramic tile panel was performed in order to evaluate the persistence of the microbial population. The obtained results indicated that the superficial contamination patterns could be related with the different environmental conditions at which panel is exposed
4	Phenolic acids are widely distributed contaminants present in industrial wastewaters, namely in cork industry. Due to their recalcitrant and bioaccumulation potential, the phenolic acids have gathered significant environmental concern. In the scope of the IAEA research project "Application of Ionizing Radiation on the Cork Wastewater Treatment", biodegradation studies are being performed to check if cork natural microbiota could help to reduce the pollutant load of these wastewaters in order to its reuse. The objective of this study was to find out if radiolytic degradation, followed by microbial degradation could increase the treatment efficiency. A natural cork wastewater bacterium was selected from the irradiated wastewater at 9 kGy. The applied methodology was based on the evaluation of growth kinetics of the selected bacteria in minimal salt medium with non-irradiated and irradiated phenolics as substrate. The growth results indicated that the selected cork wastewater natural strain, was not capable to degrade both gallic acid and esculetin (irradiated and nonirradiated) as sole carbon source, for the analyzed conditions. In turn, it was observed for both phenolics compounds and correspondent radiolytic products antimicrobial and bacteriostatic actions against the tested strain. Based on the obtained results a new methodological setup was designed.
5	There is a growing interest in indoor air quality for a better quality environment both at home and at work because many people spend at least 80% of their time indoors. In Portugal, a step forward was given when the European Directive no. 2002/91/CE relative to energetic certification of buildings was transposed to the Portuguese law with the inclusion of IAQ requirements such as comfort parameters, concentrations limits for indoor pollutants and minimum levels of air renovations. The aim of this requested service by EFACEC is to evaluate the indoor concentration of airborne bacteria and fungi in several public buildings. The concentrations of airborne bacteria and fungi were determined by impaction using the MAS-100 portable air sampler and microbial culture media.
6	The activity of antibiotics could be tested in vitro by microbiological assay methods. Based on a previous methodological validation performed in 2010 to implement the method in the Quality Control system of Iberfar pharmaceutical industry, it was requested by the industry to determine the potency of Neomycin Sulfate for a batch of the Nodryl product using the microbiological agar diffusion assay for inter-comparison purposes.

## **PAPERS**

• Nunes, N. Mesquita, S. Cabo Verde, M. J. Trigo, A. Ferreira, M. M. Carolino, A. Portugal, M. L. Botelho, Gamma radiation effects on physical properties of parchment documents: Assessment of Dmax, *Radiation*. *Physics and Chemistry*, 81, 1943-1946, (2012).

- J. Pereira, M. Oliveira, T. Silva, M. G. Lima, S. Cabo Verde, J. Cruz, M. L. Botelho, Avaliação do tratamento de alimentos por radiação ionizante para grupos de risco, 6.º Congresso do Comité Português da URSI - Aplicações das ondas electromagnéticas: da eficiência energética à bioengenharia, ANACOM (2012).
- T. Calado, A. António, S. Cabo Verde, P. Rodrigues, M. L. Botelho, L. Abrunhosa, A. Venâncio, Efeito da Radiação γ em soluções de aflatoxinas, 11º Encontro de Química dos Alimentos (2012) pp. 312.
- C.A. Ramos, S. M. Almeida, S. Cabo Verde, S. Viegas, C. Viegas, Indoor air quality in gymnasiums, European Aerosol Conference (2012) C-WG05S1P34.
- M. J. Trigo, M.B. Sousa, A. Ferreira, A.C. Ramos, S. Cabo Verde, M.L. Botelho, Efeito da irradiação ionizante na vida útil das framboesas (*Rubus idaeus* L.), Actas Portuguesas de Horticultura nº20 (2012) pp. 197-203.

#### **COMMUNICATIONS**

- Biodegradation studies on cork wastewater, <u>S. Cabo Verde</u>, Faculdade de Ciencias da Universidade de Lisboa, 12 Nov. 7 Dec. (2012), Invited Theoretical and laboratory lessons in the scope of the discipline Microbial Biotechnology.
- Avaliação do tratamento de alimentos por radiação ionizante para grupos de risco, J. Pereira, M. Oliveira, T. Silva, M. G. Lima, S. Cabo Verde, J. Cruz, M. L. Botelho, 6.º Congresso do Comité Português da URSI Aplicações das ondas electromagnéticas: da eficiência energética à bioengenharia, Lisbon, 16 Nov., (2012), Poster presentation.
- Inactivation of microorganisms/ higienisation/ preservation (determination of Dmin) on tiles and parchment samples, <u>S. Cabo Verde</u>, Regional Training Course on Radiation Technology for Cultural Heritage Preservation, Lisbon, 5-9 Nov (2012), Invited theoretical and laboratory lessons.
- Application of gamma radiation on the preservation of CH objects: parchment and tiles case studies. <u>S.</u> <u>Cabo Verde</u>, Regional Training Course on Radiation Technology for Cultural Heritage Preservation, Lisbon, 5-9 Nov (2012), Invited talk.
- Efeito da Radiação γ em soluções de aflatoxina. T. Calado, A. António, S. Cabo Verde, P. Rodrigues, M. L. Botelho, L. Abrunhosa, A. Venâncio, 11° Encontro de Química dos Alimentos, Bragança, Portugal, 16-19 Sep. (2012), Poster presentation.
- Resposta dos microrganismos à Radiação Ionizante, <u>S. Cabo Verde</u>, Faculdade de Farmácia da Universidade do Porto, 15 Jun (2012), Invited Talk.
- Effects of gamma radiation on raspberries: safety and quality issues. <u>S. Cabo Verde</u>, A. António, P. Santos, R. Melo, C. Junqueira, T. Silva, I. Nunes, M. J. Trigo, M.L. Botelho. *International Congress of Environmental Health, Lisbon, Portugal, 29May 1 June (2012)*, Oral communication.
- Sistemas de Gestão de Qualidade HACCP: Análise de Perigos e Pontos Críticos de Controlo, <u>S. Cabo</u> <u>Verde</u>, Faculdade de Ciências da Universidade de Lisboa, 16 May (2012), Invited Talk.
- Efeito da irradiação ionizante na vida útil das framboesas (Rubus idaeus L.), M. J. Trigo, M.B. Sousa, A. Ferreira, A.C. Ramos, S. Cabo Verde, M.L. Botelho, IV Colóquio Nacional da Produção de Pequenos Frutos, Faro, Portugal, 20-21 Apr. (2012), Poster presentation.
- Enhancing quality control methods and procedures for radiation technology Portuguese country report. <u>S. Cabo Verde</u>, R. Melo, P.M.P. Santos, T. Silva, I. Nunes, M.L. Botelho. Final Meeting of the IAEA RER8017 project, Vienna, Austria, Feb 6-10 (2012), Oral Communication.

### **EDUCATION / THESES SUPERVISION**

• Supervisor, M. Sc. Thesis, Avaliação do tratamento de frutas e vegetais por radiação ionizante para grupos de risco, by Joana Pereira, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 15 November 2012.

### **PROJECTS**

- Survival and Inactivation Patterns of Viral Threat Agents in the Environment: Assessment of Ionizing Radiation as Decontamination Tool, IAEA Research Contract No. 17474. IST/ITN Coordinator: S. Cabo Verde (40%).
- Ionization radiation treatment of fruits and vegetables for immuno-compromised patients feasibility study, IAEA Coordinate Research Project CRP D6-RC-1163.2 "Development of Irradiated Foods for Immuno-compromised Patients and Other Potential Target Groups", IAEA Research Contract No. 16281. IST/ITN Coordinator: S. Cabo Verde (30%).

#### Submitted projects

- "Avaliação da irradiação de alimentos frescos para doentes imunodeprimidos", FCT. Not recommended for funding.
- Comprehensive study of the effects of gamma rays in chemical and microbiological parameters of cherries, FCT-Bilateral Agreement Portugal-Tunisia. Under evaluation.

### **CONTRACTS**

- Microbiological analysis for Indoor Air Quality in the scope of the Energy Certification for Buildings, IST/ITN/N.381200002; N.381200003; N.381200004, EFACEC, Nov-Dec. 2012, 1.1 k€.
- Determination of Neomycin Sulfate for Nodryl product, IST/ITN/N.381200008, Industria Iberfar, Oct. 2012, 0.2 k€.

## **CONFDERENCE ORGANIZATION / COMMITTEES**

- Organization of the *Regional Training Course on Radiation Technology for Cultural Heritage Preservation*, Lisbon, Portugal, 5-9 November 2012.
- Member of the scientific committee of the *International Congress of Environmental Health* (ICEH), Lisbon, Portugal, 29May 1 June 2012.

### **COLLABORATIONS**

• S. Bashandy, National Centre for Radiation Research and Technology, Egypt, 9-21 April 2012, IAEA Training on Radiation sterilization of medical products based on ISO 11137.

### NAME: Victoria Corregidor Berdasco

**CATEGORY:** Auxiliary Researcher (*Ciência 2008*) **ID NUMBER:** 25463

### **R&D ACTIVITIES**

Nº	Activity Description	R&D
1	Research – Coins: Compositional Study	40%
2	Research - Collaboration, Museu Nacional de Arte Antiga e Museu Nacional de	20%
	Arqueologia, Portugal	
3	Research – Collaboration, Autónoma University of Madrid, Spain	8%
4	Research – Collaboration, Consorzio CREO, Italy	5%
5	Research – Collaboration, Imprensa Nacional - Casa da Moeda, Portugal	5%
6	Training- PhD-Collaboration CAPES	20%
7	Training Ciência viva	2%
Total		100%

# WORK SUMMARY

Nº	Work Summary and Main Achievements
1	Research – Coins: Compositional Study
	Following the work developed over the last year, the proton beam generated by the 2.5 Van de
	Graaff Accelerator was used to study the composition of silver and gold coins from different
	centuries. The main objective is to create a database composition of the coins in order to find

	representative composition for each coin according with the date and place were the coins were
	minted. In this sense, in recent silver coins minted in Portugal (2\$50) from 1943, 1945, and 1951 show
	different Ag content (slightly higher) than the value decreed by Law. Also, the coins were cut and
	it was possible to study the composition distribution along this cut. The coin from 1951 shows a
	silver surface enrichment, probably related with a cleaning process.
	Regarding the gold coins, PIXE analyses were done in order to ascertain about the authenticity
	considering the concentration of the main (gold and silver) and the trace elements.
2	Research – Collaboration, Museu Nacional de Arte Antiga e Museu Nacional de
	Arqueologia, Portugal
	Silver objects from different collections, "Vidigueira Treasure" from Museu Nacional de Arte
	Antiga and gold earrings belonging to "Pancas Treasure" from Museu Nacional de Arqueologia
	were studied by Ion Beam techniques.
	Identification and quantification of the main, minor and trace elements were done.
	Regarding the silver objects, different silver alloys were used: both between the pieces themselves
	and between elements of the same piece. Only a urn from oratory-reliquary and one of the screw
	and diffusion execution the Christ from eretery reliquery, which the Ha emplacem technique was
	gold diffusion, except on the Christ from oratory rendulary, which the fig analgam technique was
	Considering the earrings of the Pancas Treasure, dated to a period between the 5th and the 3nd
	centuries BC from the composition it was possible to establish pairs of earrings. Also the allows
	are different within the Pancas group and correspond to the compositions of objects from the south
	of the Iberian Peninsula, representative of the period of oriental influence. Further studies are
	planned to determine the trace impurities concentration.
3	Research – Collaboration, Autónoma University of Madrid, Spain
	In collaboration with the Crystal Growth Laboratory from Universidad Autónoma de Madrid
	(UAM), ZnO thin films grown on lithium niobate substrates were analysed. The ZnO thin films
	are grown by a novelty method designed by Dr. J.L. Plaza from UAM. These structures have
	several applications, for instance, biosensors, SAW filters or LEDs and lasers in the UV emission.
	By means of IBA techniques it was observed the oxygen depth distribution and a slight diffusion
	of ZnO into the substrate. More studies are required to find the pattern of the diffusion and find the
	correlation with the growth conditions.
4	Research – Collaboration, Consorcio CREO, Italy
	(Italy) The sim of this work is to apply these low dimensional structure metarials, grown on glass
	(hary). The ann of this work is to apply these low differsional structure materials, grown on glass substrates to obtain low-cost photovoltaic devices with competitive efficiency values
	Different thickness (from few nm to $\sim 650$ nm) obtained by vanour deposition on glass substrates
	have preferentially a cubic structure and their growth occurs along the [111] crystallographic
	direction, although the experimental growth conditions should however be carefully adjusted in
	order to have more control on the shape and distribution of the nanowires.
	It was also studied the influence of Bismuth in the nanostructures, which act as nucleation points.
	In fact, the diameter of the Bi2Te3 seeds (~100nm) seems to govern the widths of the nano-
	structures although the distribution of the seeds found in some regions of the glass substrate is
	quite low, suggesting that some of the seeds disappeared during the growth process, and only
	remained those with a critical thickness, ~40 monolayers, which was calculated from the RBS
	spectra.
	The influence of the metal alloy used as back electrode contact was also studied.

5	Research – Collaboration, Imprensa Nacional - Casa da Moeda, Portugal
	In collaboration with other researchers from Universidade Nova de Lisboa (Dr. J Cruz) and CTN,
	a study based on the hardness evolution of steel coinage dies when different dose implantations of
	<sup>14</sup> N <sup>+</sup> ions is under development. The implantation process promotes the formation of a nitrated
	layer on the surface of the dies, increasing the hardness and the number of coins that can be mint.
6	Training: PhD-Collaboration CAPES
	PhD Co-orientation. MSc Morgana Streicher. Title "Al influence on the electrical and optical
	properties of GaInSb crystals grown by Czochralski method". By means of the IBA techniques,
	mainly RBS and PIXE, GaSb and GaInSb crystals were characterized. The results showed a
	heterogeneous In distribution along the crystal growth direction and also the presence of Sb
	precipitates. They are related with the crystal growth conditions, mainly with the temperature
	gradients during the solidification process. The structural quality of several crystals (with different
	In content) was also investigated by channeling experiments. The results show the presence of
	punctual defects and also dislocations along the principal crystallographic orientations. The
	relationship of Ga/Sb in a GaSb ingot doped with Al was established. Along the growth direction,
	the stoichiometric composition is observed and almost constant. On the other hand, in the radial
	direction some deviations were found.
7	Training: "Ciência Viva" Program
	Training Course No. 2734, entitled: "Compositional analysis of metallic artefacts by ion beam
	techniques: determining its authenticity". Duration: 5 days (morning and afternoon). The course
	was directed to students of 11 th / 12 th grade (s) of education in the vocational area of physics.
	During the internship students participated in data acquisition, identification of the elements
	present in silver and gold and quantification. The students also discussed the results obtained and
	compared with the expected composition.

### **PAPERS**

- Q. Zheng, F. Dierre, V. Corregidor, R. Fernandez-Ruiz, J. Crocco, H. Bensalah, E. Alves, E. Dieguez, Deposition of nanometric double layers Ru/Au, Ru/Pd, and Pd/Au onto CdZnTe by the electroless method, *Journal of Crystal Growth*, 358, 89-93 (2012), http://dx.doi.org/10.1016/j.jcrysgro.2011.04.014
- J. Crocco, H. Bensalah, Q. Zheng, V. Corregidor, E. Alves, A. Castaldini, B. Fraboni, D. Cavalcoli, A. Cavallini, O. Vela, E. Dieguez, Study of asymmetries of Cd(Zn)Te devices investigated using photo-induced current transient spectroscopy, Rutherford backscattering, surface photo-voltage spectroscopy, and gamma ray spectroscopies, *Journal of Applied Physics*, 112, 7, (2012), <a href="http://dx.doi.org/10.1063/1.4754448">http://dx.doi.org/10.1063/1.4754448</a>
- Q. Zheng, F. Dierre, J. Franc, J. Crocco, H. Bensalah, V. Corregidor, E. Alves, E. Ruiz, I, Vela, J.M.Perez, E. Dieguez, Investigation of generation of defects due to metallization on CdZnTe detectors, *Journal of Physics D- Applied Physics*, 45, 17, (2012), <u>http://dx.doi.org/10.1088/0022-3727/45/17/175102</u>
- Q. Zheng, F. Dierre, V. Corregidor, J. Crocco, H. Bensalah, J.L. Plaza, E. Alves, E. Dieguez, Electroless deposition of Au, Pt, or Ru metallic layers on CdZnTe, *Thin Solid Films*, 525, 56-63, (2012), http://dx.doi.org/10.1016/j.tsf.2012.09.058
- V. Corregidor, L.C. Alves, PIXE analysis: "Arrecadas" from Museu Nacional de Arqueologia, Portugal, Report.
- V. Corregidor, L.C. Alves, Análises de PIXE do Tesouro da Vidigueira, Museu Nacional de Arte Antiga, Portugal, Report.

# **COMMUNICATIONS**

- Analysis of surface stains on modern gold coins, V. Corregidor, L.C. Alves, J. Cruz, 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, July 2012, Talk.
- CdTe nanorods for photovoltaic devices, V. Corregidor, L.C. Alves, N. Franco, N. V. Sochinskii, E. Alves, 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, July 2012, (Portugal), Poster

- Preliminary study of dye distribution in nanocrystalline TiO2 films for optoelectronic devices, M.A. Barreiros, S. Sequeira, J. Mascarenhas, M.J. Brites, L.C. Alves, V. Corregidor, , 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, July 2012, (Portugal), Poster
- The Earrings of Pancas Treasure: analytical study by X-ray based techniques, I. Tissot, M. Tissot, M. Manso, L.C. Alves, M.A. Barreiros, T. Marcelo, M.L, Carvalho, V. Corregidor, M.F. Guerra, 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, July 2012, (Portugal), Poster
- *MeV Ion Beam Microscopy: a Tool for Materials Characterization*, L.C. Alves, V. Corregidor, T. Pinheiro, L. Ferreira, *SPMicros2012 -, September 24-25, 2012, Lisbon, Portugal.* Talk by L.C. Alves.
- Analysis of a gold solidus of roman emperor Valentinian I, J. Cruz, V. Corregidor, L.C. Alves, P.A. Carvalho, M.A. Stanojev Pereira, M. Fonseca, SPMicros2012, Lisbon, 24th 25th September 2012. Poster
- Investigation of elemental distribution in cat femoral head by nuclear microprobe for Paget disease of bone studies, C. Santos, JM. Fonseca, V. Corregidor, L.C. Alves, M. Capelão, J.C. Branco, A.P. Jesus, SPMicros2012, Lisbon, 24th 25th September 2012. Poster
- External Ion Beam Analysis of "Tesouro da Vidigueira Collection", V. Corregidor, L.C. Alves, A. Candeias, L. Penalva, B. Maduro, 2nd International Workshop on Physical & Chemical Analytical Techniques in Cultural Heritage, 4-5 June 2012, Lisbon, Portugal. Talk
- Combination of IBA techniques to study art-historical objects using a microprobe, V. Corregidor, C.P. Marques, R.C. Silva, P.A. Rodrigues, M. Vilarigues, T. Silva, S. Cabo Verde, M.L. Botelho, M.I. Prudêncio, S. Coentro, V. Muralha, E. Alves, L.C. Alves, 2nd Luminescence in Archaeology International Symposium, 5-7 September 2012, Lisbon, Portugal, Poster.
- Tribological improvement of coinage dies for the Portuguese Mint by nitrogen implantation, J. Cruz, V. Corregidor, B. Nunes, E. Alves, L.C. Alves, R. Colaço, P. Alexandrino, P. Leitão, 18th International Conference on Ion Beam Modifications of Materials (IBMM2012), 2-7 September, 2012, Qingdao, China. Poster.

### **EDUCATION / THESIS SUPERVISION**

- Supervision of PhD work of Morgana Streicher, *Influência do Al nas propriedades eléctricas e ópticas em cristais de GaInSb obtidos pelo método Czochralski*, as Portuguese partner responsible of the CAPES Program, PhD in "Engenharia e Tecnologia de Materiais", from Pontificia Universidade Católica do Rio Grande do Sul, Brasil.
- Training course supervisor of the Ciência Viva Program, N° 2734, Compositional analysis of metallic artefacts by ion beam techniques: determining its authenticity.

### PROJECTS

- *HisCoin Ciência, História e Arte na Numária da República Portuguesa,* PTDC/CPC-EAT/4884/2012. Leading Institution: IST/ITN. Submetido à FCT.
- *IDonEtaCdTe Identificação dos defeitos presentes em células solares com um absorvedor extremamente delgado baseado em nanofios de ZnO e CdTe* PTDC/CTM-ENE/1727/2012. Leading Institution: IST/ITN. Submetido à FCT.

### **CONFERENCE ORGANIZATION / COMMITTEES**

- Organising committee of the 13th International Conference on Nuclear Microprobe Technology and Applications (ICNMTA 2012), Lisbon, Portugal, 22-27 July, 2012.
- Scientific Local Committee, 2nd Luminescence in Archaeology International Symposium (LAIS), Lisbon, Portugal, 5-7 September, 2012.

### **COLLABORATIONS**

• E. Diéguez, Autónoma University of Madrid, Spain, Collaboration: characterization of metal contacts on CdZnTe crystals.

- J.L. Plaza, Autónoma University of Madrid, Spain, Collaboration: characterization of ZnO on lithium niobate.
- Dr. N. Shockinski, Consorzio CREO, L'Aquila (Italy). Collaboration: ion beam techniques applied to CdTe nano-structures for photovoltaic applications.
- M. A. Barreiros, Laboratório Nacional de Energia e Geologia, Lisboa, Portugal, Collaboration: characterization of TiO<sub>2</sub> nano-structures for optoelectronic devices.
- B. deDavid, Pontifícia Universidade Católica do Rio Grande do Sul, Av. Ipiranga, 6681 Porto Alegre/RS Brasil, Collaboration: characterization of GaSb and GaInSb single crystals.
- L. Penalva, Museu Nacional de Arte Antiga, Portugal. Characterization of silver objects by Ion beam techniques.
- B. Maduro, A. Candeias, Instituto dos Museus e da Conservação, Portugal. Characterization of Cultural Artifacts by Ion beam techniques.
- M. Vilarigues, Vicarte, Dept. of Conservation and Restoration from FCT-UNL Characterization of glass objects by Ion beam techniques.
- I. Tissot, M. Tissot, Museu de Arqueologia, Portugal, Characterization of gold objects by Ion beam techniques.
- Collaboration with Imprensa Nacional Casa da Moeda, Portugal.

### **TRAINING PARTICIPATION**

- Microscopy training course "SPMicros2012 Microscopy: A tool for the advancement of science", organized by Instituto Superior Técnico, Lisbon, 26 27 September 2012
- Training course entitled "Enhancing the Characterization, Preservation and Protection of Cultural Heritage Artefacts", organized by Atomic Energy Agency (IAEA) no IST/ITN, 5-6 November, 2012.