
MATERIALS CHARACTERIZATION WITH NUCLEAR RADIOACTIVE TECHNIQUES

Annual Activity Report 2013

UNIT: Physics and Accelerators

TEAM

Name	Category	R&D (%)
João Guilherme Martins Correia	Principal Researcher	100%
Ulrich Wahl	Principal Researcher (Habilitation)	90%
Katharina Lorenz	Researcher	15%
Eric Bosne	BI CERN-FP-123585-2011 & FCT - SFRH/BD/95865/2013	100% from 20-08-2012 up to 01-02-2014 (got a PhD FCT grant)
Ângelo Costa	BI CERN-FP-123585-2011 & FCT - SFRH/BD/86386/2012	100% from 01-11-2012 up to 31-04-2013 (got a PhD FCT grant)
Paulo Velho	BI CERN-FP-123585-2011	100% from 01-06-2013 up to 31-01-2014
Ana Henriques	BI CERN-FP-123585-2011	100% from 01-06-2013 up to 31-01-2014

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 nine orders of magnitude lower concentrations of active probe elements 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 sites of radioactive probe nuclei and characterize their atomic interactions with the host, by probing the charge distribution and magnetic fields in their surroundings at the atomic scale.

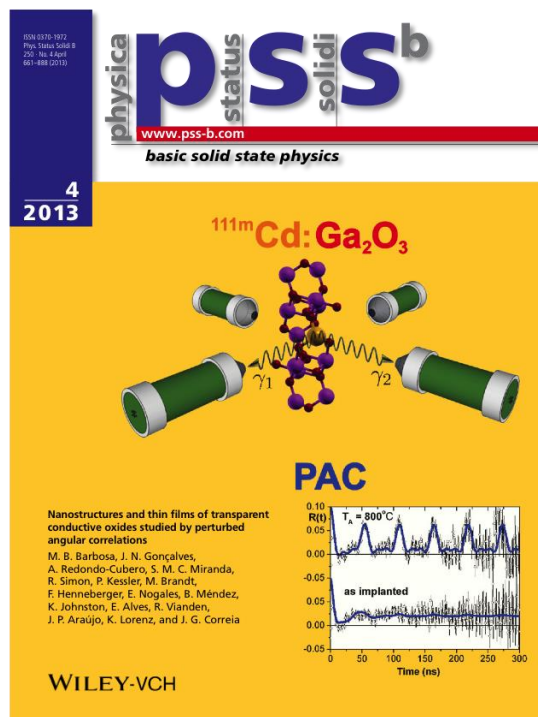
Approved scientific proposals:

- IS585 Interaction and Dynamics of add-atoms with 2-Dimensional Structures (PAC studies of mono- and low- number of stacking layers). Spokesperson: V. S. Amaral CICECO, Contact Person J. G. Correia CTN (JGC) (approved in 2013).
- IS580 Emission Channeling with Short-Lived Isotopes: lattice location of impurities in semiconductors and oxides. Spokesperson: L.M.C. Pereira IKS-Leuven, Contact Person JGC. (approved in 2013).
- 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.
- IS487 Study of local correlations in magnetic and multiferroic materials. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.

- IS481 The role of In in III-nitride ternary semiconductors. Spokesperson: K. Lorenz CTN, Contact person JGC.
- IS453 Emission channeling lattice location experiments with short-lived isotopes. Spokesperson: U. Wahl CTN, Contact Person (JGC).
- EDUCATION & TRAINING objectives are inherent to the execution of the scientific and R&D projects, since our working strategy is fully oriented at obtaining Diploma, MSc and PhD theses.
- R&D, MAINTENANCE and MISSION costs are fully supported by funding projects resources.

MAIN ACHIEVEMENTS

- IS453 – with the 2013 temporary shutdown of accelerators at CERN-ISOLDE, we have run experiments with the ^{59}Fe (45 d) long-lived isotope, performed data analysis of previous experiments and published finalised work. In order to investigate the involvement of Fe-B pairs on the identified lattice sites, ^{59}Fe emission channeling experiments were done in p^+ -Si, aiming to dissociate the pairs with laser light and later with temperature. In spite of published works observing the pair breakup under illumination, we could not observe significant changes in emission channeling, e.g. a reversible decrease in the fraction of interstitial Fe under light exposure or at elevated temperature. We notice that above 300°C annealing Fe changes from displaced substitutional positions to completely interstitial with a fraction at the bond centre (BC) site - with Fe sitting between two Si vacancies - and a fraction at the tetrahedral interstitial site. Only at 900°C Fe could be promoted to substitutional Si sites, irreversibly. Most likely the very high concentration of B acceptors [$6 \times 10^{19} \text{ cm}^{-3}$] hindered the observation of the pair breakup, with a recombination rate much higher than the breakup rate. The experiment shall be repeated with a significantly lower concentration of B centres. Other experiments were performed with ^{59}Fe implanted GaFeN(0.25%Fe) thin films with the aim of observing the formation of Fe(Ga) – V(N), vacancy complexes. However, this experiment was inconclusive, since a large fraction of the implanted ^{59}Fe segregated to low symmetry lattice sites, probably clustering with other Fe. This situation revealed to be different from what was observed for GaMnN where the formation of Mn(Ga)-V(N) complexes is confirmed. We also report the noticeable fact that in 2013 three young Portuguese scientists working at the IS453 EC-SLI experiment have won awards at international scientific conferences. First, Dr. Lino M.C. Pereira, was runner up in the “Young Researcher for Best Manuscript Competition” (sponsored by Elsevier BV) at the 21st International Conference on Ion Beam Analysis (IBA-21), which took place in Seattle, Washington, from 23.-28.6.2013. Following his PhD studies, which were a joint project between the former ITN (now CTN-IST), KULeuven and Universidade do Porto, he has recently won a post-doc scholarship at Instituut voor Kern- en Stralingsfysica (IKS) of KULeuven in Belgium. The topic of his contribution was “Emission channeling studies on a challenging case of impurity lattice location: “Cation versus anion substitution in transition-metal doped GaN and ZnO”. Then, Lígia Marina Amorim, a PhD student with a joint project between the former ITN (CTN-IST) and KULeuven, won the “Award for Best Student Oral Presentation” at the 17th International Conference on Radiation Effects in Insulators (REI-17), in Helsinki, Finland, 30.6.-5.7.2013. The topic of her contribution was “Lattice sites of implanted Mg in the group-III nitrides”. Last but not least, Daniel José da Silva a PhD student with a joint project between the former ITN (CTN-IST) and Universidade do Porto won the prestigious J.W. Corbett prize at the 27th International Conference on Defects in Semiconductors (ICDS-27), in Bologna, Italy, 21.-



IS481 - PAC data + DFT simulations show that implanted Cd (potential p-type dopant) in Ga_2O_3 sits only at the octahedral (Ga) site surrounded by 6 oxygen atoms. <http://dx.doi.org/10.1002/pssb.201200923>

26.7.2013. The prize is named in memory of James W. Corbett, one of the pioneers in the field of defects in semiconductors, who always helped and encouraged young researchers. The topic of his contribution was “Influence of the doping on the lattice sites of Fe in Si”.

- IS481 - Perturbed angular correlations (PAC) has been used to study Ga_2O_3 , which is a conductive oxide with transparency down to 260nm and is now emerging as promising material for high power electronics. Still, p-type doping could not yet be achieved. PAC with $^{111\text{m}}\text{Cd}/^{111}\text{Cd}$ ($t_{1/2}=48$ min) and $^{111}\text{In}/^{111}\text{Cd}$, using Cd - a possible acceptor candidate - as a probe, aims at studying the electronic properties around the Cd atom, in particular defects that may compensate p-type conductivity. Preliminary results obtained in 2012, have shown the successful incorporation of Cd at only the octahedral substitutional Ga-sites in all morphologic forms, single-crystal, pellets and the highly interesting nanowires. In 2013 this work was illustrated at the back-cover of *Physica Status Solidi b* 4. Still in 2013, in parallel with data analysis of the remaining data, off-line experiments using $^{111}\text{In}/^{111}\text{Cd}$ - where In was inserted by diffusion - were done on single crystals and pellets. Unexpectedly, electronic intrinsic defects were found at the SCs, which are inexistent at the Pellets that may be due to higher n-type carrier concentrations in the single crystals that compensate p-type conductivity. These studies will continue in 2014 at a higher range of temperatures and on nano-wire materials, as well as upon combining e- γ and γ - γ PAC on $^{111\text{m}}\text{Cd}/^{111}\text{Cd}$, looking forward to have a larger extension of measurements, materials and techniques to be able to fully characterize the defects and their origin.
- IS515 (cleaning waters using magnetic nanoparticles) No further experiments could be done but the data analysis has been finished showing that Hg can still bind to the SiO_2 external encapsulation of the nanoparticle without the dithiocarbamate (DTC) vector. Two sites / configurations have been identified where Hg has different coordination with oxygen atoms (linear / non-linear). On nanoparticles using the DTC vector the trapping efficiency is much greater suggesting that S-Hg-S linear bonds fully prevail over the O-Hg-O bonds. Simulations are on-going to detail the atomistic configurations. Stability studies should proceed in 2014.
- IS487 During 2013 we started studying magnetic systems with geometric frustration (e.g. frustrated networks as triangular, Kagomé, fcc or pyrochlore lattices). In a world where frustrated magnets seem to be the goal for materials where the control of electric properties by magnetic fields is possible, still exist a myriad of proposed (unknown) mechanisms to explain the origins of relaxor and multiferroic behaviour. In this context, in parallel with data analysis and publishing of previous experiments, during the CERN-ISOLDE radioactive beam shutdown we have used the PAC technique at CFNUL with the $^{111}\text{In}/^{111}\text{Cd}$ probe, in collaboration with the Garcia de Horta Hospital and CTN - to start studying CdCr_2S_4 , CdMn_2O_4 , ZnCr_2O_4 and CdCr_2O_4 . Our aim is to understand how these systems lift the frustration at the local - atomic scale - as a function of temperature, and achieve an ordered state. In particular we try to pinpoint how they show such a strong coupling between ferroelectric and ferromagnetic orders.

MAIN ACHIEVEMENTS

Successful mounting, tests and commissioning of two new fast VATAGP7 Si pad detectors (1 mm thick) – denominated as Pad_8 and Pad_9. One of the detectors, Pad_9, has no dead pixels in the central region, making it an ideal detector for EC-SLI experiments. Still the relatively high leakage current will require permanent cooling in vacuum around 2°C, what is easily done with water-cooling with the help of a chiller.

Successful redesign and manufacture of a new concept for the small heating element working at the high precision new Panmure goniometer in use at the EC-SLI setup. Integrated thermocouple (type K) elements of both T1 and T2 alloys will allow in the future to mount and dismount the sample holder without further cabling attachment. Due to the reduced dimensions, complicated design and hardness of the T1 and T2 materials this was a difficult and quite challenging task to accomplish.

Redesign of the holding, stand-up and manipulation frame of the heavy pad_1 (He) goniometer, which is required to fit in and work in the new laboratories, building 508, at ISOLDE.

RELEVANT PAPERS

- A. M. L. Lopes, J. G. Correia, V. S. Amaral and J. P. Araujo: “Local probe studies in the weakly Jahn-Teller distorted LaMnO₃.08 manganite”, Physica Status Solidi B -Basic Solid State Physics, 1-4 (2013). <http://dx.doi.org/10.1002/pssb.201350075> .
- L. M. C. Pereira, U. Wahl, J. G. Correia, M. J. Van Bael, K. Temst, A. Vantomme and J. P. Araujo: “Paramagnetism and antiferromagnetic interactions in single-phase Fe-implanted ZnO”, J. Phys.: Condens. Matter 25, 416001/1-15 (2013). <http://dx.doi.org/10.1088/0953-8984/25/41/416001> .
- A. M. L. Lopes, V. S. Amaral, J. G. Correia and J. P. Araujo: “Jahn–Teller distortion relaxation across the LaMnO₃+Δ phase diagram”, J. Phys.: Condens. Matter 25, 385602/1-7 (2013). <http://dx.doi.org/10.1088/0953-8984/25/38/385602> .
- L. M. C. Pereira, U. Wahl, J. G. Correia, L. M. Amorim, D. J. Silva, E. Bosne, S. Decoster, M. R. da Silva, K. Temst, and A. Vantomme: “Minority anion substitution by Ni in ZnO”, Applied Physics Letters 103, 091905/1-4 (2013). <http://dx.doi.org/10.1063/1.4820254> .
- D. J. Silva, U. Wahl, J. G. Correia, and J. P. Araújo, “Influence of n1 and p1 doping on the lattice sites of implanted Fe in Si”, Journal of Applied Physics 114, 103503/1-9 (2013). <http://dx.doi.org/10.1063/1.4819210> .
- M.A. Nagl, M.B. Barbosa, U. Vetter, J. G. Correia, H.C. Hofsäss: “A new tool for the search of nuclides with properties suitable for nuclear solid state physics based on the Evaluated Nuclear Structure Data Files“, Nuclear Instruments and Methods in Physics Research A 726, 17–30 (2013). <http://dx.doi.org/10.1016/j.nima.2013.05.045> .
- M. R. Silva, U. Wahl, J. G. Correia, L. M. Amorim, and L. M. C. Pereira: “A versatile apparatus for on-line emission channeling experiments”, Review of Scientific Instruments 84 073506/1-8 (2013). <http://dx.doi.org/10.1063/1.4813266> .
- M. B. Barbosa, J. N. Goncalves, A. Redondo-Cubero, S. M. C. Miranda, R. Simon, P. Kessler, M. Brandt, F. Henneberger, E. Nogales, B. Mendez, K. Johnston, E. Alves, R. Vianden, J. P. Araujo, K. Lorenz, and J. G. Correia: “Nanostructures and thin films of transparent conductive oxides studied by perturbed angular correlations”, Physica Status Solidi B-Basic Solid State Physics 250, 801-808 (2013), <http://dx.doi.org/10.1002/pssb.201200923>, open access: <http://cds.cern.ch/record/1641914>

FUNDS

Project/Service	Reference	Timeframe	2013
Perturbed Angular Correlations and Electron Channeling Experiments at ISOLDE - applied materials research with nuclear techniques, training and development.	CERN-FP-123585-2011 RD0187	01-06-2012 to 31-12-2014	61,648.65 €

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. It is our responsibility to organize the work, orienting the synergies and sharing the efforts among the different participants, in such way that there will be always an added value for students, with training and conclusion of thesis with their consequent academic degrees. Under Portuguese leadership there are today 6 INTC approved proposals (mentioned at “Objectives”): IS453, IS481, IS487, IS515, IS580 and IS585 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: C2TN/IST, 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, U of the Witwatersrand, Johannesburg
- Japan: CERC Tsukuba, U Tokyo
- South Korea: Sungkyunkwan University
- Russia: Kurchatov Institute Moscow
- Chile: U Talca, U de Chile, Santiago
- USA: IBM T.J. Watson research lab, Yorktown heights, New York
- Since 6 years we also collaborate with the MEDIPIX collaboration, which provides us with highly segmented position sensitive Si detectors, aimed for high-resolution EC experiments.

TEAM RESEARCHERS

NAME: João Guilherme Martins Correia

CATEGORY: Principal Researcher

IST/ID: 5451

ACTIVITIES

Nº	Activity Description	R&D
1	Project management	20%
2	SCIENTIFIC Work	20%
3	R&D Work	20%
4	Students and training	40%
Total		100%

WORK SUMMARY

Nº	Work Summary and Main Achievements
1	<p>1.1 Coordination of the work, report and funding management of project FCT-CERN-FP-123585-2011 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.</p> <p>1.2 Approved scientific proposals (IS) and Letter-of-intent (LOI)</p> <p>IS585 Interaction and Dynamics of add-atoms with 2-Dimensional Structures (PAC studies of mono- and low- number of stacking layers). Spokesperson: V. S. Amaral CICECO, Contact Person <u>J. G. Correia</u> CTN (JGC) (approved in 2013).</p> <p>IS580 Emission Channeling with Short-Lived Isotopes: lattice location of impurities in semiconductors and oxides. Spokesperson: L.M.C. Pereira IKS-Leuven, Contact Person JGC, (approved in 2013).</p> <p>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.</p> <p>IS487 Study of local correlations in magnetic and multiferroic materials. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.</p> <p>IS481 The role of In in III-nitride ternary semiconductors. Spokesperson: K. Lorenz</p>

	<p>CTN, Contact person JGC.IS487 Study of local correlations in magnetic and multiferroic materials. Spokesperson: V.S. Amaral CICECO, Contact person: JGC.</p> <p>IS453 Emission channeling lattice location experiments with short-lived isotopes. Spokesperson: U. Wahl CTN, Contact Person (JGC).</p>
2	<p>1.3 Scientific Main Results 2013</p> <p>Work presented as a résumé for each Scientific Proposal:</p> <p>IS453 - ^{59}Fe (44.5d) $\text{p}^+\text{-Si}$ experiments have been done looking forward to identify a reversible behaviour of interstitial Fe with laser light or temperature. Still, the breakup of Fe-B pairs could not be observed on these samples probably due to the very high p-dopant (B) concentration. For the GaFeN case the observation of Fe(Ga) – V(N) complex was hindered by the implanted Fe segregation due to low stability of the doped GaN film. In both cases new experiments are envisaged with new samples – with lower B concentration for Si and less Fe for the GaFeN thin films. Still this year three of our students got important conference prizes (detailed at the group “Main Achievements”) and several publications have been concluded.</p> <p>IS481 - Perturbed angular correlations (PAC) with $^{111}\text{In}/^{111}\text{Cd}$ ($T_{1/2} = 2.8\text{d}$) using Cd as a potential p-type dopant and a probe has been used to study single crystals and pellets of the transparent conductive oxide Ga_2O_3. Unexpectedly, electronic intrinsic defects were found at the SCs that are inexistent at the Pellets, which may be due to the higher n-type carrier concentrations in the single crystals that compensate to p-type conductivity. Previous results showing the unique occupation of implanted Cd at the octahedral Ga site were published and illustrated at the back-cover of Physica Status Solidi b 4 in 2013.</p> <p>IS515 (cleaning waters using magnetic nanoparticles) Two sites / configurations have been identified where Hg has different coordination with oxygen atoms (linear / non-linear) at the SiO_2 external encapsulation of the nanoparticle without the dithiocarbamate (DTC) vector. On nanoparticles using the DTC vector the trapping efficiency is much greater, further showing that S-Hg-S linear bonds fully prevail to the O-Hg-O bonds.</p> <p>IS487 During 2013 we start studying magnetic systems with geometric frustration (e.g. Frustrated networks as triangular, Kagomé, fcc or pyrochlore lattices). In this context, in parallel with data analysis and publishing of previous experiences, during the CERN-ISOLDE radioactive beam shutdown we have used the PAC technique at CFNUL with the $^{111}\text{In}/^{111}\text{Cd}$ probe, in collaboration with the Garcia de Horta Hospital and CTN - to start studying CdCr_2S_4, CdMn_2O_4, ZnCr_2O_4 and CdCr_2O_4. Our aim is to understand how these systems lift the frustration at the local - atomic scale - as a function of temperature, and achieve an ordered state. In particular we try to pinpoint how they show such a strong coupling between ferroelectric and ferromagnetic orders.</p>
3	<p>R&D Main Results</p> <p>Successful mounting, tests and commissioning of two new fast VATAGP7 Si pad detectors (1 mm thick) – denominated as Pad_8 and Pad_9. One of the detectors, Pad_9, has NO dead channels in the central region making it an ideal detector for EC experiments. Still the relatively high leakage current will require permanent cooling in vacuum around 2°C, what is easily done with a chiller.</p> <p>Successful redesign and manufacture of a new concept for the small heating element working at the high precision new Panmure goniometer in use at the EC-SLI setup. Integrated thermocouple (type K) elements of both T1 and T2 alloys will allow in the future to mount and dismount the sample holder without further cabling attachment. Due to the reduced dimensions, complicated design and hardness of the T1, T2 materials this was a difficult but quite challenging task to accomplish.</p> <p>Redesign of the holding, stand-up and manipulation frame of the heavy pad_1 (He) goniometer, which is required to fit in and work in the new laboratories, building 508, at ISOLDE.</p>

4	<p>Students and training</p> <p>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.</p> <p>In 2013, directed related to our projects and proposals, we had 6 PhD students (4 FCT-grant, 1 IKS-Leuven, 1 project funded) and 2 MSc students (project funded), one undergraduate (IST) student, project funded, and one IKS-Leuven summer student at ISOLDE, which are working with us.</p>
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PAPERS

- A. M. L. Lopes, J. G. Correia, V. S. Amaral and J. P. Araujo: “Local probe studies in the weakly Jahn-Teller distorted LaMnO₃.08 manganite”, *Physica Status Solidi B*, 1-4 (2013). <http://dx.doi.org/10.1002/pssb.201350075> .
- L. M. C. Pereira, U. Wahl, J. G. Correia, M. J. Van Bael, K. Temst, A. Vantomme and J. P. Araujo: “Paramagnetism and antiferromagnetic interactions in single-phase Fe-implanted ZnO”, *J. Phys.: Condens. Matter* 25, 416001 (2013). <http://dx.doi.org/10.1088/0953-8984/25/41/416001> .
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- M. B. Barbosa, J. N. Goncalves, A. Redondo-Cubero, S. M. C. Miranda, R. Simon, P. Kessler, M. Brandt, F. Henneberger, E. Nogales, B. Mendez, K. Johnston, E. Alves, R. Vianden, J. P. Araujo, K. Lorenz, and J. G. Correia: “Nanostructures and thin films of transparent conductive oxides studied by perturbed angular correlations”, *Physica Status Solidi B-Basic Solid State Physics* Volume: 250 Issue: 4 Pages: 801-808 Published: APR 2013, <http://dx.doi.org/10.1002/pssb.201200923>, open access: <http://cds.cern.ch/record/1641914>

COMMUNICATIONS

Invited Talks

- *Radioactive isotopes ion beams and applications*, J. G. Correia, *IP SCHOOL, Physics and materials science of nanostructures probed by nuclear methods and intense particle beams, KU Leuven, Belgium, 22 April 2013.*
- *Applied Physics with Accelerators at ISOLDE*, J. G. Correia, *CERN Lectures Public Divuligation Series for Portuguese teachers, 03 September 2013.*

Talks

- “Lattice location and thermal stability of the implanted transition metals Fe, Co and Ni in silicon by Emission Channeling”, D.J. Silva (Talk), U. Wahl, J. G. Correia, L.M.C. Pereira, L. Amorim, M. Ribeiro da Silva, J.P. Araújo, *Gettering and Defect Engineering in Semiconductor Technology 2013, Oxford UK, 22nd to 27th September 2013.*
- “Emission Channeling with Short-Lived Isotopes (EC-SLI) at CERN’s ISOLDE facility”, U. Wahl (Inv.Talk), A. Costa, J. G. Correia, L.M.C. Pereira, L.M. Amorim, V. Augustyns, K. Temst, A. Vantomme, M.R. da Silva, D.J. Silva, J.P. Araújo, E. Bosne, P. Miranda, K. Bharuth-Ram, *The first International African Symposium on Exotic Nuclei (IASEN-2013) Cape Town, South Africa, 2-6 December, 2013.*
- “Emission channeling studies on transition-metal doped GaN and ZnO: cation versus anion substitution”, L. M. C. Pereira (Talk), S. Decoster, L. M. Amorim, K. Temst, A. Vantomme, U. Wahl, M. R. da Silva, J.G. Correia, D.J. Silva, J.P. Araújo, *21st International Conference on Ion Beam Analysis (IBA – 2013), Seattle, Washington, USA 23-28 June 2013.*
- “Lattice sites of implanted Mg in GaN and AlN”, L. Amorim (Talk), U. Wahl, J. G. Correia, L. M. Pereira, S. Decoster, D. Silva, K. Temst, A. Vantomme, *10th International Conference on Nitride Semiconductors, (ICNS 2013) Washington – DC Metropolitan Area, USA, August 25-30, 2013.*
- “Dynamic off-centering of Cr³⁺ ions and short-range magneto-electric clusters in CdCr₂S₄”, G.N.P. Oliveira (Talk), A.M. Pereira, J.S. Amaral, A.M. Santos, T.M. Mendonça, C.T. Sousa, Y. Ren, V.S. Amaral, J. G. Correia, J.P. Araújo, A.M.L. Lopes, *ISOLDE Workshop and Users meeting 2013, CERN, Geneva Switzerland, 25-27 November 2013.*
- “Lattice location and thermal stability of the implanted transition metals Fe, Ni and Co in silicon of different doping types”, D.J. Silva (Talk), U. Wahl, J. G. Correia, L.M.C. Pereira, L. Amorim, V. Augustyns, A. Costa, E. Bosne, M. R. Silva and J.P. Araújo *ISOLDE Workshop and Users meeting 2013, CERN, Geneva Switzerland, 25-27 November 2013.*
- “Local Probing of multiferroics”, J. N. Gonçalves (Talk), V. S. Amaral, J. G. Correia, A. Stroppa, A. S. Fenta, A. Baghizadeh, S. Picozzi, *Joint European Magnetic Symposia 2013, Rhodes, Greece, 25-30 August 2013.*
- “Ab-initio Modelling of Multiferroic Materials”, J. N. Gonçalves (Talk), V. S. Amaral, J. G. Correia, A. S. Fenta, A. Baghizadeh, A. Stroppa, S. Picozzi, *Jornadas CICECO-Aveiro-Portugal, April 2013.*
- “Position Sensitive Detectors for RBS/Channeling Experiments”, P.A. Mirandav (Talk), U. Wahl, J. G. Correia, N. Catarino, E. Bosne, M.R. da Silva, and E. Alves, *Latin American Symposium on Nuclear Physics and Applications-Montevideo-Uruguay, December-2013.*
- “Cation Versus Anion Substitution in Transition-Metal Doped ZnO”, L.M.C. Pereira (Talk), U. Wahl, J. G. Correia, L. Amorim, D.J. Silva, J.P. Araujo, K. Temst, A. Vantomme, *Materials Research Society 2013, (MRS FALL 2013) Fall Meeting & Exhibit, Boston, Massachusetts, USA, December 1-6, 2013.*
- “Lattice sites of implanted Mg in GaN and AlN”, Lúcia Amorim (Talk), U. Wahl, J. G. Correia, L. M. Pereira, S. Decoster, D. Silva, K. Temst, A. Vantomme, *THE 17th International conference on radiation effects in insulators (REI-2013), Helsinki, Finland, June 30- July 5 2013.*

Posters

- “Lattice location of implanted ⁵⁹Fe in 3C-SiC”, A. Costa (Poster), U. Wahl, J. G. Correia, L. Amorim, L.M. Pereira, M.R. da Silva, D.J. Silva., K. Bharuth-Ram, *ISOLDE Workshop and Users meeting 2013, CERN, Geneva Switzerland, 25-27 November 2013.*
- “Can we dope the wide gap Ga₂O₃ semiconductor? – ion implantation and hyperfine interactions studies”, M.B. Barbosa (Poster), K. Lorenz, J. G. Correia, J. P. Araújo, *ISOLDE Workshop and Users meeting 2013, CERN, Geneva Switzerland, 25-27 November 2013.*
- “Electric field gradient and magnetic hyperfine field calculations and measurements in multifunctional materials”, J. N. Gonçalves (Poster), V. S. Amaral, J. G. Correia, A. S. Fenta, A. Baghizadeh, A. Stroppa, S. Picozzi, *Trends, challenges and emergent new phenomena in multifunctional materials (MAMA-TREND 2013), Sorrento (NA), Italy, May 20-23, 2013.*

- “*Hyperfine Techniques Studies of Graphene Layers Using isolated add-atom probes*”, A.S. Fenta (Poster), J. N. Gonçalves, A. Gottberg, K. Johnston, M. Stachura, C. Vyas, M. Correia, Y. Kadi, T. Trindade, C. Lopes, V. S. Amaral, J. G. Correia, *Jornadas CICECO-Aveiro-Portugal, April 2013*.
- “*Study of the local environment of implanted Cd in Ga₂O₃ nanowires, single- and polycrystals*”, M. B. Barbosa (Poster), E. G. Vllora, E. Nogales, B. Méndez, J. P. Araújo, K. Lorenz, J. G. Correia, *European Materials Research Society SPRING MEETING (E-MRS Spring 2013), Strasbourg, France, May 27-31 2013*.
- “*Lattice sites of implanted Mg in GaN and AlN*”, L.M. Amorim (Poster), U. Wahl, S. Decoster, L.M.C. Pereira, J. G. Correia, D.J. Silva, K. Temst and A. Vantomme, *European Materials Research Society SPRING MEETING (E-MRS Spring 2013), Strasbourg, France, May 27-31 2013*.
- “*Emission channeling studies on Mn-doped GaAs: High thermal stability of interstitial Mn in the low Mn-doping regime*”, L. M. C. Pereira (Poster), U. Wahl, J. G. Correia, L. M. Amorim, D. J. Silva, S. Decoster, M. R. da Silva, J. P. Araújo, K. Temst, and A. Vantomme, *21st International Conference on Ion Beam Analysis (IBA – 2013), Seattle, Washington, USA, 23-28 June 2013*.
- “*Influence of the doping on the lattice sites of Fe in Si*”, D. J. Silva (Poster), U. Wahl, J. G. Correia, J. P. Araújo, *27th International Conference on Defects in Semiconductors 2013, (ICDS 2013) Bologna, Italy, 21 to 26 July 2013*.
- “*Emission channeling lattice location of implanted Na in ZnO*”, U. Wahl (Poster), L.M.C. Pereira, L. Amorim, S. Decoster, M.R. da Silva, and J. G. Correia, *27th International Conference on Defects in Semiconductors 2013, (ICDS 2013) Bologna, Italy, 21 to 26 July 2013*.
- “*Mn-implanted GaAs: interstitial vs substitutional sites*”, L.M.C. Pereira (Poster), U. Wahl, J. G. Correia, L.M. Amorim, D.J. Silva, S. Decoster, M. R. da Silva, J. P. Araújo, K. Temst, A. Vantomme, *27th International Conference on Defects in Semiconductors 2013, (ICDS 2013) Bologna, Italy, 21 to 26 July 2013*.

EDUCATION

- *Eric David Bosne*, “Sistema de deteção Timepix e FitPix na análise de materiais em RBS/C” (Advisor CTN/IST-UL: U. Wahl; Co-advisor CTN/IST-UL: J.G.M. Correia; PhD IST-UL since 22-09-2013) - scholarship FCT - SFRH/BD/95865/2013.
- *Carlos de Oliveira Amorim*, “Multiscale studies of magnetic and electric effects in confined multiferroic materials” (Advisor DF-UA: V. Amaral; Co-advisor CTN/IST-UL: JGMCorreia; PhD UA since 22-09-2013) - scholarship FCT - SFRH/BD/93336/2013.
- *Marcelo Baptista Barbosa*, “Atomistic view of the functionalization of wide gap semiconductor nanowires – defects recombination rates and excited states”, (Advisor DF-UP: J.P.E. Araújo; Co-advisor CTN/IST-UL: J.G.M. Correia; PhD UP since 22-09-2013) - scholarship FCT - SFRH/BD/97591/2013.
- *Ângelo Rafael Granadeiro Costa*, “Ion implantation doping of SiC” (Advisor CTN/IST-UL: U. Wahl; Co-advisor CTN/IST-UL: J.G.M. Correia; PhD IST-UL since since 02-07-2012) - scholarship FCT - SFRH/BD/86386/2012.
- *Abel Eduardo Silva Fenta*, “Hyperfine Techniques Studies of surfaces and interfaces using isolated ad-atom radioactive probes”, (Advisor DF-UA: V. Amaral; Co-advisor CTN/IST-UL: JGMCorreia; PhD UA) since 02-07-2012) - scholarship FCT - SFRH/BD/84743/2012.
- *João Nuno Santos Gonçalves*, “Study of hyperfine properties of multiferroic materials and low dimensional structures (graphene and other carbon layered and nanostructured materials)” (Advisor DF-UA: V. Amaral; Co-advisor CTN/IST-UL: JGMCorreia; pos-DOC UA since 27-06-2011) - scholarship FCT - SFRH/BPD/82059/2011.

PROJECTS

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

SCIENTIFIC COMMITTEES

- J.G. Correia, member of the Hyperfine Interactions (HI) and Nuclear Quadrupole Interactions (NQI) International Advisory Committee.

NAME: Ulrich Wahl

CATEGORY: Principal Researcher (Habilitation)

IST/ID: 5480

N°	Activity Description	R&D (%)
1	Project participation: Perturbed Angular Correlations and Electron Channeling Experiments at ISOLDE - applied materials research with nuclear techniques, training and development, FCT-CERN-FP-123585-2011	40
2	Supervision of students	55
3	Project participation: SPIRIT (Support of Public and Industrial Research Using Ion Beam Technology) FP7 contract Nr. 227012)	5
Total		100

ACTIVITIES

N°	Work Summary and Main Achievements
1	<p>An integral part of the above-mentioned FCT project 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 CERN experiment IS453 “Emission channeling lattice location experiments with short-lived isotopes”, 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. The experimental work was in 2013 restricted by the fact that ISOLDE was, along with all other accelerators at CERN, in temporary shutdown, which in case of ISOLDE is also being used for a major upgrade of the facility. Consequently no beam times took place. However, a number of experiments were performed with p^+-Si and GaFeN samples containing the long-lived isotope ^{59}Fe ($t_{1/2}=45$ d), which still had been produced before the shutdown in Dec. 2012.</p> <p>In addition, the activities on experimental modelling and data analysis were intensified. As an example, work was started on simulating electron emission channeling patterns from GaN with an angular step width of 0.025° and up to an electron energy of 10 MeV, which is required for analysing future experiments with high-resolution pixel detectors.</p>
2	<p>In 2013 I have been supervisor or co-supervisor of the following theses:</p> <p>Lígia Amorim: PhD Thesis on “Lattice site location of electrical dopant impurities in group III-nitrides”, Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, Belgium, since Jan 2010.</p> <p>Daniel Silva, PhD thesis on “Lattice location of transition metals in Si by means of high-resolution emission channeling”, Faculdade de Ciências da Universidade do Porto, since Jan. 2011.</p> <p>Ângelo Costa: PhD thesis on “Ion implantation doping of SiC”, Instituto Superior Técnico, Universidade de Lisboa, since Nov 2012.</p> <p>All theses mentioned above make use of the emission channeling technique for lattice location of implanted radioactive probes, using the ISOLDE facility at CERN.</p> <p>Eric Bosne: Masters thesis on “Timepix and FitPix detection system for RBS/C materials analysis”, Faculdade de Ciências da Universidade de Aveiro, Sept 2012-Dec 2013.</p> <p>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.</p>
3	ITN’s task within the SPIRIT project of exploring the application of position-sensitive

<p>detectors for Rutherford Backscattering/Channeling (RBS/C) experiments was brought to its successful conclusion in 2013 by a series of experiments with the TimePix detector (a pixel detector developed by the CERN-Medipix collaboration, consisting of a $1.5 \times 1.5 \text{ cm}^2$ Si wafer, with 256×256 pixels, pixel size $55 \text{ }\mu\text{m}$) at the Van De Graaff accelerator of IST/ITN. The experiments measured the RBS/C effects along different crystallographic directions of a number of AlInN thin films deposited on GaN buffer layers on sapphire. From the offset of the channeling effect of 4He backscattered from In atoms in the thin film and Ga atoms in the buffer layer, the strain state of the thin AlInN films could be characterized.</p>
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PUBLICATIONS

- L.M.C. Pereira, J.P. Araújo, U. Wahl, S. Decoster, M.J. Van Bael, K. Temst, A. Vantomme, Searching for room temperature ferromagnetism in transition metal implanted ZnO and GaN, *Journal of Applied Physics* 113, 023903/1-10 (2013), doi: 10.1063/1.4774102.
- M.R. Silva, U. Wahl, J.G. Correia, L.M. Amorim, L.M.C Pereira, A versatile apparatus for on-line emission channeling experiments, *Review of Scientific Instruments* 84, 073506/1-8 (2013), doi: 10.1063/1.4813266.
- R.P. Borges, B. Ribeiro, M.M. Cruz, M. Godinho, U. Wahl, R.C. da Silva, C. Magén, Nanoparticles of Ni in ZnO single crystal matrix, *European Physical Journal B* 86, 254/1-7 (2013), doi: 10.1140/epjb/e2013-40008-5.
- L.M.C. Pereira, U. Wahl, J. G. Correia, L.M. Amorim, D.J. Silva, E. Bosne, S. Decoster, M.R. da Silva, K. Temst, A. Vantomme, Minority anion substitution by Ni in ZnO, *Applied Physics Letters* 103, 091905/1-4 (2013), doi: 10.1063/1.4820254.
- D.J. Silva, U. Wahl, J.G. Correia, J.P. Araújo: Influence of n^+ and p^+ doping on the lattice sites of Fe in Si, *Journal of Applied Physics* 114, 103503/1-9 (2013), doi: 10.1063/1.4819210.
- L.M.C. Pereira, U. Wahl, J.G. Correia, M.J. Van Bael, S. Decoster, K. Temst, A. Vantomme, J.P. Araújo, Paramagnetism and antiferromagnetic interactions in phase-pure Fe-implanted ZnO, *Journal of Physics: Condensed Matter* 25, 416001/1-15 (2013), doi: 10.1088/0953-8984/25/41/416001.
- B. De Vries, U. Wahl, S. Ruffenach, O. Briot, A. Vantomme, Influence of crystal mosaicity on axial channeling effects and lattice site determination of impurities, *Applied Physics Letters* 103, 172108/1-4 (2013), doi: 10.1063/1.4826705.
- L.M. Amorim, U. Wahl, L.M.C. Pereira, S. Decoster, D.J. Silva, M.R. da Silva, A. Gottberg, J.G. Correia, K. Temst, A. Vantomme, Precise lattice location of substitutional and interstitial Mg in AlN, *Applied Physics Letters* 103, 262102/1-5 (2013), doi: 10.1063/1.4858389.

COMMUNICATIONS

Invited Talks

- *Emission Channeling with Short-Lived Isotopes (EC-SLI) at CERN's ISOLDE facility*, U. Wahl, A. Costa, J.G. Correia, L.M.C. Pereira, L.M. Amorim, V. Augustyns, K. Temst, A. Vantomme, M.R. da Silva, D.J. Silva, J.P. Araújo, E. Bosne, P. Miranda, K. Bharuth-Ram, *The first International African Symposium on Exotic Nuclei (IASEN 2013)*, iThemba LABS, Cape Town, South Africa, Dec 1-6 (2013), invited talk presented by U. Wahl.
- *Emission channeling and blocking experiments using position-sensitive detectors*, U. Wahl, *The first International African Symposium on Exotic Nuclei (IASEN 2013)*, iThemba LABS, Cape Town, South Africa, Dec 1-6 (2013), invited tutorial talk presented by U. Wahl.
- *Solid state diffusion studied by means of radioactive isotopes*, U. Wahl, *The first International African Symposium on Exotic Nuclei (IASEN 2013)*, iThemba LABS, Cape Town, South Africa, Dec 1-6 (2013), invited tutorial talk presented by U. Wahl.

Oral Presentations

- *Emission channeling studies on a challenging case of impurity lattice location: cation versus anion substitution in transition-metal doped GaN and ZnO*, L.M.C. Pereira, U. Wahl, J.G. Correia,

- L.M. Amorim, D.J. Silva, S. Decoster, M.R. da Silva, J.P. Araújo, K. Temst, A. Vantomme, *21st International Conference on Ion Beam Analysis (IBA), Seattle, Washington, June 23-28 (2013)*, oral given by L.M.C. Pereira, **runner up in the “Young Researcher for Best Manuscript Competition” (sponsored by Elsevier BV)**.
- *Lattice sites of Mg in the group-III nitrides*, L.M. Amorim, U. Wahl, S. Decoster, L.M.C. Pereira, J.G. Correia, D.J. Silva, K. Temst, A. Vantomme, *17th International Conference on Radiation Effects in Insulators (REI), Helsinki, Finland, June 30-July 5 (2013)*, oral presented by L.M. Amorim, **honoured by the Best Student Oral Presentation Award**.
 - *Lattice location experiments of Mg in GaN and AlN: implanted Mg occupies the octahedral site*, L.M. Amorim, U. Wahl, S. Decoster, L.M.C. Pereira, J.G. Correia, D.J. Silva, K. Temst, A. Vantomme, *10th International Conference on Nitride Semiconductors (ICNS), Washington DC, Aug 25-30 (2013)*, oral presented by L.M. Amorim.
 - *Lattice location and thermal stability of the implanted transition metals Fe, Co and Ni in silicon by Emission Channeling*, D.J. Silva, U. Wahl, J.G. Correia, L.M.C. Pereira, L. Amorim, M. Ribeiro da Silva, J.P. Araújo, *Gettering and Defect Engineering in Semiconductor Technology (GADEST 2013), Oxford, United Kingdom, Sept 22-27 (2013)*, oral presented by D.J. Silva.
 - *Lattice location and thermal stability of the implanted transition metals Fe, Co and Ni in silicon of different doping types*, D.J. Silva, U. Wahl, J.G. Correia, L.M.C. Pereira, L.M. Amorim, V. Augustyns, A. Costa, E. Bosne, M.R. da Silva, J.P. Araújo, *2013 ISOLDE Workshop and Users Meeting, CERN, Geneva, Switzerland, Nov 25-27 (2013)*, oral presented by D.J. Silva.
 - *Position Sensitive Detectors for RBS/Channeling Experiments*, P.A. Miranda, U. Wahl, J.G. Correia, N. Catarino, E. Bosne, M.R. da Silva, E. Alves, *X Latin American Symposium on Nuclear Physics and Applications, Montevideo, Uruguay, Dec 1-6 (2013)*, oral presented by P.A. Miranda.

Poster Presentations

- *Lattice sites of implanted Mg in GaN and AlN*, L.M. Amorim, U. Wahl, S. Decoster, L.M.C. Pereira, J.G. Correia, D.J. Silva, K. Temst, A. Vantomme, *2013 Spring Meeting of the European Materials Research Society (E-MRS), Symposium L “Group III nitrides”, Strasbourg, France, May 27-31 (2013)*, poster presented by L.M. Amorim.
- *Emission channeling studies on Mn-doped GaAs: high thermal stability of interstitial Mn in the low Mn-doping regime*, L.M.C. Pereira, U. Wahl, J.G. Correia, L.M. Amorim, D.J. Silva, S. Decoster, M.R. da Silva, J.P. Araújo, K. Temst, A. Vantomme, *21st International Conference on Ion Beam Analysis (IBA), Seattle, Washington, June 23-28 (2013)*, poster presented by L.M.C. Pereira.
- *Influence of the doping on the lattice sites of Fe in Si*, D.J. Silva, U. Wahl, J.G. Correia, J.P. Araújo, *27th International Conference on Defects in Semiconductors (ICDS), Bologna, Italy, July 21-26 (2013)*, poster presented by D.J. Silva, **winner of the J.W. Corbett Prize for Best Young Scientist contribution**.
- *Emission channeling lattice location of implanted Na in ZnO*, U. Wahl, L.M.C. Pereira, L. Amorim, S. Decoster, J.G. Correia, *27th International Conference on Defects in Semiconductors (ICDS), Bologna, Italy, July 21-26 (2013)*, poster presented by U. Wahl.
- *Mn-implanted GaAs: interstitial vs substitutional sites*, L.M.C. Pereira, U. Wahl, J.G. Correia, L.M. Amorim, D.J. Silva, S. Decoster, M. R. da Silva, J. P. Araújo, K. Temst, A. Vantomme, *27th International Conference on Defects in Semiconductors (ICDS), Bologna, Italy, July 21-26 (2013)*, poster presented by U. Wahl.
- *Properties of Fe in ion-implanted ZnO monitored with ⁵⁷Fe Mössbauer spectroscopy*, K. Johnston, R. Mantovan, H. Masenda, T. E. Mølholt, L. Pereira, K. Bharuth-Ram, H. P. Gíslason, H. P. Gunnlaugsson, G. Langouche, D. Naidoo, S. Ólafsson, U. Wahl, G. Weyer, M. B. Madsen, *27th International Conference on Defects in Semiconductors (ICDS), Bologna, Italy, July 21-26 (2013)*, poster presented by K. Johnston.
- *Lattice location of implanted ⁵⁹Fe in 3C-SiC*, A. Costa, U. Wahl, J.G. Correia, L.M. Amorim, L.M.C. Pereira, M.R. da Silva, D.J. Silva, K. Bharuth-Ram, *2013 ISOLDE Workshop and Users Meeting, CERN, Geneva, Switzerland, Nov 25-27 (2013)*, poster presented by A. Costa.
- *Cation Versus Anion Substitution in Transition-Metal Doped ZnO*, L.M.C. Pereira, U. Wahl, J.G. Correia, L.M. Amorim, D.J. Silva, J.P. Araujo, K. Temst, A. Vantomme, *2013 Fall Meeting of the*

Materials Research Society (MRS), Symposium on "Oxide Semiconductors", Boston, Massachusetts, Dec 1-6 (2013), poster presented by A. Vantomme.

EDUCATION

- Sept 2012/Jan 2013: supervisor of Valérie Augustyns, ERASMUS student at IST from KU Leuven.
- Jury member, Master thesis defence of Eric David Bosne, "Timepix and FitPix detection system for RBS/C materials analysis", Faculdade de Ciências da Universidade de Aveiro, Portugal, Dec 13, 2013.

SCIENTIFIC COMMITTEES

- Since Jan. 2013: Member of the advisory committee and board of referees on the "Use of large scale facilities for condensed matter research" of the German Federal Ministry for Education and Research.
- May-Dec. 2013: Member of the International Advisory Committee for the 1st International African Symposium on Exotic Nuclei (IASEN-2013), 2.-6.12.2013 in Cape Town, South Africa.

COLLABORATIONS

- Mehluli Ncube, 25.5.-13.7.2013, PhD student, University of the Witwatersrand, Johannesburg, South Africa, received training in the data analysis of emission channeling experiments on ⁵⁷Mn in Si, jointly performed at ISOLDE/CERN.
- Daniel José Silva, 1.-4.7.2013, and 3.-14.6.2013, PhD student, Porto University, discussion of data analysis and common publications in the field of emission channeling lattice location of transition metals in silicon.