## Nuclear Instruments and Methods

## Introduction

The activity of the Group included (a) modelling and simulation of gamma, electron and neutron fields; (b) modelling and simulation of low temperature gas discharges; (c) development of nuclear methods, techniques and instrumentation for measurement and control; (d) technical assistance and supply of equipment and services.

The work in the field of modelling and simulation of gamma, electron and neutron fields, carried out using the MCNP code, was the following:

- Dose calculations in the Portuguese Gamma Irradiation Facility, in order to establish isodose distributions;
- Dose calculations in linear accelerators for radiotherapy applications;
- Dose calculations in brachytherapy applications;
- Feasibility studies of adapting the horizontal access of the RPI thermal column for a BNCT installation;
- Calculation of fast neutron and gamma radiation spectra inside a lead hollow cylinder from a planar source of fission neutrons and reactor gamma photons.
- Response of superconducting detectors (Sn and Re) to electron irradiation;

The work in modelling and simulation of low temperature gas discharges included:

- Study of the electron kinetics in Ar-Cu and Ne-Cu discharges, with applications to gas *lasers* and magnetron discharges;
- Re-engineering of a software code for solution of the stationary homogeneous Boltzmann equation for electrons.

The work in the design of instrumentation included:

- Small-Angle Neutron Scattering Instrument EPA
  - conclusion of the design of the EPA Sample Chamber (including the design of a sample positioning system);
  - participation in the design of the neutron detector's positioning system;
  - participation in the mechanical and electrical tests of the neutron velocity selector.
- Hot-Bird High-Resolution High-Temperature Double-Crystal X-ray Diffractometer, for *in-situ* studies on crystalline materials:
  - conclusion of the temperature controller and specialised power supply of the High Temperature Chamber;
  - a Data Acquisition Board (DAQ) was bought and software for the Diffractometer control was developed; also a PCB for interfacing the DAQ with the Diffractometer was designed and manufactured;
  - numerical optimization of the geometry of the spectrometer
  - participation in testing of the X-ray generator.
- Laboratory prototype of the new Gama Densimeter

Technical assistance and services in the field of electronics and information technologies were extended to different ITN Groups and to external users.

## Research Team

Researchers –	8	(8 PhD or equivalent)
Technicians –	2	

## **Publications**

Journals –	2	(and 5 in press)
Proceedings –	3	(and 1 in press)
Special publ		2 in press
Conf. Commun. –	15	

	10 <sup>3</sup> PTE
Expenditure:	8 516
Missions:	1 409
Other Expenses:	5 105
Hardware & Software:	151
Other Equipment:	1 851

Funding:		8 423
External Projects:	1997 1998	562 <sup>(1)</sup> 2 070
Others		5 791
<sup>(1)</sup> Funding not used in 1997		

## **Dose rate Determinations in the Portuguese Gamma Irradiation Facility: Monte Carlo Simulations and Measurements**

#### C. Oliveira, J. Salgado and A. Ferro de Carvalho

Nuclear and Technological Institute, Est. Nac. 10, 2685 Sacavém, Portugal

#### Abstract

A simulation study of the Portuguese Gamma Irradiation Facility, UTR, is being carried out using the MCNP code. The work focused on the optimisation of the dose distribution inside the irradiation cell, in order to obtain higher doses and a better homogeneity, dose calculations inside irradiated samples and dose calculations in critical points for protection purposes.

Calculations were carried out in points inside and outside the irradiation cell, where it was expected different behaviour (distance from the source, radiation absorption and scattering in irradiator structure and walls). The contributions from source, irradiator structure, sample material, carriers, walls, ceiling and floor for the photon spectra and doses in those points are reported and discussed.

Dose measurements were also carried out using an ionisation chamber. Good agreement was found between experimental and calculated doses.

Radiation Physics and Chemistry (submitted).

## Photoelectric Emission Induced by Resonance Radiation in Discharges with Azimuthal Symmetry

#### Nuno Rombert Pinhão

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#### Abstract

We present a computation of the photoelectric emission induced by the resonance radiation produced in gas discharges with azimuthal symmetry. These conditions apply to discharges between concentrically cylindrical electrodes and discharges between plane parallel electrodes. The photoelectric emission is computed with resource to a radiation escape matrix taking account of radiation transmission and geometrical factors. Both thin plasma conditions and radiation imprisonment for a full range of opacity values are considered. A constant line profile and complete redistribution of frequencies are assumed for radiation imprisonment. Radiation escape matrix are computed for Doppler and collisional broadening but can easily be generalised to a Voigt line profile. Finally, the results are applied to a case study.

Comunication to: *Fourteenth European Conference on the Atomic and Molecular Physics of Ionised Gases*, Malahide, Ireland, August 26-29, 1998. *J. Phys. D. Appl. Physics* (submitted).

## Design Optimisation of a High-temperature X-ray Diffractometer for in-situ Residual Stress Analysis and Lattice Mismatch Determination - The hot-bird

F. M. A. Margaça, N. R. Pinhão and A. D. Sequeira

Nuclear and Technological Institute, Physics Department, Est. Nac. 10, P-2685 Sacavém, Portugal

#### (see Condensed Matter Physics)

*EPDIC - 6, European Powder Diffraction International Conference,* Budapest, 22-25 August (1998) *Materials Science Forum* (submitted).

## Monte Carlo Calculation of Fast Neutron Spectra inside a Lead Hollow Cylinder

Isabel F. Gonçalves, Eduardo Martinho, José Salgado Nuclear and Technological Institute, Est. Nac. Nº10, 2685 SACAVÉM, Portugal

(see Nuclear Engineering - Modelling and simulation)

Kerntechnik (submitted).

**Preparation of a Beam Tube of the Portuguese Research Reactor to be Used in BNC and Other Activities** 

A.J. G. Ramalho<sup>1</sup>, I. F. Gonçalves<sup>1</sup>, I. C. Gonçalve<sup>1</sup>s, J. Salgado<sup>1</sup>, M. Castro<sup>2</sup> and A. F. P. Fernandes<sup>2</sup>

<sup>1</sup> Nuclear and Technological Institute, Est. Nac. 10, Apartado 21, 2686-953 Sacavém, Portugal <sup>2</sup>Centro de Estudos de Farmacologia Experimental e Clínica, Fac. de Medicina de Lisboa, Portugal,

(see RPI - Dosimetry)

8<sup>th</sup> Symposium on Neutron Capture Therapy for Cancer, La Jolla, Califórnia, 1998. Proc. "Frontiers in Neutron Capture Therapy", Publishing Corporation (submitted).

## **Current Status of Nucleonic Gauges in Portugal**

J. Salgado, F. G. Carvalho, J. Manteigas, C. Oliveira, I. F. Gonçalves, J. Neves and C. Cruz

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#### Abstract

The main users of NCS in Portugal are: cement, chemical, basic metal, paper, textile, wood industries, as well as civil engineering, mining and agriculture. These industries are interested in level monitoring, thickness and density measurements, moisture content monitoring and XRF

measurements. There is no local industrial firm producing nucleonic gauges. There are several commercial firms selling foreign equipment, but they do not provide local assistance concerning the radiation sources. There is no research in the Universities related with this matter, and nucleonic gauging technology has not been included in the curricula. The ITN is the unique Portuguese institution that has been working in this field and has developed some cooperation with industrial users. The Monte Carlo code is being used for design optimisation of nucleonic instrumentation, such as prompt gamma neutron activation analysis. The ITN provides assistance in maintenance, calibration and operation of the equipment and techniques. The main difficulties to overcome are, on one hand, the mistrust of potential clients of the local expertise and quality of our equipment and, on the other hand, the fear of using radiation in their process control.

Report of the ADVISORY GROUP MEETING on "Emerging new applications of nucleonic control systems (NCS) in industry", (Vienna, 5-8 May), to be published as an IAEA TECDOC.

### **Prompt Gamma Neutron Activation Analysis (PGNAA)**

#### C. Oliveira. J. Salgado and F. G. Carvalho

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#### Abstract

Prompt Gamma Neutron Activation Analysis (PGNAA) is a multi-elemental analytical technique based on the detection of  $\gamma$ -rays emitted by excited nuclei following neutron radioactive capture or neutron inelastic scattering. The accumulated count rate relative to the  $\gamma$ -ray energy characteristic of a certain isotope depends on its concentration. The measurements take place during sample irradiation. The technique can provide accurate information on the elemental composition of materials in a broad range of cases: raw materials, mineral exploration, contaminants, detection of forbidden products, such as drugs and explosives, inspection of containers and applications in health care. Among the main advantages of the PGNAA technique are: faster results; non-destructiveness; flexible sample requirements; bulk sample analysis; in situ application by direct on-line measurement; detectable unique signatures for most elements; improved accuracy for short-lived elements; low residual activity. On the other hand, the most significant limitations are: higher detection limits as compared with delayed gamma neutron activation analysis (DGNAA); longer irradiation times; single (one-cycle) sample irradiation; impracticability of enhancing a specific isotope contributions by radiochemical or physical (half-life) separation techniques; requirement of relatively larger samples.

*Encyclopaedia of Analytical Chemistry: Instrumentation and Applications, John Willey and Sons.* in publication as an invited paper.

## **Dose Determinations by Monte Carlo - a Useful Tool in Gamma Radiation Process**

#### C. Oliveira, J. Salgado, M. L. Botelho and L. M. Ferreira

Nuclear and Technological Institute, Est. Nac. 10, Apartado 21, 2686-953 Sacavém, Portugal

#### Abstract

Monte Carlo simulations can be used as a predictive tool of dose measurements thus reducing the amount of experimental work with dosimeters. However, some validation measurements must be performed.

The paper presents results on absorbed dose calculations carried out using the Monte Carlo N-Particle (MCNP) code in the Portuguese Gamma Irradiation Facility. The facility has a planar <sup>60</sup>Co source with an actual activity of 3 PBq. The irradiator consists of 30 stainless steel tubes containing 156 <sup>60</sup>Co sources, doubly encapsulated in welded stainless steel. The irradiation chamber has 28 irradiation positions; carriers suspended from an overhead monorail conveyor carry the products. Each carrier can be loaded with 4 boxes.

The model was applied to a dummy product and a natural product - Lyomer -, which will be in the future irradiated to sub-lethal doses. The computer running time is chosen in order that the statistical errors are always less than 5%.

Dose measurements using Amber and Ceric-Cerous dosimeters were also carried out in order to validate the calculations. The Amber Perspex dosimeter is a PMMA routine dosimeter with an uncertainty of 6% ( $\alpha$ =0.05) in the range of 1 to 30 kGy. The determination of the absorbed dose is made indirectly through spectrophotometric evaluation of the absorbance at  $\lambda$ =651 nm. The Ceric-Cerous dosimeter is a chemical liquid system classified as reference standard with an overall uncertainty of 3.5% ( $\alpha$ =0.05). The dose measurement is made according to Compu-Dose System from Nordion International Inc. (potentiometric method). A low range (1-10 kGy) batch of Ceric-Cerous dosimeters was used.

A good agreement between simulated and experimental data was obtained. This fact indicates that the model is appropriate for the particular application, namely: (a) the code has been used in a correct way (cross sections, variance reduction techniques, cut-offs); (b) source and geometry of the installation were well defined (all important components have been included with enough detail); and (c) dimension, composition and density of the product have been correctly established.

Comunication (accepted) to: 11<sup>th</sup> International Meeting on Radiation Processing, Melbourne, 1999.

# MC Simulation of a Linear Accelerator Treatment Head – EGS4 and MCNP-4B Intercomparison

M. Fragoso<sup>1</sup>, A. Chaves<sup>2</sup>, C. Alves<sup>2</sup>, C. Oliveira<sup>3</sup>, J. Seco<sup>1,\*</sup>, L. Peralta<sup>1</sup>, M. C. Lopes<sup>2</sup> <sup>1</sup>Lab. de Intrum. & Física Experimental de Partículas, Lisboa, Portugal <sup>2</sup>Centro Regional de Oncologia de Coimbra – IPOFG, Portugal <sup>3</sup> Nuclear and Technological Institute, Est. Nac. 10, Apartado 21, 2686-953 Sacavém, Portugal \*Presently at the Institute of Cancer Research, Sutton, UK

**Introduction:** The codes EGS4 and MCNP-4B are used to simulate the treatment head of a Siemens Mevatron linear accelerator from the *Centro Regional de Oncologia de Coimbra*. In this work, the 6 MV energy spectra simulated by both codes are compared. These spectra are then used to simulate the PDD curves and are compared with the experimental data from Coimbra. The 4B version of the MCNP code has an improved electron transport treatment which allowed it to join the list of MC codes applied to Radiation Therapy, where EGS4 is already well benchmarked.

**Methods:** The detailed study of the 6 MV energy spectra is presented, following the beam direction from the target to a water phantom surface, through the primary collimator, flattening filter and jaws. Energy cut-offs criteria and several variance reduction techniques are used during both codes optimisation.

**Results:** The simulated beams have been used to calculate depth dose curves in water at SSD=100 cm. The results have been compared with experimental data obtained in a MP3-PTW water phantom with an ionisation chamber of 0.125 cc (PTW type 233642).

**Conclusions:** Both codes describe well the experimental data and the general agreement is better than 3%.

5<sup>th</sup> Biennial Meeting on Physics in Clinical Radiotherapy, Göttingen, 6-10 April (1999) (submitted).

A Monte Carlo Study of a Linear Accelerator Head. Optimization of the Running Time to Obtain the Phase Space Source

A. Chaves<sup>1</sup>, C. Oliveira<sup>2</sup>, M. C. Lopes<sup>1</sup> and J. Salgado<sup>2</sup>

1-Centro Regional de Oncologia do IPOFG, Coimbra, PORTUGAL 2- Nuclear and Technological Institute, Est. Nac. 10, Apartado 21, 2686-953 Sacavém, Portugal

**Introduction:** The MCNP is a general Monte Carlo code (from Los Alamos National Laboratory) which simulates the transport and interactions of neutrons, photons and electrons. In the latest version (4B) the electron treatment has been improved enabling to extent its field of application to medical physics, namely to the dosimetry calculation. The code, running on a Pentium PC and on a Unix workstation, was used to simulate the linear accelerator head of a Siemens Mevatron in 6MV photon mode. This work is the first part of a study in order to obtain the DDC (Depth Dose Curve) in water, 100 cm source surface distance. The goal of this work is to efficiently obtain the phase space source (PSS) just upstream the jaws.

**Methods:** In order to decrease the running time, different energy cut-offs were studied. Initially, the photon fluence is calculated with the cut-offs adjusted for the currently used values of 10 keV and 50 keV for photons and electrons respectively. However, taking into account the electron cross sections and the electron fluence in the different system components, the electron cut-offs were increased to 700 and 500 keV in the target and in the remaining components respectively. Other simplifications were also tested (modifications in the primary collimator, photon energy cut off, and elimination of secondary electrons

**Results:** The statistical analysis of the photon fluence proves that the higher values for electron energy cut-off are valid, enabling a substantial increase of the number of particles transported for a given error (a factor of 3.2). On the other hand, when geometrical cuts in collimator are considered, the photon fluences are significantly different from those without such cuts.

**Conclusion:** The results, discussed in this work, show that the use of appropriate energy cutoff can improve the efficiency of Monte Carlo calculation building the phase space source to be used in subsequent runs.

5<sup>th</sup> Biennial Meeting on Physics in Clinical Radiotherapy, Göttingen, 6-10 April (1999) (submitted).

## Measurements Validation of the Dose Distribution of Ir-192 Wires in Acrylic and Water Phantom Simulated with MCNP and Plato

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<sup>(1)</sup> - Escola Superior de Tecnologia da Saúde - Lisbon, Portugal

<sup>(2)</sup>- Instituto Português de Oncologia - Lisbon, Portugal

<sup>(3)</sup>- Instituto Tecnológico e Nuclear - Sacavém, Portugal

#### Abstract

A comparative study has been carried out between absorbed dose values, obtained by two simulation methods: MCNP, a Monte Carlo simulation code and the Plato, the computerised treatment planning system, used in interstitial brachytherapy; for the measurements "in vitro", are used TLD dosimeters. This study is part of a global work that evaluates the viability of the use of continuous sources of iridium (with manual insertion), face to the point iridium source of the PDR system. This work will involve, also, the analysis of the dose behaviour, in a heterogeneity medium. The MCNP code, version 4B, simulates the emission and the transport of photons and electrons (and neutrons) in any tridimensional geometry, doing a dose calculation in a homogeneous, as well as in a heterogeneous medium, with a similar accurate and precision. The Plato, is a software that is developed based on semi-empirical algorithms, like the Meisberger and Van-Kleffens, that calculates a dose distribution, around a radioactive source, in a homogeneous medium, the water.

An acrylic phantom obtained with the superposition of several acrylic plates is used for the "in vitro" measurements, with interior channels for the insertion of the sources and the TLDs rods  $(6x0.9 \text{ mm}^2)$ . The linear activity of the sources is normalised to 0.1 mCi/mm. Plans with 2 to 8 Ir wires of 6 cm were simulated. The separation between wires was from 6 to 20 mm. Based on these different arrangements of the sources dose distributions were obtained. The dose calculations using the Plato and MCNP code in water show a good agreement. The validation of those results is made by TLD measurements.

Annual Brachytherapy Meeting GEC - ESTRO, Utrech-Zeist, 11-12 May (1999) (submitted).

## Current Work

# Technical Assistance in the Field of Engineering Applications of Radiations and Radioisotopes

#### J.B.Manteigas, F.G. Carvalho, J. Salgado

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Assistance to industrial companies in the field of Engineering Applications of Radiations and Radioisotopes is linked to the development of prototypes and equipment fabrication for specific applications. Assistance takes mainly the forms of specialised consultant engineer advice; installation of nuclear gauges, including calibration; maintenance and repair; supply of locally produced radioisotope sources (Pt-Ir) and recharging of gauges with imported sources. A summary of the more relevant services rendered in 1998 is presented below in the Table.

Activity	Number	Client	
Supply of laboratory equipment for the determination			
of radioactive element traces by electrodeposition	2	JRC/Ispra	
Disposable cell bodies with lid in PVC	150	JNC/Ispia	
Constant current power supply, DC	2		
Supply of laboratory equipment for the determination		ID C /	
of radioactive element traces by electrodeposition	2	JRC/Ispra	
Disposable cell bodies with lid in PVC	500		
Supply of laboratory equipment for the determination		Modern Technologies Corp.	
of radioactive element traces by electrodeposition	1	(USA)	
Supply of laboratory equipment for the determination		Environmental Physics, Inc.	
of radioactive element traces by electrodeposition	1	(USA)	
Supply of electrode plating disks	500	DGA	
Supply of teflon cells	5	DGA	
Supply of gamma level detector units	2	Cimpor/Souselas	
Source recharging	2	SOPORCEL	
Supply of gamma level indicators DNG2	6	CMP – Maceira e Pataias, SA	
Supply of <sup>192</sup> Ir gamma sources	21	Siderurgia Nacional, SA	
	3	Aeroporto de Tires	
Supply of Personal Dosimeters RAD X 100	4	SATIS, Lda	
	1	Ortognática	
Technical Assistance	-	Instituto Geológico e Mineiro,	
		Instituto Superior de Agronomia,	
		Solvay Portugal, CAIMA	

# Dose Distributions in the Portuguese Gamma Irradiation Facility Calculated Using the MCNP Code

#### Carlos Oliveira and José Salgado

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A systematic study of the dose distribution in the Portuguese Gamma Irradiation Facility (Cavaco 1991) is being carried out using the MCNP code in order to establish isodose curves in the sample carriers. Each carrier can be loaded with 4 cardboard boxes  $(0.4 \times 0.4 \times 0.4 \text{ m}^3)$ . Each box was divided in eight equal cubes.

Absorbed dose rate, gamma flux per energy interval and average gamma energy were calculated inside the eight cubes. For comparison purposes, boxes filled with air and "dummy" boxes loaded with layers of folded and crumpled newspapers to reach the desired density were used. The dose uniformity (the ratio of maximum to minimum dose rates absorbed in each box) was also calculated. The contributions from source, irradiator structures, samples material and other origins (ceiling, floor and walls) for the total photon spectra are also calculated. The Figure shows the average dose rate and dose uniformity in both carrier rows.

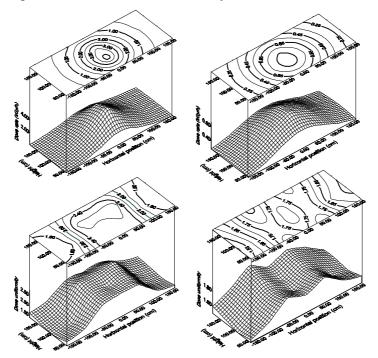


Fig. - Dose rates and dose uniformity in the internal carrier row, facing the source plane (left) and in the external row (right).

The dose distribution is symmetrical in parallel lines to the source plane and is slightly shifted toward the lower region as experimental results (Cavaco 1991) have already shown.

M.C. Cavaco *et al.*, "Dosimetry commissioning for an Industrial Cobalt-60 Gamma-radiation Facility", *Appl. Radiat. Isot.* **42** (12) (1991) 1185-1188.

## Monte Carlo Calculation of Gamma Radiation Spectra Inside a Lead Hollow Cylinder

Isabel F. Gonçalves, Eduardo Martinho, José Salgado Nuclear and Technological Institute, Est. Nac. N°10, 2685 SACAVÉM, Portugal

(see - Nuclear Engineering - Modelling and Simulation)

## Upgrading of the Automatic Control of the Cooling, Ventilation and Alarm Systems of the UTR Facility

#### C. Cruz, J.E. Oliveira\*

Nuclear and Technological Institute, Est. Nac. 10, Apartado 21, 2686-953 Sacavém, Portugal \* EDP Sul, Évora

This work involved, in a first phase, the identification of the electrical and sensors networks of the UTR facility, in order to make possible to choose and install a Programmable Logic Controller, PLC for the automatic control of the cooling, ventilation and alarm systems. The second phase is the design of a logic program for the PLC. In the third phase the PLC system will be connected, through the "campus" network, to a PC for remote monitoring of the PLC status.

## Simulation of Implantation Profiles by Plasma Immersion Ion Implantation in Pieces with Complex Shapes

#### Nuno Pinhão and Rui M. C. Silva

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Ion implantation is an effective technique for surface modification of materials, improving wear, corrosion, fatigue and friction properties. Over the last decade a new implantation technique has been under development, in the USA and, independently, in Australia - the *Plasma Immersion Ion Implantation, PIII*. More recently the importance of this new technology was recognised in Europe, especially in Germany, where the first experimental system was established five years ago. In *PIII*, the target is placed directly in the plasma source and is pulse biased to a high negative potential relative to the chamber walls. A plasma sheath is formed around the target and sheath ions are accelerated to the target. However, in order to explore the full potentialities of this technique, a number of scientific and technological problems remain to be solved.

Among those problems is the dose uniformity in pieces with complex shapes. In this work the implantation profiles for different distributions in energy, angle and composition, of the ion at the surface will be simulated with a standard program – TRIM.

## Numerical Simulation of a Hollow-Cathode Magnetron Discharge

Nuno R. Pinhão<sup>1</sup>, Mário J. G. Pinheiro<sup>2</sup>, Manuel J. P. Maneira<sup>3</sup>, Manuel Ribau Teixeira<sup>3</sup>, Idalino J. A. Franco<sup>3</sup>

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<sup>2</sup> Instituto Superior Técnico, Centro de Electrodinâmica, Av. Rovisco Pais, 1, Lisboa

<sup>3</sup> FCT / Universidade Nova de Lisboa, Quinta da Torre, Monte da Caparica

A self-consistent hybrid Monte Carlo-fluid model will be developed and applied to a hollow cathode magnetron. Fast particles (electrons, energetic ions and sputtered particles) and the cathode fall will be described by a test particle Monte Carlo method tracing the history of a specific number of particles in 3D. Slow electrons magnetically confined above the cathode fall will be described by fluid equations. Taking into account the symmetry of the problem, the fluid equations can be solved in 2D, with a fully implicit procedure. The combined output of the fluid and MC models allows a self-consistent computation of the electric field by solving the Poisson equation. The result will be compared with measurements on experimental hollow-cathode magnetrons, currently under construction in FCT/UNL.

# **Co-ordination and Technological Supervision of UTR, Technological Assistance and Irradiation Services to Institutions and Companies**

L. M. Ferreira, J.B. Manteigas, N. Coelho, J. Venâncio, A. Góis and V. Damas

(see Radiation Technologies: Processes and Products)