APPLICATIONS OF LOW ENERGY MEV ION BEAMS AND COMPUTER SIMULATION TO SURFACE ANALYSIS OF MATERIALS

J. A. R. Pacheco de Carvalho [1,2], C. F. F. P. Ribeiro Pacheco [1], A. D. Reis [1,2]

[1] APTEL Research Group, 2 Departamento de Física, Universidade da Beira Interior, 6201-001 Covilhã, Portugal
E-mails: pacheco@ubi.pt; a17597@ubi.pt; adreis@ubi.pt

ABSTRACT
This work is about surface analysis by nuclear techniques, which are essentially non-destructive, and computer simulation. The energy analysis method for nuclear reaction analysis is used. Elastic scattering is a particular and important case. Energy spectra are computer simulated and compared to experimental data, giving target composition and concentration profile information. The simulations use, mainly, target parameterization and available nuclear data. The method is successfully applied to determination of a uniform concentration profile of ^{18}O from the (p,α) reaction in a thick oxide target. Uniform concentration profiles of ^{12}C are obtained from the (d,p) reaction for a thick target. Uniform concentration profiles of ^{16}O are also obtained from (d,p) and (d,α) reactions along large depths. Elastic scattering is used for depth profiling of Al and O in a thick target. *Keywords*: Surface analysis; Nuclear reaction analysis; Carbon; Oxygen; Elastic scattering; Computer simulation**.**

INTRODUCTION
A broad range of surface analysis techniques has been developed, involving e.g. ion, electron and photon beams interacting with a solid target. The techniques are, generally, complementary and provide target information for depths near the surface. Both nuclear and non-nuclear techniques have been available. Nuclear techniques, which are essentially non-destructive, provide for analysis over a few microns close to the surface giving absolute values of concentrations of isotopes and elements. Their main applications have been in areas such as scientific, technologic, industry, arts, archaeology and medicine, using low energy MeV ion beams [1-6]. Nuclear reaction analysis permits tracing of isotopes with high sensitivities. We use ion-ion reactions and the energy analysis method where, at a conveniently chosen energy of the incident ion beam, an energy spectrum is recorded of ions from the reaction, coming from several depths in the target. Θ_L and Θ_R are the laboratory detection and the target rotation angles, respectively. Such spectra are computationally predicted, giving target composition and concentration profile information [4-6]. Elastic scattering is a particular and important case. A computer program has been developed in this context, mainly for flat targets [4-6]. The non-flat target situation arises as an extension. Applications of the method are given using (p,α), (d,p), (d,α) reactions and elastic scattering of $(^4He)^+$ ions.

RESULTS AND CONCLUSIONS
Energy spectra were obtained for four main samples. Published nuclear data, namely for reaction differential cross section and stopping power, were used in the computer predictions. Sample S1 was a fairly flat pyrolitic graphite target, as checked with SEM microscopy. S1 was analysed through a deuteron beam at a bombarding energy E_d=1.86 MeV, Θ_R=-30° and Θ_L=165°. A good computer fit to data of the $^{12}C(d,p_0)^{13}C$ reaction was obtained, as shown in Figure 1. A probed depth with X_1=15 μm and uniform concentration profile of ^{12}C were found. Sample S2 was an austenitic steel sample. It was obtained by high temperature oxidation in $C^{18}O_2$ gas. A 4.2 μm oxide thickness was provided by weight gain measurements. A uniform concentration profile of ^{18}O was expected. SEM microscopy has shown a reasonably flat oxide. S2 was analysed through a proton beam at a bombarding energy E_p=1.78 MeV, an energy

slightly above the resonance energy at 1.766 MeV in the differential cross section of the $^{18}O(p,\alpha_0)^{15}N$ reaction, $\Theta_R=27^o$ and $\Theta_L=165^o$. A good computer fit to data was obtained, as shown in Figure 2. A uniform concentration profile of ^{18}O was found with $X_1=4.5$ µm. Sample S3 was a thick flat sample of quartz (SiO_2) with a very thin surface film of carbon. S3 was analysed through a deuteron beam at $E_d=0.993$ MeV, $\Theta_R=0^o$ and $\Theta_L=135^o$. A good computed fit to data was obtained. A very thin surface film of ^{12}C was found with uniform concentration and thickness $X_1=0.061$ µm. A uniform step concentration profile distribution of ^{16}O was found in the quartz substrate. The corresponding thickness parameters X_2 of the predictions were, by diminishing order, 5.49 µm for (d,p_0), 5.20 µm for (d,p_1) and 3.39 µm for (d,α_0). Details of the fit are shown in Figure 3. Sample S4 was a thick flat sample of sapphire (Al_2O_3). Uniform distributions of Al and O were expected in the sapphire substrate. S4 was analysed through a $(^4He)^+$ beam at $E_\alpha=1.5$ MeV, $\Theta_R=0^o$ and $\Theta_L=165^o$. A good computer fit to data was obtained, as shown in Figure 4. Uniform concentration profiles of Al and O were obtained with X_1 parameters of 0.53 and 0.23 µm, respectively.

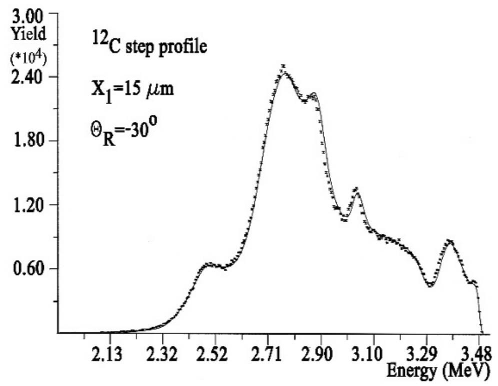

Figure 1. Computed fit to data of the $^{12}C(d,p_0)^{13}C$ reaction from the pyrolitic graphite target, (S1), for $E_d=1.86$ MeV, $\Theta_R=-30^o$, $\Theta_L=165^o$.

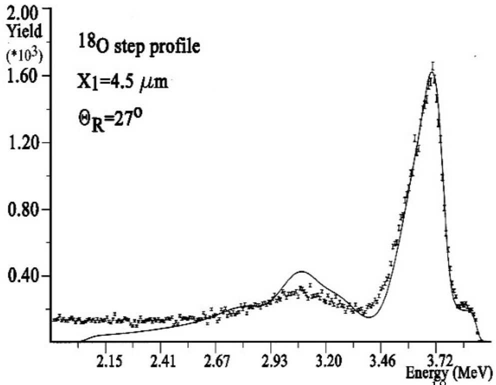

Figure 2. Computed fit to data of the $^{18}O(p,\alpha_0)^{15}N$ reaction from the oxidised steel target, (S2), for $E_p=1.78$ MeV, $\Theta_R=27^o$, $\Theta_L=165^o$.

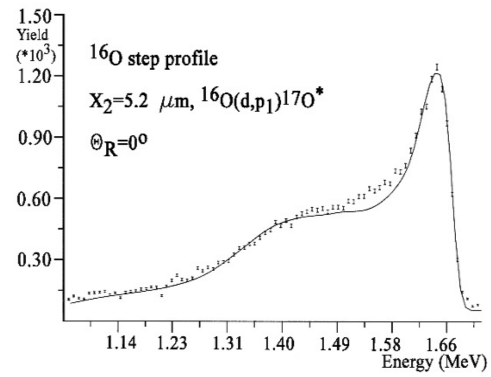

Figure 3. Computed fit to data of the $^{16}O(d,p_1)^{17}O^*$ reaction peak from the quartz target, (S3), for $E_d=0.993$ MeV, $\Theta_R=0^o$,$\Theta_L=135^o$.

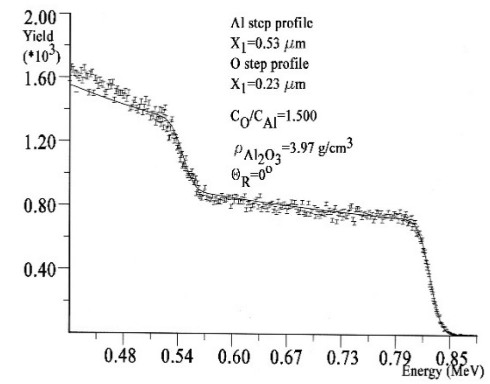

Figure 4. Computed fit to the elastic scattering data from the sapphire target, (S4), for $E_\alpha=1.5$ MeV, $\Theta_R=0^o$, $\Theta_L=165^o$.

Nuclear techniques have shown to be highly powerful and important analytical tools in surface analysis. The results presented would be very difficult to obtain by non-nuclear techniques.

REFERENCES

[1] Wang Y., Nastasi M. (Eds.): Handbook of Modern Ion Beam Materials Analysis, 2nd edition, Materials Research Society, Pittsburgh, PA, U. S. A., 2009.

[2] Amsel G., Battistig G.: The impact on materials science of ion beam analysis with electrostatic accelerators, Nucl. Instr. and Meth. B, 240,1-12, 2005.

[3] Calvert J. M., Derry, D. J., Lees, D. G.: Oxygen diffusion studies using nuclear reactions, J. Phys. D: Appl. Phys., 7, 940-953, 1974.

[4] Pacheco de Carvalho J. A. R., Ph. D. Thesis, University of Manchester, England, 1984.

[5] Pacheco de Carvalho J. A. R., Reis A. D.: Differential cross-section measurements for the $^{12}C(d,p_0)^{13}C$ reaction and applications to surface analysis of materials, Nucl. Instr. and Meth. B, 266, 10, 2263-2267, 2008.

[6] Pacheco de Carvalho J. A. R., Ribeiro Pacheco C. F. F. P., Reis A. D.: Applications of spectral computer simulation to surface analysis of materials, Nucl. Instr. and Meth. B, 269, 24, 3054-3056, 2011.

Project funded by FCT (Fundação para a Ciência e a Tecnologia)/PEst-OE-FIS/UI0524/2014 (Projecto Estratégico-UI524-2014).