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Nuclear Techniques and Computer Simulation in Surface Analysis of Materials

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Introduction – A broad range of surface analysis techniques has been developed. They are, generally, complementary and give target information for depths near the surface. Nuclear techniques, which are non-destructive, permit analysis over a few microns close to the surface giving absolute values of concentrations of isotopes and elements. They have been applied in areas such as scientific, technologic, industry, arts, archaeology and medicine, using low energy MeV ion beams [1-7]. Nuclear reactions permit detection of isotopes with high sensitivities. Ion-ion reactions and the energy analysis method are used in the present work. For a conveniently chosen energy of the incident ion beam, an energy spectrum is collected 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. Predictions of the spectrum are computed, giving information of target composition and concentration profile [4-8]. Elastic scattering arises as a particular and important case. A computer program has been developed in this context, mainly for flat targets [4-7]. The method is applied to determination of an ^{18}C concentration profile in a thick sample using a (p,α) proton induced reaction in ^{18}O. Elastic scattering of $(^4He)^+$ ions is applied to depth
profiling of Al and Ag, Au thin films.

Experimental details - Experimental details have been given [4]. The main targets used for acquisition of charged particle spectra were: 1) *S1*, a thick steel sample oxidised at high temperature in $C^{18}O_2$ gas; An oxide thickness X_1=4.2 μm was given by weight gain measurements. A uniform concentration profile of ^{18}O was expected. A reasonably flat oxide was found by SEM microscopy. 2) *S2*, a flat sample obtained by sequential vacuum evaporation of Ag and Au thin films on a thick flat high purity Al substrate (Al/Ag/Au). Nominal thicknesses were X_1=0.0648 μm and X_2=0.1333 μm for the Au and Ag films, respectively. Spectra were acquired from: 1) *S1,* using the ^{18}O (p,α_0) ^{15}N reaction at E_p=1.78 MeV, an energy slightly above the 1.766 MeV cross-section resonance, Θ_R=27° and 165°. 2) *S2,* using elastic scattering of $(^4He)^+$ ion beams at 1.5 and 2.9 MeV, and 165°.

Results and Discussion - Published nuclear data were used in the computer predictions. Good fits to experimental data were obtained. For *S1*, an ^{18}O step concentration profile was found with thickness X_1=
4.5 μm. For *S2* it was found that it is best described by a structure Al/Ag/(Au,Ag) where the surface film consists of a mixture of Au and Ag. Step concentration profiles were used for Au and Ag in the surface layer with X_1=0.060 μm and for Ag in the middle layer with X_2=0.126 μm, close to the nominal values. A relative atomic density C_{Ag}/C_{Au} of 5.6% in the mixture was found.

Conclusions - The computer simulated predictions have given good descriptions of experimental spectra both for thick target and thin film cases. Nuclear techniques have shown as very powerful tools for surface analysis of materials. Present results would be difficult to obtain by non nuclear techniques.

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