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Determination and theoretical analysis of the differential cross sections of the ^{2}H(d,p) reaction at energies and detection angles suitable for NRA (Nuclear Reaction Analysis)

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Abstract. The accurate determination of deuteron depth profile presents a strong analytical challenge for all the principal IBA (Ion Beam Analysis) techniques. As far as NRA (Nuclear Reaction Analysis) is concerned, the ^{2}H(d,p) reaction, seems to be a promising candidate, especially in the case of complex matrices, or for the study of deep-implanted deuteron layers. In the present work differential cross-section values for the ^{2}H(d,p) reaction have been determined at 140^{o}, 160^{o} and 170^{o}, for $E_{d,lab}$=900-1600 keV, with an energy step of 50 keV, using a well-characterized, thin C:D target deposited on a polished Si wafer. The experimental results were analyzed using the R-matrix calculations code AZURE.

1 Introduction

Deuterium accounts for approximately 0.0156% (or on a mass basis: 0.0312%) of all the naturally occurring hydrogen. Despite its low abundance, however, it has a large number of technical and scientific uses, being the most common nuclide employed in nuclear fusion reactor designs, especially in combination with tritium.

Deuterium and hydrogen show, as isotopes of the same element, a similar chemical behavior, forming analogue compounds. However, if the speed of a reaction is limited by diffusion, the former reacts slower than the latter, a criterion that distinguishes the two isotopes. Because of this property, among others, deuterium is extensively used as a non-radioactive, stable isotopic tracer in investigations of chemical, environmental and biochemical reactions involving hydrogen. Moreover, deuteron implantation has been extensively used in the past for the modification of the physical properties of metals, compounds and semiconductors.

The accurate determination of the deuteron depth profile presents a strong analytical challenge for all the principal IBA (Ion Beam Analysis) techniques. Among these, ERDA (Elastic Recoil Detection

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Analysis) has been successfully employed in the past for the study of ultra-thin deuteron layers, being close to the target's surface, whereas the ^{2}H(d,p) reaction, has been proposed for in-beam monitoring purposes [1], and indeed seems to be a promising candidate (along with the standard and widely used ^{2}H(^{3}He,p) reaction [2]), especially in the case of complex matrices, or for the study of deep-implanted layers.

NRA (Nuclear Reaction Analysis), a well-established IBA technique nowadays, presents important advantages, such as high isotopic selectivity, enhanced sensitivity for many nuclides, capability of least-destructive depth profiling, and possibility of simultaneous analysis of more than one light element in near–surface layers of materials. The creation of IBANDL (http://www-nds.iaea.org/exfor/ibandl.htm), a specially designed library supported by IAEA, which contains differential cross-sections suitable for IBA that can be directly incorporated in widely used analytical programs, has significantly enhanced the analytical power of NRA, and d-NRA in particular. However, the most reliable differential cross-sections are the theoretically evaluated ones, and for d-NRA a lot of key reactions, such as the ^{2}H(d,p) one, still need to be addressed.

In the present work differential cross-section values for the ^{2}H(d,p) reaction have been determined at 140^{o}, 160^{o} and 170^{o}, for $E_{d,lab}$=900-1600 keV, with an energy step of 50 keV, suitable for NRA purposes, using a well-characterized, thin C:D target, deposited on a polished Si wafer. The results, in graphical and tabular form, will soon be available to the scientific community through IBANDL. Moreover, an initial theoretical analysis has been attempted, using the R-matrix calculations code AZURE [3]. It has to be noted though, that, in the case of d–NRA, such an analysis presents strong and interesting theoretical challenges; particularly the problem of taking into account the co-existence of two reaction mechanisms (direct and compound) with energy-dependent contributions seems to be of vital importance, as shown by the obtained results.

2 Experimental setup and procedure

The experiments were performed using the deuteron beam of the 5.5 MV TN11 Tandem Accelerator of N.C.S.R. "Demokritos", Athens, Greece. The deuterons, accelerated to $E_{d,lab}$= 900–1600 keV in steps of 50 keV were led to a cylindrical scattering chamber of large dimensions. The energy of the deuteron beam entering the scattering chamber was determined by nuclear magnetic resonance measurements (NMR) with an estimated ripple of ∼0.16%, as verified by the 991.89 keV resonance of the ^{27}Al(p,γ)^{28}Si reaction at the beginning and at the end of the experiment, using a HPGe detector (of 80% relative efficiency). The excellent linearity of the magnet for the energy range under investigation has been examined in the past by implementing the ^{16}O(d,n)^{17}F reaction ($E_{threshold}$=1829 keV). The deuteron energy, for each measurement, corresponds to the half of the target's thickness (according to the usual convention), after its proper correction according to the results of the accelerator calibration. The energy loss and the energy straggling in the target, in all cases, were calculated using the computer code SRIM [4]. The deuteron energy values were determined with an overall accuracy of ∼3 keV over the whole studied energy range. The deuteron beam was collimated to a 2x2 mm^{2} spot onto the target, while the vacuum was kept constant at 5x10^{-7}mbar. The beam current did not exceed 50 nA during all measurements, in order to avoid any possible deterioration of the deuteron concentration, through excessive heating. The detection system consisted of three silicon surface barrier (SSB) detectors (thickness of 1000 μm) placed at a distance of ∼11-13 cm from the target, at the appropriate angles, along with the corresponding electronics. The spectra from all detectors were simultaneously recorded for each energy step. No absorber foils were placed in front of the detectors, whereas the angular uncertainty was reduced to less than ±1^{o}, with the use of orthogonal slits (4x8 mm^{2}) placed in front of the detectors.

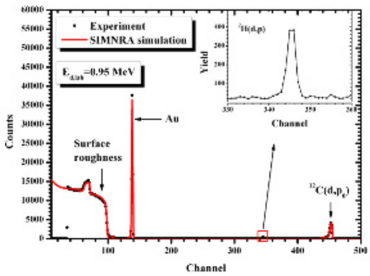

Figure 1. A typical experimental spectrum taken at $E_{d,lab}$=950 keV. The roughness was taken into account using SIMNRA's incorporated model. The inset presents the peak corresponding to the ^{2}H(d,p) reaction.

For the differential cross-section measurements, the thin target used, was a well-characterized (via the implementation of the ^{2}H(^{3}He,p) reaction), C:D layer, on top of polished Si. The target thickness was determined to be ~9x10^{17} at/cm^2. An ultra thin carbon foil (~10 μg/cm^2), with a slight amount of Au evaporated on top, was mounted in front of the target, for charge and detector solid angle normalization purposes. The thickness of the gold layer was determined by SIMNRA [5] calculations and fitting procedures. SIMNRA was also used to verify the whole composition of the target, at various beam energies and detection angles. A typical experimental spectrum taken at $E_{d,lab}$=950 keV is shown in fig.1. The inset presents the peak corresponding to the ^{2}H(d,p) reaction. As it can be seen in this figure, the relevant proton peak was isolated, with a relatively low background, and this was the case for the whole energy range studied, above which strong perturbations occured, due to (d,p) and (d,α) reactions in the Si isotopes. Unfortunately, despite the polished Si substrate, the problem of roughness was evident, yielding significant lateral inhomogeneities. The roughness was taken into account using repeatedly SIMNRA's incorporated model, and was partly studied with the use of optical microscopy, as shown in fig.2. The target roughness caused lateral fluctuations in the D content, and thus to the D:Au ratio, reaching values as high as 9%, as verified experimentally with control measurements (returning to the highest energy, after every 4-5 steps). These fluctuations, constituted the dominant factor in the overall uncertainty of the obtained differential cross-section values. In the cases where the inhomogeneities caused serious ambiguities in the obtained results, the corresponding differential cross-section values were omitted from the graphs, as shown in the following section.

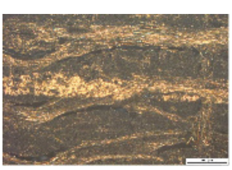

Figure 2. Optical microscopy image of the target after the formation of the C:D layer (golden color), showing evidence of roughness and lateral inhomogeneity.

3 Results, discussion and conclusions

Differential cross sections for the d+d system, were determined following relative measurements, compared to the differential cross-section values of the ^{197}Au(d,d$_0$)^{197}Au reaction, which is purely Rutherford, for the same scattering angle and accumulated charge. Peak integration yielded an uncertainty of the total number of the backscattered deuterons and emitted protons not greater than 2-5% in most of the cases (including counting statistics and background subtraction). The uncertainty of the yields, as well as the lateral inhomogeneity of the target were the main contributing factors to the overall uncertainty, which - because of the latter - reached values that even exceeded 10% in some cases.

This overall uncertainty was used as input to the AZURE R-matrix code, in order to simultaneously fit the data through χ^2 minimization.

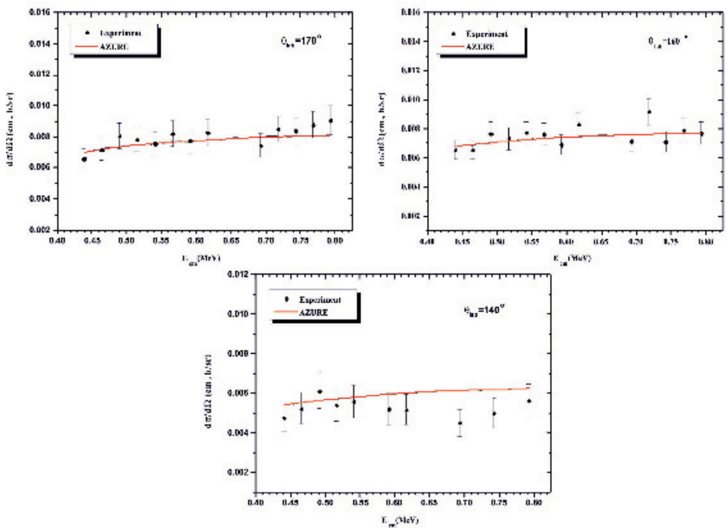

Figure 3. R-matrix calculations with AZURE [3], showing an excellent agreement with experimental data at 170^o and 160^o, angles particularly suitable for NRA. The agreement is only fair, however, at less backward detection angles, as in the case of 140^o.

As shown in fig.3, using the existing (e.g. http://www.nndc.bnl.gov/chart/) broad resonance data (energies, Γ, Γ_p, Γ_n) for the compound nucleus ^{4}He, there is an excellent agreement between the R-matrix calculations and the experimental results for 170^o and 160^o, which are among the most important detection angles for NRA applications. However, the agreement is less satisfactory at 140^o, implying that further calculations are required in order to take into account the contribution from the co-existing direct reaction mechanism. Another, non hard-sphere, R-matrix code will also be tested in the near future [6]. Moreover, currently ongoing experimental runs, which cover the angular range between 110^o and 150^o are expected to facilitate the analysis, aiming at finally achieving the theoretical evaluation of the differential cross-section values of the ^{2}H(d,p) reaction for NRA purposes.

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