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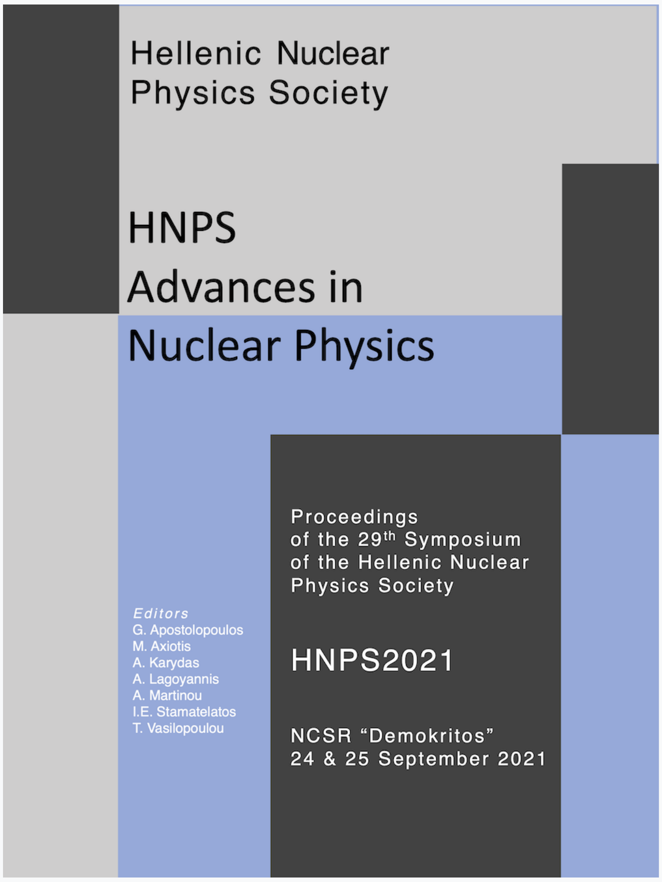

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R-matrix Calculations for Proton Elastic Scattering on ^{nat}Mg in the Energy Range E = 2.45 - 4.25 MeV, Suitable for EBS

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Abstract In the present work R-Matrix calculations regarding the differential cross sections of the ^{nat}Mg(p,p$_0$)^{nat}Mg elastic scattering for $E_{p,lab}$ = 0.70 – 4.25 MeV were implemented using the Azure2 code [1]. A coherent set of differential cross sections, the first to cover the $E_{p,lab}$ = 2.45 – 4.25 MeV energy range [2], measured at the Tandem Accelerator laboratory of NCSR "Demokritos" was used as a basis for the calculations. These results were able to accurately reproduce both the experimental dataset as well as the current evaluation [3] which covers the $E_{p,lab}$ = 0.7 to 2.7 MeV energy range.

Keywords Ion Beam Analysis, EBS, R-Matrix, Cross Section Measurements, ^{nat}Mg

INTRODUCTION

Natural magnesium consists of three isotopes, ^{24}Mg (78.99%), ^{25}Mg (10%) and ^{26}Mg(11.01%), with its alloys exhibiting remarkable light weight, heat dissipation and damping ability. These characteristics, along with their wide availability, have established their use in a variety of industries and applications, with their most prominent implementation being in the electronics and construction sector for the creation of lightweight materials. Due to the wide use of such alloys, the need to precisely determine and quantify depth profile concentrations of ^{nat}Mg in near surface layer in various matrices naturally arises.

Ion Beam Analysis (IBA) refers to a group of highly accurate experimental methods that, through nuclear reactions, are able to accomplish the above for a variety of isotopes, while causing the least amount of damage to the samples under study. To implement these techniques, however, reliable differential cross section data regarding the employed nuclear reactions are needed. Evaluated datasets, in particular, which are the product of theoretical calculations based on a number of experimental data from different sources, are considered the most trustworthy and desirable. In addition, as these industries and applications evolve over time, the probing of greater depths is needed, which in turn requires cross-section data for higher beam energies. From the available IBA techniques proton backscattering spectroscopy (p-EBS) is ideal for such measurements at greater depths since the lower mass and charge of protons results in smaller losses in the beam energy.

Specifically for the case of the ^{nat}Mg(p,p$_0$)^{nat}Mg elastic scattering the current evaluated cross-section data covers the $E_{p,lab}$ = 0.7 – 2.7 MeV energy range. In addition, there are no available published experimental datasets in the literature for energies higher than 2.7 MeV. In the present work, the first coherent set of cross sections for the ^{nat}Mg(p,p$_0$)^{nat}Mg elastic scattering for $E_{p,lab}$ = 2.45 – 4.25 MeV was used to implement R-Matrix theoretical calculations that reproduce accurately both the experimental data, as well as the current evaluation. These calculations could form the basis for a future expansion of the current evaluation once more experimental data become available and the experimental and theoretical results of this work are subjected to benchmarking experiments from independent laboratories.

EXPERIMENTAL DETAILS

The measurements were performed at the Van de Graff Tandem 5.5 MV Accelerator of the Institute of Nuclear and Particle Physics of NCSR "Demokritos". The final Ion Beam energy was determined via Nuclear Magnetic Resonance (NMR). The energy calibration of the accelerator was implemented using the known resonance of the ^{27}Al(p,γ) reaction at the 991.89 keV proton energy determining a ripple of 4.7 keV along with a 5.1 keV beam offset. These values were considered constant for the duration of the experiment since non-linear deviations of the magnet have not been observed before.

The beam was directed into a cylindrical scattering chamber containing a high precision goniometer with an accuracy of 0.1^{o} atop of which 6 Silicon Surface Barrier (SSB) detectors were positioned along with their respective electronics in the detection angles θ = 120^{o}, 130^{o}, 140^{o}, 150^{o}, 160^{o} and 170^{o}. A thin foil consisting of three different layers and constructed at NCSR "Demokritos" was used as target for the cross-section measurements. Specifically, the target consisted of a thin ^{12}C foil that acted as the backing of the target, upon which ^{nat}Mg was evaporated and finally, an ultra-thin layer of ^{197}Au was evaporated on the surface of the target for normalization and wear protection purposes (figure 1). To estimate the target stoichiometry the SIMNRA code version 7.01 [4] was used along with three dedicated experimental measurements for $E_{p,lab}$ = 1900, 2300 and 2550 keV for the 150^{o}, 160^{o} and 170^{o} detection angles. These energies were chosen due to the availability of evaluated cross-section data for all elements of interest in this energy range from the SigmaCalc 2.0 online calculator [5] http://sigmacalc.iate.obninsk.ru. The chamber was held under constant high vacuum for the whole duration of the measurements.

The experiment proceeded in three distinct phases. Firstly, the measurements for the accelerator energy calibration were implemented. The measurements for the determination of the target composition followed and finally the cross-section measurements were performed with protons accelerated from 2450 to 4250 keV.

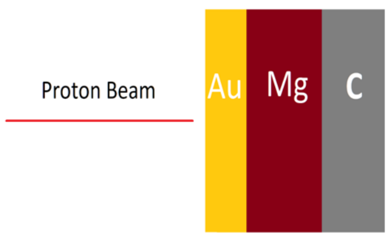


Figure 1: *A graphical representation of the target composition that was used for the differential cross section measurements.*

RESULTS AND DISCUSSION

To determine the differential cross-section values from the acquired experimental data the relative measurement technique was used, which is described by the following formula

$$\left(\frac{d\sigma}{d\Omega}\right)^{E,\theta}_{nat_{Mg}} = \left(\frac{d\sigma}{d\Omega}\right)^{E',\theta}_{Au} \frac{N_{t,Au}}{N_{t,nat_{Mg}}} \frac{Y_{nat_{Mg}}}{Y_{Au}} \tag{1}$$

where E refers to the proton beam energy at the half of the target thickness, having taken into account the accelerator energy calibration, E' refers to the calibrated proton beam energy and θ to the detection angle. The term $\left(\frac{d\sigma}{d\Omega}\right)^{E',\theta}_{Au}$ corresponds to the cross-section values for the elastic scattering of protons on ^{197}Au, calculated analytically by the Rutherford formula and corrected for the electronic screening effect using the formula by L'Ecuyer [6]. The term $\frac{N_{t,Au}}{N_{t,nat_{Mg}}}$ refers to the ratio of the atomic aerial densities of ^{197}Au ($N_{t,Au}$) and ^{nat}Mg ($N_{t,^{nat}Mg}$) of the target, as they were determined using the SIMNRA code. Lastly, the term $\frac{Y_{nat_{Mg}}}{Y_{Au}}$ refers to the ratio of the integrated yields of the proton elastic scattering peaks of ^{nat}Mg (Y^{nat}_{Mg}) and ^{197}Au (Y_{Au}) in the experimental spectra. For the integrations and the spectral analyses, the SPECTRW code [7] was used.

The ratio of the determined cross section values to the ones according to the Rutherford formula are shown in figure 2 for all 6 detection angles, along with their corresponding statistical uncertainties, which did not exceed 6.9%. No systematic uncertainties are shown in the figure. These could mainly originate in the accuracy of the implemented stopping power model that was used in the determination of the $\frac{N_{t,Au}}{N_{t,nat_{Mg}}}$ term (ZBL stopping power compilation [8]) and in possible lateral inhomogeneities of the target.

The differential cross sections did not exhibit a strong angular dependence on their values. Strong resonant behavior however was observed with most Breit–Wigner resonances corresponding to excited energy states of the ^{25}Al* compound nucleus [9].

To implement the R–Matrix calculations, the Azure2 code was used, following the standard hard–sphere approach. The aim of these calculations was to determine a single set of parameters that could reproduce the current evaluation, which covers the $E_{p,lab}$ = 0.7 – 2.7 MeV energy range in addition to the acquired cross-section data that cover the $E_{p,lab}$ = 2.45 to 4.25 MeV energy range. The calculations were based on the compound nucleus of the p-^{24}Mg reaction, ^{25}Al* following the Few-Channel, Multi-Level approach. Specifically, two reaction channels were used, namely the elastic channel ^{24}Mg(p,p$_0$) and the first excited ^{24}Mg(p,p$_1$) reaction channel with a nucleus radius of 4.86 fm for both channels. A total of 14 levels of the ^{25}Al* compound nucleus were used in the calculations with occasional small deviations from the values found in the literature for the level's nominal energy and total width Γ. In addition, two artificial levels were inserted in order to simulate the influence of the ^{25}Mg and ^{26}Mg isotopes in the cross section. It should be noted that the small deviations from the values found in the literature and the insertion of artificial levels are considered to be a standard practice in this kind of calculations and are no cause for concern. The results of the R–Matrix calculations (red line) along with the current evaluation (blue line) and the acquired cross-section data (black squares) are shown in figures 3a-f for all the measured detection angles

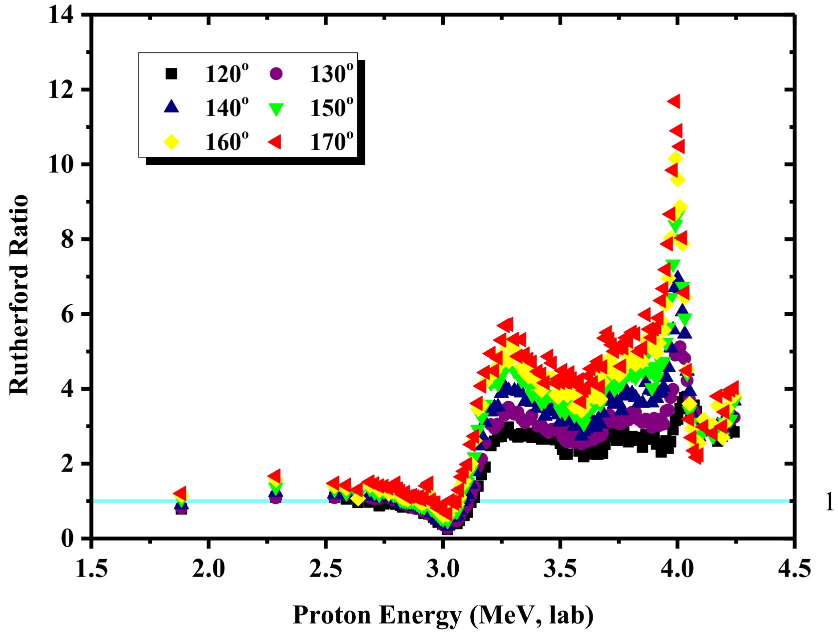
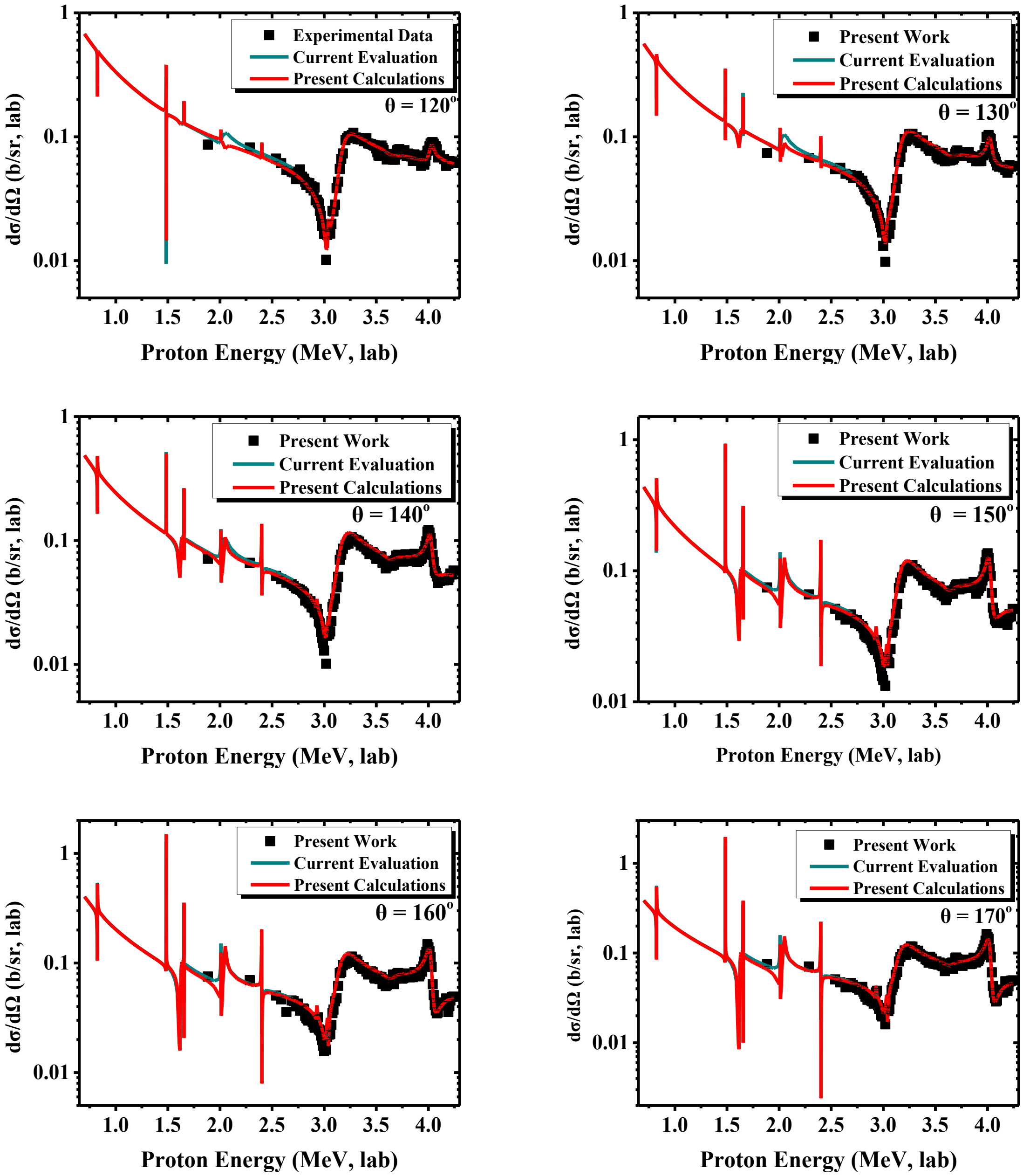


Figure 2: *Ratio of the measured differential cross section values (mb/sr) with respect to the values calculated via the Rutherford formula for $E_{p,lab}$ = 2450 – 4250 keV (nominal beam energy) for the 120°, 130°, 140°, 150°, 160° and 170° backscattering angles. The blue horizontal line indicates a ratio equal to 1.*

As it can be seen from figures 3 a – f, the present R–Matrix calculations were able to reproduce both the current evaluation, as well as the acquired data with accuracy. More specifically, for the 0.7 to 2.7 MeV energy range some small deviations in the maxima and minima of the resonances can be observed between the present calculations and the current evaluation, however, these can mostly be attributed to differences between the energy step in the calculations. A greater deviation is observed in the resonance at 2.035 MeV. No existing energy state of the ^{25}Al nucleus corresponds to this resonance, most likely the result of the influence of the ^{26}Mg in the cross section. To accommodate for this extra level an artificial one was inserted in the calculations. With respect to the 2.4 to 4.25 MeV energy range, the present calculations were able to reproduce all the resonances that were observed in the acquired experimental data quite accurately, with discrepancies not surpassing ~ 6%. The only exception to this was the resonance around $E_{p,lab}$ = 3 MeV in the lower detection angles, for which the discrepancies between the calculations and the experimental data reached ~13%. Finally, it should be noted that the acquired data were in good agreement with the current evaluation for the overlapping energy region.



Figures 3 a – f: *Comparison between the present R – Matrix calculations (red line), the current evaluation (blue line) and the acquired experimental data (black squares) for an energy range between Ep,lab = 0.7 to 4.25 MeV for the detection angles 120º. 130º, 140º, 150º, 160º and 170º.*

CONCLUSIONS

In the present work, R-Matrix calculations were implemented using the Azure2 code for the elastic scattering of protons on ^{nat}Mg in the energy range $E_{p,lab}$ = 0.7 to 4.25 MeV. These calculations were based on the first coherent set of differential cross-section data for the ^{nat}Mg(p,p$_0$)^{nat}Mg elastic scattering in the $E_{p,lab}$ = 2.45 – 4.25 MeV energy range, for detection angles from 120º to 170º with a 10º step. The excited energy states of the ^{25}Al* compound nucleus along with two artificial levels were used in the calculations. The results were compared to the current evaluation which covers the 0.7 to 2.7 MeV energy range and the aforementioned experimental data. The calculations were able to accurately reproduce both datasets using a single set of parameters. Thus, they allow the interpolation of cross section values for energies between 0.7 to 4.25 MeV and for detection angles ranging from 120^o to 170^o. In addition, these calculations can form the basis of a future expansion of the current evaluation, once more experimental datasets become available and both the experimental and theoretical results of this work are tested in benchmarking measurements from independent laboratories.

References

[1] R. Azuma et al., Physical Review C 81
[2] E. Alvanou et al., HNPS Adv. Nucl. Phys. (2019)
[3] A. F. Gurbich et al., Nucl. Instr. and Methods in Physics B, Vol. 268, p. 1703 (2010)
[4] M. Mayer, Nucl. Instr. And Methods in Physics B, (2014), Vol. 332, p. 176
[5] A.F. Gurbich, Nucl. Instr. and Methods in Physics B, Volume 371 (2016)
[6] Pages 27-32, J. L'Ecuyer et al., Nucl. Instr. Methods 160 337-346 (1979)
[7] C. A. Kalfas et al., Nucl. Instr. and Methods in Physics A, Vol. 830, p. 265 (2016)
[8] J.F. Ziegler et al., The Stopping and Range of Ions in Solids. Vol. 1. The Stopping and Ranges of Ions New York: Pergamon Press, (1985)
[9] R.B. Firestone, Nucl. Data Sheets 110, 1691 (2009)