Benchmarking the natSi(p,p0) and natO(d,d0) elastic scattering and the 16O(d,p0,1,α0) reactions for IBA purposes

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**Benchmarking the $^{\text{nat}}\text{Si}(p,p_0)$ and $^{\text{nat}}\text{O}(d,d_0)$ elastic scattering and the $^{16}\text{O}(d,p_0,1,\alpha_0)$ reactions for IBA purposes**

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**Abstract**

The benchmarking experimental procedure in IBA (Ion Beam Analysis) is carefully designed in order to validate evaluated and experimental differential cross-section datasets of charged particles via the acquisition of EBS and NRA spectra from thick targets of known composition, followed by their simulations.

In the present work, such benchmarking measurements have been performed at the laboratory of the Institute for Nuclear and Particle Physics “Demokritos”, for the elastic scattering of protons on $^{\text{nat}}\text{Si}$ in the energy range of 1.1 – 3.5 MeV at four backward angles, at 140°, 150°, 160° and 170°. In addition, measurements were performed for the elastic scattering of deuterons on $^{16}\text{O}$ in the energy range of 1.1 – 1.7 MeV at four backward angles, at 140°, 150°, 165° and 170°. More specifically, a thick non-polished Si target with Au evaporated on top and a Nb$_2$O$_5$ tablet were used.

The spectra acquired were compared with simulated ones using the SIMNRA program along with the evaluated differential cross-section datasets from IBANDL. All the experimental parameters were thoroughly investigated. The obtained results, the observed discrepancies and the encountered problems during the benchmarking process are discussed and analyzed.

**Keywords** Benchmarking, EBS, NRA, IBA

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**INTRODUCTION**

The benchmarking experimental procedure in IBA (Ion Beam Analysis) [1] is a means to validate microscopic differential cross-section data of charged-particle reactions, via the acquisition of EBS (Elastic Backscattering Spectroscopy) and NRA (Nuclear Reaction Analysis) spectra from appropriate thick targets of known composition, followed by their simulations.
The importance of the benchmarking procedure lies in the requirements of the IBA depth profiling techniques. All of these techniques largely depend on the accuracy of the available experimental differential cross-section datasets for the reactions involved, which are unfortunately quite rare and usually discrepant. This implies that their credibility is questionable at best; thus a carefully designed validation procedure is mandatory, even for evaluated datasets, which are regarded as being the most reliable ones. Benchmarking can also provide the necessary feedback for a small adjustment of the parameters of the nuclear model used in the evaluation process, as well as indicate the best experimental datasets if evaluated ones are not available.

In the present work, benchmarking measurements have been performed for the study of proton elastic scattering on natSi, in the energy range between 1.1 and 3.5 MeV, at four backward detection angles, namely at 140°, 150°, 160° and 170°. Also, additional measurements were performed for the study of deuteron elastic scattering on natO, which also included the 16O(d,p0,1) and 16O(d,α0) reactions, widely implemented for oxygen depth profiling, in the deuteron beam energy range between 1.1 and 1.7 MeV, at four backward detection angles, namely at 140°, 150°, 165° and 170°. In all cases, evaluated differential cross section datasets were tested via extensive simulations.

EXPERIMENTAL DETAILS

The experiment was carried out using the proton beam of the 5.5 MV Tandem HV T11 accelerator, which impinged on the targets set inside a goniometric chamber, depicted in the picture below. The electrically insulated target column in the center of the chamber can be moved vertically and it can be rotated as well. In this column two thick targets were appropriately placed.

The backscattered protons were simultaneously detected by four silicon SSB detectors, initially set in pairs, at 10° intervals, in two independently rotating tables of 0.01° angular precision. During the experiment, the chamber was sealed and high vacum of the order of 10^{-6} Torr was applied.

A thick non–polished crystalline Si target with a thin layer of Au evaporated on top for normalization purposes and a high-purity Nb2O5 pressurized pellet were used throughout the measurements.
The beam energies were selected before and after the resonances, but also in some intermediate regions in order to scan the whole excitation function as shown below.

Evaluated datasets, obtained from SigmaCalc 2.0 in IBANDL, the Ion Beam Analysis Nuclear Data Library, were used for the benchmarking process.

RESULTS AND DISCUSSION

After determining the accelerator energy calibration and the energy resolution of each detector, the spectra were analyzed by comparing the experimental datasets with the simulations performed via SIMNRA, using evaluated data from SigmaCalc 2.0.
Some characteristic spectra are shown in the next figure. The integration regions are defined by the vertical, dashed lines and extend in an equivalent depth of 250 keV from the silicon surface edge.

The $^{nat}$Si(p,p$_0$) elastic scattering at 1733 keV is shown in the top left panel of the figure. The agreement between experimental and simulated data is quite good since the deviation does not exceed 5.2%. An even better agreement is obtained at 2157 keV, as shown in the top right panel. The deviation is only 3.0%. As the energy of the beam increases, the deviations are enhanced. At 2997 keV the deviation reaches 44.2%, as shown in the bottom left panel. At 3397 keV the deviation exists not only in the integrated yield but also in the very form of the simulation, which overestimates the experimental result by 14.8%.

A similar pattern is observed in all studied angles.

In the following figure, the results from the $^{nat}$O(d,d$_0$) elastic scattering and the results from the $^{16}$O(d,p$_{0,1}$,a$_0$) reactions are also presented.

The integration regions are defined by the vertical, dashed lines and extend over a depth of 200 keV from the oxygen surface edge for the elastic scattering.

In the top left panel the agreement is satisfactory, since the deviation is only 4.11%. As the energy of the beam increases, the deviations are enhanced. In the top right panel, at 1650 keV, the deviation reaches a value of ~32%.

![Fig. 3 Comparison between experimental data and simulations based on evaluated data for the $^{nat}$Si(p,p$_0$) elastic scattering](http://epublishing.ekt.gr)
As far as the nuclear reactions are concerned, as shown in the bottom left panel, the integration window is huge, approximately 1502 keV, starting from 1200 keV, due to level overlap. The agreement is satisfactory, since the deviation does not exceed 4.55% over the whole energy range. In the bottom right panel, the integration window is approximately 1275 keV, starting from 1600 keV. The agreement is rather mediocre, with the deviation reaching a value of 22.47%, the largest part of which can be attributed to the poor reproduction of low-energy resonances.

CONCLUSIONS

In this work, a systematic effort was made to validate the evaluated differential cross-section datasets based on the R-matrix theory, whose parameters were tuned according to already existing experimental ones. More specifically, benchmarking measurements were made to evaluate the differential cross sections for the elastic scattering of protons on natSi as well as for the elastic scattering of deuterons on natO, along with the 16O(d,p0,1,α0) reactions. For this purpose high-purity thick targets of known stoichiometry were implemented.

The results from this work are expected to effectively complement the existing differential cross section datasets and provide the necessary feedback for a re-tuning of the nuclear parameters used in R-matrix theory calculations, especially for high proton beam energies.
References