

HNPS Advances in Nuclear Physics

Vol 24 (2016)

HNPS2016



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doi: [10.12681/hnps.1860](https://doi.org/10.12681/hnps.1860)

To cite this article:

Preketes-Sigalas, K., Lagoyannis, A., & Axiotis, M. (2019). Development of a simulation code for material analysis using the PIGE technique. *HNPS Advances in Nuclear Physics*, 24, 162–166. <https://doi.org/10.12681/hnps.1860>

Development of a simulation code for material analysis using the PIGE technique

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Abstract Particle Induced Gamma ray Emission (PIGE) is a well known and widely used Ion Beam Analysis (IBA) technique for non-destructive material analysis, usually in conjunction with Proton Induced X-ray Emission (PIXE). The main drawback in the applicability of PIGE regarding the quantification of light elements in various heavy element substrates is the need for many reference targets with similar matrices to the one under study, because of the importance of the ion energy loss in the calculations. In order to overcome this problem, an appropriate simulation code that uses as inputs the experimental spectrum and the relevant differential cross sections, with the output being the quantification of the concentration depth profiles of the isotopes of interest is needed. A code like this is currently being developed in C++ and it is compatible with Windows, Linux and Mac.

Keywords Differential cross section, PIGE, PiGreCo, code, yield

INTRODUCTION

A major drawback for PIGE measurements is that until now they are carried out by mainly using the relative technique. However, because of the unavoidable variations in the stopping power of the samples, each time a reference target is required, with a matrix similar to the analyzed one's, so each laboratory needs to own an extensive set of such standards. In order to overcome this problem, standardless measurements should be conducted. Thus, if the respective cross sections, σ , are well measured and the composition of the analyzed sample is quantified, the accumulated yield, Y_{sam} , could be determined using the equation:

(1)

where Y_{init} is the yield from zero up to an energy E_{init} below which no cross section value exists in literature, E_b is the energy of the incident beam particles and S_{sam} corresponds to stopping power correction. This equation is accurate due to the fact that although the stopping power correction is not constant, it is integrated over the same energy range. On the contrary, in relative measurements the accumulated yield is approximated using the equation:

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where Y_{std} is the yield from the standard sample at the same energy, C_{sam} and C_{std} correspond to the concentrations of the analyzed isotope in the measured sample and standard, respectively, and S_{std} is the stopping power correction of the standard target. In this case, stopping power corrections are calculated only at the bombarding energy, E_b , so equation (3) is not so precise.

The calculation of the yield using equation (4) would be more convenient and the sample analysis could be automated if there existed an appropriate analytical code. Several attempts have been presented in the past, with ERYA [1–6] being the most prominent candidate. Unfortunately, this code operates only in Windows 64-bit version-based computers, because it is developed in LabVIEW (National InstrumentsTM), and moreover, it is not compatible with R33 differential cross section standard input files.

THE PIGRECO PROGRAM

PiGreCo, which stands for Particle Induced Gamma-Ray Emission Code, is a code developed in C++ and it uses Qt Libraries for the Graphical User Interface (GUI). It operates in Windows, Linux and Mac, and it is compatible with R33 files as obtained from the Ion Beam Analysis Nuclear Data Library (IBANDL, <https://www-nds.iaea.org/exfor/ibandl.htm>).

In the present version, the target has to be a homogeneous monolayer, the initial composition of which is given by the user. The code, taking into account the experimental conditions (accumulated charge, detector efficiency, etc.), calculates the expected yield for the reaction under study. Using successive iterations it fits the concentration of the sample isotopes until the experimental yield is reproduced within a certain accuracy. The energy loss in the target is calculated using the Ziegler, Biersack and Littmark (the so-called "ZBL") stopping for each element and then the Bragg's rule for the determination of the stopping power in compounds. The differential-cross-section files should be in R33 format and the user can give an initial yield for the lowest energy that the cross section is available. Taking into account the aforementioned parameters, the yield is calculated using equation (5).

The most important function of PiGreCo is that it can also work in the inverse way. The user should additionally provide an estimated target composition and the experimental yield, Y_{exp} , and the code, by doing repeated iterations, is able to converge, checking at each step the ratio between the calculated and the experimental yield, Y_{sam}/Y_{exp} , while doing the respective modification in the target composition, in order to approach unity (Fig. 1). For each element of the target there are three choices ("fit", "fixed" and "free"). "Fit" is for the fitted elements and there should be at least one in the target (and up to five in the current version), "fixed" is for the elements whose percentage in the target is known and also, by definition, at least one element should be set as "free" in order for the code to maintain the total percentage equal to 1 (or 100%) (Fig. 2).

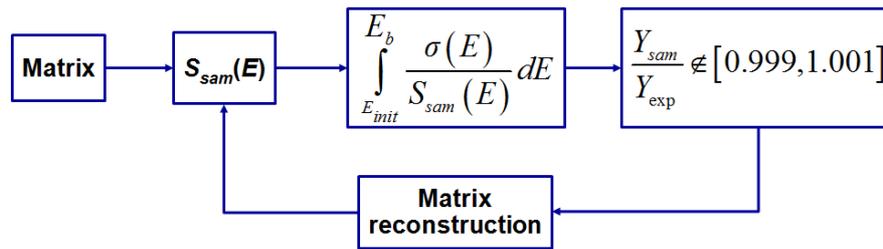


Fig. 3. Loop procedure for concentration estimation. The ratio of calculated and experimental yield, Y_{sam}/Y_{exp} , should be in the given range (which can be adjustable) in order to have convergence. If not, the suitable concentration adaptation (matrix reconstruction) is done.

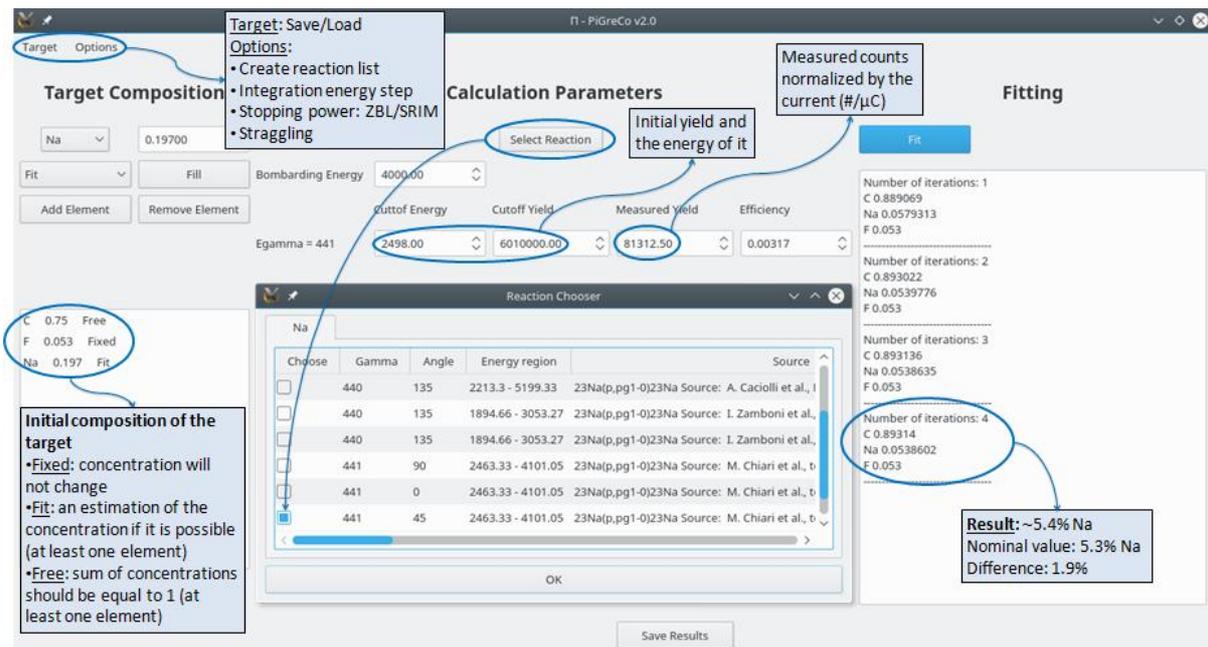


Fig. 4. Interface and main functions of PiGreCo. In this specific case, a measurement was carried out using a homemade thick target of NaF (5.3% Na and 5.3% F in C). The cross section and the initial thick-target yield used for sodium were taken by M. Chiari et al. [8,9]. The difference between the result and the nominal value is lower than 2%.

EVALUATION OF THE CODE

In order to evaluate the code, an experiment was conducted in the Tandem Accelerator Laboratory, INPP, NCSR “Demokritos” with two (2) NIST samples, namely a phosphate rock (SRM 120b) one and a multicomponent glass (SRM 1412). The proton beam energy range was $E_p=1.5 - 4.0$ MeV, using variable steps, and two (2) HPGe detectors were implemented, set at 55° and 90° .

In Tables 1 and 2 details are shown about each reaction used along with the differences between nominal and estimated (using the code) concentrations for the phosphate rock and multicomponent targets for the proton beam energies of 4000 and 3500 keV, respectively. It has to be noted that the

elements have been simultaneously fitted for each target. The maximum difference between the certified and calculated concentration for the NIST certified elements is 4%.

| Element | Reaction | E_γ (keV) | Initial yield (#/sr/ μ C) | Cross section | Difference |
|----------|--|------------------|-----------------------------------|-------------------|------------|
| Fluorine | $^{19}\text{F}(p,p'\gamma_{1-0})^{19}\text{F}$ | 110 | 5.1×10^6 @ 2500 keV [10] | Chiari et al. [8] | 2.3% |
| Sodium | $^{23}\text{Na}(p,p'\gamma_{1-0})^{23}\text{Na}$ | 440 | 6.01×10^6 @ 2498 keV [9] | Chiari et al. [8] | 4% |

Table 3. Phosphate rock (NIST 120b) at $E_p=4000$ keV.

| Element | Reaction | E_γ (keV) | Initial yield (#/sr/ μ C) | Cross section | Difference |
|-----------|--|------------------|--------------------------------------|------------------------|-------------------|
| Sodium | $^{23}\text{Na}(p,p'\gamma_{1-0})^{23}\text{Na}$ | 440 | 6.01×10^6 @ 2498 keV [9] | Chiari et al. [8] | 2.8% |
| Lithium | $^7\text{Li}(p,p'\gamma_{1-0})^7\text{Li}$ | 478 | 10^7 @ 2002 keV* | Fonseca et al. [11] | 9.6% [†] |
| Boron | $^{10}\text{B}(p,p'\gamma_{1-0})^{10}\text{B}$ | 718 | 2.4×10^4 @ 2002 keV* | Lagoyannis et al. [12] | 0.3% |
| Magnesium | $^{25}\text{Mg}(p,p'\gamma_{2-1})^{25}\text{Mg}$ | 390 | 2.4×10^4 @ 2400 keV [13,14] | Preketes et al. [15] | 1.9% |
| | $^{25}\text{Mg}(p,p'\gamma_{1-0})^{25}\text{Mg}$ | 585 | 8.5×10^4 @ 2416.2 keV* | Preketes et al. [15] | 3% |
| | $^{25}\text{Mg}(p,p'\gamma_{2-0})^{25}\text{Mg}$ | 975 | 2.2×10^4 @ 2400 keV [13,14] | Preketes et al. [15] | 4% |

Table 4. Multicomponent glass (NIST 1412) at $E_p=3500$ keV.

CONCLUSIONS

In conclusion, PiGreCo can calculate elemental concentrations in a quite satisfactory way. In the near future an in-depth debugging should be done and as an upgrade the Vavilov/Lorentzian distribution will be added for beam energy straggling calculations in order to facilitate the studies of

* Interpolation between existing data, available for downloading from the IBANDL database

[†] Not certified

thin layers. Following these steps, the code will be freely distributed to the scientific community through the Institute's web page. The open and modular architecture of the code will allow for extra features to be added in the future upon user request. A possible important extension of the algorithm could concern the determination of resonant depth profiles via different types of regularization, in order to effectively treat the ill-posed mathematical problem of the deconvolution of the cross section in the case of complex, multilayered matrices. Finally, users will have the capability to add multiple layers and simultaneously fit more than five light isotopes coexisting in a target.

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