

HNPS Advances in Nuclear Physics

Vol 28 (2021)

HNPS2021

Hellenic Nuclear Physics Society

HNPS
Advances in
Nuclear Physics

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Proceedings
of the 29th Symposium
of the Hellenic Nuclear
Physics Society

HNPS2021

NCSR “Demokritos”
24 & 25 September 2021

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doi: [10.12681/hnps.4798](https://doi.org/10.12681/hnps.4798)

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To cite this article:

Bari, Z., Chasapoglou, S., Kalamara, A., Vasilopoulou, T., Axiotis, M., Lagoyannis, A., Kokkoris, M., Vlastou, R., & Stamatelatos, I. (2022). Fast Neutron Activation Analysis at the NCSR Tandem Accelerator facility: Prognosis and Optimization. *HNPS Advances in Nuclear Physics*, 28, 257–260. <https://doi.org/10.12681/hnps.4798>

Fast Neutron Activation Analysis at the NCSR D Tandem Accelerator facility: Prognosis and Optimization

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Abstract Neutron Activation Analysis Prognosis and Optimization (NAAPRO) code was applied for the prognosis of the activation products, their activities, the number of counts recorded in the detector, the minimum detection limits as well as the gamma spectrum obtained in fast neutron activation analysis experiments. Simulations were performed for geological and biological reference materials irradiated with 14 MeV neutrons at the 5.5 MV NCSR D tandem accelerator facility. The results of the study demonstrated the fast neutron analytical capabilities of the accelerator and, moreover, allowed for the optimization of the FNAA parameters, while avoiding the performance of difficult and time-consuming experimental tests at the accelerator facility.

Keywords: fast neutron activation analysis, NAAPRO

INTRODUCTION

Neutron activation analysis is a nuclear analytical technique enabling qualitative and quantitative multi-element analysis in samples from a wide range of materials [1]. Typically, the technique is performed with thermal neutron capture reactions at research reactors due to the very high sensitivity achieved for many elements. However, it can also be performed in neutron beams produced at particle accelerators utilizing threshold reactions [2], even though this case is limited by lower neutron fluence rates, lower cross sections, shorter irradiation times due to limited target life and interfering reactions. In this work, the Fast Neutron Activation Analysis (FNAA) capabilities of the NCSR D 5.5 MV Tandem accelerator facility are investigated. The study was performed using Neutron Activation Analysis Prognosis and Optimization (NAAPRO) code [3].

METHOD

The NAAPRO code predicts the results and main characteristics of neutron activation analysis experiments. Specifically, it predicts detection limits, determination limits, measurement limits and relative precision of the analysis, gamma dose rates and the count rate of the spectrometry system used are predicted for different cooling times after sample irradiation. The code provides visualization of the spectrometer efficiency, background spectrum, as well as response spectrum from the sample. Simulations were performed for samples representing biological (IAEA A-13) and geological (IAEA Soil 7) materials, irradiated under 14 MeV ($10^{10} \text{ cm}^{-2} \cdot \text{s}^{-1}$) neutron beam. The spectrum was calculated on a HPGe detector of 80% relative efficiency. Several irradiation, cooling and measurement time cycles were tested (Table 1). The sample mass was 0.1 g.

Table 1. Time properties of irradiation-cooling-measurement cycles

	Cycle 1	Cycle 2	Cycle 3	Cycle 4	Cycle 5
Irradiation time	60 s	300 s	0.5 h	3 h	24 h
Cooling time	60 s	300 s	0.5 h	3 h	24 h
Measurement time	60 s	300 s	0.5 h	3 h	24 h

RESULTS AND DISCUSSION

Tables 2 and 3 show the main detected elements for the Soil-7 and the A-13 samples for the irradiation, cooling and measurement cycles examined. In these tables the detected elements, the optimum cycle for the measurement, the reference concentration in the sample (C), the reactions, the product main gamma ray energy used for the analysis, as well as the Minimum Detection Limit (MDL) computed by the code are presented.

From Table 2, it can be seen that in the geological sample “Soil-7” Si, Ca, Cd, As, Ni and Sb can be detected in significantly low concentrations. Concerning Cd and As, that are toxic metals of particular analytical interest for environmental studies in soil and other geological samples, very low detection limits are achieved for cycles 4 and 5, respectively. Furthermore, by implementing cycle 5, the detection of Ni and Sb is possible with low detection limits, which is important especially for Sb, since it belongs to potentially hazardous trace metals. However, Si and Ca present quite high values of MDLs, indicating that the neutron activation technique under the parameters used in the present work is not proposed for analysis, unless quite large concentrations of Si and Ca (above 2440 ppm and 41300 ppm, respectively) are expected.

Table 2. Calculated results for the geological sample IAEA Soil 7

Cycle	Element	C (ppm)	Reactions	Energy (keV)	MDL (ppm)
1	Si	1.8E+05	$^{29}\text{Si}(\text{n},\text{p})^{29}\text{Al}$ (98.95%) + $^{30}\text{Si}(\text{n},\text{d})^{29}\text{Al}$ (1.05%)	1273.368	2.01E+03
2	Ca	1.63E+05	$^{48}\text{Ca}(\text{n},\text{g})^{49}\text{Ca}$	3084.4	2.44E+03
4	Ca	1.63E+05	$^{43}\text{Ca}(\text{n},\text{p})^{43}\text{K}$ (80.99%)+ $^{44}\text{Ca}(\text{n},\text{np})^{43}\text{K}$ (15.28%)+ $^{44}\text{Ca}(\text{n},\text{d})^{43}\text{K}$ (3.68%)+ $^{46}\text{Ca}(\text{n},\text{a})^{43}\text{Ar}(\text{B}-)^{43}\text{K}$ (0.05%)	396.861	4.13E+04
4	Cd	1.3E+00	$^{116}\text{Cd}(\text{n},\text{p})^{116}\text{Ag}(\text{B}-)^{116}\text{Cd}(\text{n},\text{a})^{113}\text{Pd}(\text{B}-)$ $^{113m}\text{Ag}(\text{IT})^{113}\text{Ag}$	298.6	1.96E-01
5	As	1.34E+01	$^{75}\text{As}(\text{n},2\text{n})^{74}\text{As}$	634.78	5.40E+00
5	Ni	2.6E+01	$^{58}\text{Ni}(\text{n},2\text{n})^{57}\text{Ni}$	1377.63	9.59E+00
5	Sb	1.7E+00	$^{123}\text{Sb}(\text{n},2\text{n})^{122}\text{Sb}$ (99.82%)+ $^{121}\text{Sb}(\text{n},\text{g})^{122}\text{Sb}$ (0.17%)+ $^{121}\text{Sb}(\text{n},\text{g})^{122m}\text{Sb}(\text{IT})^{122}\text{Sb}$ (0.01%)	564.24	6.51E-01

From Table 3, it can be seen that in the biological sample “A-13” P, K, Na, Ca, Fe, Mg and Zn can be detected. However, K has a quite high value of MDL (1390 ppm) and therefore,

under the parameters used in the present work, FNAA is not the optimum choice for its determination [4]. Concerning detection of Fe, cycle 3 provides the best option which also allows for the detection of Mg that is a trace element which plays a significant role in human health and disease, along with the Zn. The latter can be detected with a very low MDL by implementing cycle 5, which also makes possible the detection of Fe, Ca and Na.

Table 3. Calculated results for the biological sample IAEA A-13

Cycle	Element	C (ppm)	Chain	Energy (keV)	MDL (ppm)
1	P	9.40E+02	$^{31}\text{P}(\text{n},\text{a})^{28}\text{Al}$	1778.85	3.09E+01
2	K	2.50E+03	$^{41}\text{K}(\text{n},\text{a})^{38}\text{Cl}$ (74.67%) + $^{41}\text{K}(\text{n},\text{a})^{38m}\text{Cl}(\text{IT})^{38}\text{Cl}$ (25.33%)	2167.405	1.39E+03
3	Fe	2.40E+03	$^{56}\text{Fe}(\text{n},\text{p})^{56}\text{Mn}$ (99.78%) + $^{57}\text{Fe}(\text{n},\text{np})^{56}\text{Mn}$ (0.19%) + $^{57}\text{Fe}(\text{n},\text{d})^{56}\text{Mn}$ (0.02%)	846.754	1.69E+01
3	Mg	9.9E+01	$^{24}\text{Mg}(\text{n},\text{p})^{24m}\text{Na}$ (IT) ^{24}Na (B-) $^{24}\text{Mg}(\text{n},\text{p})^{24m}\text{Na}$ (IT) ^{24}Na	2754.028	1.33E-05
5	Ca	2.86E+02	$^{48}\text{Ca}(\text{n},2\text{n})^{57}\text{Ca}(\text{B}-)^{47}\text{Sc}$	159.381	4.08E+00
5	Fe	2.40E+03	$^{54}\text{Fe}(\text{n},\text{a})^{51}\text{Cr}$	320.082	2.54E+02
5	Na	1.26E+04	$^{23}\text{Na}(\text{n},2\text{n})^{22}\text{Na}$	1274.53	2.92E+01
5	Zn	1.3E+01	$^{66}\text{Zn}(\text{n},2\text{n})^{65}\text{Zn}$ (99.76%) + $^{64}\text{Zn}(\text{n},\text{g})^{65}\text{Zn}$ (0.24%)	1115.539	1.69E+00

CONCLUSIONS

The results of the study demonstrate the fast neutron analytical capabilities of the NCSR D Tandem accelerator for biomedical and geological studies. Although the reaction cross sections, neutron fluence rate and irradiation time achieved in a particle accelerator, such as the 5.5 MV Tandem at the NCSR D, do not allow the analytical sensitivities observed in a research nuclear reactor, certain elements with analytical importance can be detected using the (n,p), (n,α) or (n,2n) reactions induced by fast neutrons. Moreover, the employment of NAPRO code allows for the optimization of the FNAA parameters, while avoiding the performance of difficult and time-consuming experimental tests at the accelerator facility. Our future work will be aimed towards experimental verification of the results.

Acknowledgements

We acknowledge support of this work by the project “CALIBRA/EYIE” (MIS 5002799) which is implemented under the Action “Reinforcement of the Research and Innovation Infrastructure”, funded by the Operational Programme “Competitiveness, Entrepreneurship and Innovation” (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

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