Cross Sections of Gadolinium Isotopes in Neutron Transmission Simulated Experiments with Low Energy Neutrons up to 100 eV

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Abstract. The Gd nucleus is of interest in fundamental and applicative fields. This nucleus has many isotopes and from tables of resonance parameters it follows that many other undetermined parameters like neutron and gamma widths exist. By neutron capture many isotopes of this nucleus form also stable isotopes or pass into radionuclides which are difficult to observe by Instrumental Neutron Activation Analysis (INAA).

In this work a simulated neutron transmission experiment (NT) for the evaluation of the properties of some Gd isotopes was realized. A sample containing trace elements as natural Gd in a matrix with other heavy and medium nuclei and also some major elements like C, H, N is considered. For the sake of simplicity from each nucleus (trace or major elements) is considered just one resonance for incident neutrons energy range up to some hundreds of eV's. In the computer modeling the neutron and gamma spectra are obtained. From these spectra the concentration of trace elements including the Gd isotopes were extracted. It is shown that a succession of gamma and NT experiments can improve significantly the measurement of Gd isotopes concentration.

1. INTRODUCTION

The Gd nucleus is metal from the IIIrd group of Medeleev periodical Table of Elements and belongs to Lanthanides. This metal is important in applications in the field of modern nuclear energetic, electronics and others. In the process of neutron capture by Gd isotopes are produced mainly stable isotopes and two nuclides that are not suitable for INAA. From Table 1 results that Gd nucleus and its isotopes are a good neutrons absorber and therefore they can be used in NTE. The abundance data in Table 1 are from [1,2,3] and the capture cross section for thermal neutrons (E_n = 0.0253 eV) are from [4,5].

Table 1. Gd nucleus and its natural isotopes.

	Isotope	Abundance [%]	Cross Section [b]
1	nat Gd		49000±1000
2	^{152}Gd	0.20	1100±100
3	^{154}Gd	2.18	85±12
4	^{155}Gd	14.80	61000±500
5	^{156}Gd	20.47	1.5±1.2
6	^{157}Gd	15.65	254000±2000
7	^{158}Gd	24.84	2.5±0.5
8	^{160}Gd	21.86	0.77±0.02

For our first evaluations we have chosen the ^{160}Gd isotope. This isotope by neutron capture passes in ^{161}Gd with time of life $\tau = 3.7\ min$ which it turns in ^{161}Tb by β^- process [6]. The thermal capture cross section is low but for resonance neutrons we have chosen a resonance with a quit high capture cross section about one hundred barns. In the process of interaction of thermal and resonance neutrons with Gd isotopes only the scattering and capture channels can be considered in the calculations. Other channels like proton and alpha can be neglected because these channels have a very low value of the cross sections in comparison with scattering and capture processes.

2. THEORETICAL BACKGROUND

2.1. The Breit-Wigner Single Level Formula

In the capture process of the slow neutron by nucleus a compound nucleus with finite time of life, definite properties (like spin, parity and others) and described by quantum states or resonant states is formed. After a time much longer than the time necessary to neutron to pass the nucleus the compound nucleus is decaying on possible channels. If the resonant states are well defined and far away from each other (isolated) the cross section of emission of x particle from the compound nucleus can be described by single – level Breit – Wigner formula [7]:

$$\sigma_{nx}^{rez} = g\pi\lambda\!\!\!^{-2} \frac{\Gamma_n \Gamma_x}{(E - E_{rez})^2 + \frac{\Gamma_{tot}^2}{4}} \tag{1}$$

where $g = \frac{(2J+1)}{(2I+1)(2s+1)}$ J, I, s = spin of compound nucleus, target nucleus and neutron; $\lambda\!\!\!^{-} = \frac{\lambda}{2\pi}$ = reduced neutron wavelength; $\Gamma_n, \Gamma_x, \Gamma_{tot}$ = neutron, x-emitted particle and total widths; $\Gamma_{tot} = \Gamma_n + \Gamma_{n'} + \Gamma_\gamma + \Gamma_p + \Gamma_\alpha + \Gamma_d + ...$ = total width; E_S = resonance energy.

The widths necessary in (1) are taken from nuclear data table and they are extracted from measurements for a better description of experimental data. The neutron widths are in according with neutron resonance parameters and for other particles are used averaged widths [4,5,8].

2.2. Potential scattering

Potential scattering depends weak on energy and in our calculations we consider it constant according with the formula [7,8]:

$$\sigma_{scatt} = 4\pi R_i^2 \tag{3}$$

R_i = radius if i^{th} nucleus; $R_i = R_0 A^{1/3}$[fm], $R_0 = 1.45$ fm; A = nucleus atomic mass;

2.3. Neutrons transmission

NTE is an efficient method in neutron and nuclear physics for the evaluation of cross section, neutron widths, resonance energies, etc. In this method an incident neutron beam is

attenuated by passing trough a target and from the neutron spectra (which are not interacting) are extracted the above mentioned parameters. The emergent neutron intensity is [9]:

$$T = Exp\left[- \sum_{i=1}^{nr\_elem} n_i \sigma_{tot}^i \right],\ \sigma_{tot}^i = \sigma_{nx}^{rez,i} + \sigma_{scatt}^i \qquad (4)$$

where n_i = concentration of i-th element from the target [m^{-2}], σ_{tot}^i = total cross section of i-th element, *nr_elem* = number of elements from the target.

3. RESULTS AND DISCUSSIONS

For the simulated NT experiment a computer code was performed which consists of the following main parts: 1) Theoretical data generation 2) Experimental data generation 3) Least square method for data processing 4) Error evaluation of (pseudo) experimental data 5) Extraction of necessary information 6) Graphic representation section with export option on ACII files for other graphical tools.

Theoretical data simulation is based on the main formulas presented in the theoretical background paragraph. Starting from simulated theoretical data we have generated the (pseudo) experimental data. It is supposed that every value of experimental data is obeying to the Gauss law. In this case the simulated experimental values have the expression:

$$x_{sim} = x_{theor} - s\sqrt{2}InverseErf[0,1-2r] \qquad (4)$$

where x_{sim} = simulated data; x_{theor} = theoretical data; s = standard error; r $\in$ [0,1) random number.

In the computer experiment a sample containing six trace elements and three major elements was considered. These elements and some of their properties of the interest in the simulation are shown in Table 2. The trace element with number 6, the ^{160}Gd nucleus is the searched element.

The major elements in the target have resonances very far from the energy range of incident neutrons (up to 1 keV) so therefore they will contribute to the cross sections only by potential scattering and their contribution act like a background. For the sake of simplicity from each element just one resonance was taken into evaluation.

In a previous work we have simulated a NT experiment with the main purpose to obtain the concentration of ^{160}Gd together with all other trace elements. Initially in the simulation process it was considered that the concentrations of trace elements are with three orders of magnitude lower than those indicated in Table 2. The concentrations of the all 6 trace elements were obtained just in the case of a very long time of measurement which is not corresponding with the real case. Further we have increased the concentrations at the levels indicated in the Table 2. In this case the concentration of ^{160}Gd isotope was obtained with a good precision. The results are presented in Table 3.

Table 2. The trace and major elements in the target

Trace elements				
	Element	**Resonance (eV)**	**Conc. (m^{-3})**	**$\sigma_{n\gamma}$[b]**
1	$^{95}_{42}Mo$	44.7	$1.26 \cdot 10^{23}$	8448.16
2	$^{64}_{28}Ni$	14300	$1.40 \cdot 10^{23}$	0.0476
3	$^{54}_{26}Fe$	7760	$6.65 \cdot 10^{23}$	0.834
4	$^{35}_{17}Cl$	-180	$1.71 \cdot 10^{24}$	-
5	$^{87}_{38}Sr$	3.54	$3.54 \cdot 10^{23}$	1143
6	$^{160}_{64}Gd$	**904.6**	**$2.99 \cdot 10^{23}$**	**83**
Major elements				
7	$^{12}_{6}C$	-2020000	$1.50 \cdot 10^{27}$	0
8	$^{16}_{8}O$	2351000	$1.12 \cdot 10^{27}$	0
9	$^{14}_{7}N$	997000	$1.12 \cdot 10^{27}$	0

Table 3. 3th column – initial concentrations. 4th column – extracted concentrations by NTE

	Element	**Conc. (m^{-3})**	**Extracted conc [m^{-3}]**
1	$^{95}_{42}Mo$	$1.26 \cdot 10^{23}$	$1.14 \cdot 10^{23} \pm 3.16 \cdot 10^{22}$
2	$^{64}_{28}Ni$	$1.40 \cdot 10^{23}$	$1.07 \cdot 10^{23} \pm 1.61 \cdot 10^{22}$
3	$^{54}_{26}Fe$	$6.65 \cdot 10^{23}$	$6.46 \cdot 10^{23} \pm 1.25 \cdot 10^{22}$
4	$^{35}_{17}Cl$	$1.71 \cdot 10^{24}$	$2.42 \cdot 10^{24} \pm 3.16 \cdot 10^{24}$
5	$^{87}_{38}Sr$	$3.54 \cdot 10^{23}$	$5.32 \cdot 10^{23} \pm 8.04 \cdot 10^{23}$
6	$^{160}_{64}Gd$	**$2.99 \cdot 10^{23}$**	**$3.02 \cdot 10^{23} \pm 2.31 \cdot 10^{22}$**

The (pseudo) experimental data were generated with a relative error of 1% according with relation (4), using initial concentrations from third column of Table 3 and data from Table 2. The extracted concentrations were obtained by least square method and are in the fourth column of Table 3. As shown the concentration of ^{160}Gd was obtained with a convenient precision. The concentration of ^{35}Cl nucleus was not obtained satisfactorily. In the evaluation for this nucleus in the simulation it was considered just one so-called negative resonance which means that the concentration can be extracted only by fitting the low energy part of the spectra where the law *1/v* is working. In this part of spectra the background given by the potential scattering of major elements or the values of resonance capture cross section of other elements can influence significantly the obtained results. One test with the initial relative error of simulated data lower than 0.1% gives a good value of 10% error for ^{35}Cl and about 1% for ^{160}Gd nucleus. But this test is a very time consuming and this is leading to a long time of measurements.

The results from the fourth column of Table 3 are more or less expectable and confirmed by some preliminary measurements on other nuclei. Further we try to show how it is possible to improve the results on concentrations of trace elements.

Table 4. Initial concentrations of first trace elements

	Element	Conc. (m^{-3})
1	$^{95}_{42}Mo$	$1.26 \cdot 10^{21}$
2	$^{64}_{28}Ni$	$1.40 \cdot 10^{21}$
3	$^{54}_{26}Fe$	$6.65 \cdot 10^{21}$
4	$^{35}_{17}Cl$	$1.71 \cdot 10^{22}$
5	$^{87}_{38}Sr$	$3.54 \cdot 10^{21}$

Table 5. Obtained concentration of ^{160}Gd by simulated NTE. Initial concentration - 3th column. 2nd column – different relative errors for NTE

	NT rel. err.	Conc [m^{-3}]	Extracted conc [m^{-3}]
1	0.01	$2.99 \cdot 10^{21}$	$2.22 \cdot 10^{21} \pm 4.41 \cdot 10^{21}$
2	0.005	$2.99 \cdot 10^{21}$	$2.48 \cdot 10^{21} \pm 4.43 \cdot 10^{20}$
3	0.001	$2.99 \cdot 10^{21}$	$2.75 \cdot 10^{21} \pm 4.39 \cdot 10^{20}$

The first five trace elements in principle could be extracted with the help of other method. We have chosen to measure the gamma spectra obtained in a NT setup. In this case the concentrations of the first five elements are in Table 4 and they are with three orders of magnitude lower than in the case of Table 2 and 3. Later we generated the gamma spectra with an error of 10%. From generated gamma spectra the concentrations of the first five elements were obtained with a relative error about of 10%. The obtained data of concentrations of the first five elements are used in the generation of NTE necessary for the extraction of ^{160}Gd which is also initially with three orders of magnitude lower than in Table 2 and 3. Because the scattering resonance cross section of ^{160}Gd is about of 80 b (very low in comparison of some others trace elements) it was necessary to test different relative errors of NT generated data. The results are shown in the fourth column of Table 5. We consider them as very good taking into account the initial level of trace elements concentrations.

4. CONCLUSIONS

The simulated experiment presented in this paper has demonstrated in principle the possibility to evidence the presence of Gd nucleus and its isotopes in different samples by NT experiments. It was chosen the ^{160}Gd isotope which is situated in a sample with other five trace elements and three major elements. This isotope of Gd has a small capture cross section for thermal neutrons and a relative high value of resonance neutron scattering in comparison with other elements in the sample.

In the simulations mainly two cases were tested. In the first case the concentrations of trace elements can be extracted by a simple NT measurement if the trace elements have their concentrations with three orders of magnitude lower than major elements. These results can be explained by the values of the cross sections and concentrations introduced in the evaluations. Relative to ^{160}Gd we can say that the relative low value of resonant capture cross section in comparison with other elements, the background induced mainly by major elements

have influenced the possibility to extract the concentration of this isotope with an order of 10^{-3} in comparison with major elements in a NT measurement.

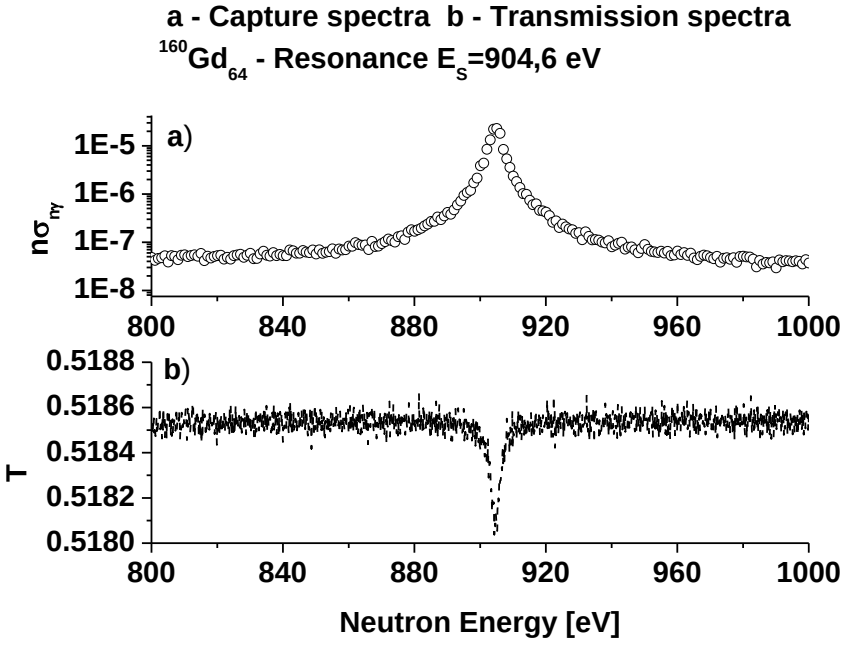

Figure 1. Generated a) gamma spectra and b) NT spectra for ^{160}Gd at the resonance E_S = *904.6* eV

In order to improve the extraction of the concentration of ^{160}Gd it was proposed a second way as follows. In the second test by a simulation of gamma spectra of the first 5 trace elements from Table 4 their concentrations were obtained. The concentrations of these elements determined above were introduced in a new NTE experiment on ^{160}Gd. It is observed that the value of extracted concentration was significantly improved. This can be explained by the fact that the resonances from Table 1 are well separated and far one from which other. By gamma measurements practically the influence of background coming from major elements is much reduced and the concentrations of first five elements are extracted quit well which was very useful in the NTE experiment on ^{160}Gd. As we have noted above the first five trace elements from Table 1 can be obtained by the help of other methods as well.

Another isotope that will be tested in the future is ^{155}Gd isotope. This isotope has about the same abundance like ^{160}Gd but has much greater capture cross section for thermal neutrons which could be used in NTE.

Some improvements: (1) one of them is to take into consideration more resonances from each element; (2) The flux of neutron source was considered constant in the present work; then another improvement is to introduce a non constant neutron flux; (3) In Table 1 the resonance are well separated and therefore will also it will be interesting to analyze how will influence the measurement of the Gd concentration by NTE when the resonances will overlap in more or less degree.

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