Proposal of a new method for determination of light nuclei using low energy neutrons

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Abstract

A new neutron activation method that utilizes a suite of nuclear neutron reactions for the determination of the presence of a light nuclei (as Be, Li, B, F, etc.) via their radioisotopic indicators is shown to give a good selectivity of the measured product radioisotopes in the presence of interferences that overload the spectra recorded by the use of a GeLi detector. Firstly by activation methods the concentrations of medium and heavy nuclei were evaluated.

Then it is necessary to evaluate the concentration of the main elements in the matrix sample. For example for biological samples the matrix of main elements are *C, O, N* and these elements also can not be determined by neutron activation methods due to the small values of thermal neutron capture cross section. The nest step is to obtain the neutron spectra obtained in a transmission experiment using the analyzed sample. From the transmission spectra the contribution of main elements from sample matrix and of medium and heavy nuclei is extracted.

In this work was realized a Monte-Carlo simulation for the evaluation of a light element cross-section (for example, ^{6}Li) in a sample of known matrix composition with the possibility to extend this method to other light nuclei. The proposal of experiment described in this work is intended for IREN, the new neutron source of FLNP – JINR Dubna.

Introduction

The presence in medium and heavy nuclei of resonance states in case of their interaction with low energy neutrons makes possible the determination the cross section and other physical parameters with a good precision by neutron activation methods. In thermal and epithermal region supposing that the resonances are well distinguished (not overlapping, isolated, far one from each other) then the cross section has the following (Breit-Wigner) form [1]:

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

$$g = \frac{(2J+1)}{(2I+1)(2s+1)}$$

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

$\Gamma_{tot} = \Gamma_n + \Gamma_{n'} + \Gamma_\gamma + \Gamma_p + \Gamma_\alpha + \Gamma_d + \Gamma_t + \Gamma_{He^3} + \Gamma_f + \ldots$ = total width

$x = n, n', p, d, t, He^3, \alpha, f$ + other nuclear clusters, E_S = resonance energy

For a better description and comparison of cross sections with experimental data generally the neutron resonance parameters and widths from [2] are used because they usually are obtained experimentally.

For light nuclei relation (1) is also valuable but the resonance appears in the region of hundred of *keV's* and this fact makes very difficult the evaluation of cross section by neutron activation method in this region due to the overlapping of resonance from others elements from samples. Therefore in this work we will use a combination between NAA and neutron transmission experiments (NTE) for evaluation of cross sections and other parameters of light nuclei. By NAA methods we extract the necessary data for medium and heavy nuclei. These data will be used in neutron transmission experiments in order to obtain new data for light nuclei.

In NTE the attenuation of neutrons beam is measured by passing trough a target (or sample). The NTE is a very powerful and efficient way for evaluation of cross sections, widths, concentrations and various effects (like parity violation) for a wide range of nuclei [3]. In the presence of one nucleus in the target the neutron transmission can be written as:

$$T = \frac{N}{N_0} = \exp\left(-n\sigma_{tot}\right) \tag{2}$$

N, N_0 = the number of neutron counts in the presence of the target and in the absence of the target, respectively

n = the thickness of the target in number of nuclei per cm^2

σ_{tot} = total cross section.

Simulated computer experiment

Let us consider a sample containing five medium and heavy elements with very well expressed *S* resonance in thermal and epithermal region and only a light nucleus as ^6Li. The ^6Li nucleus has a high value of (n, α) cross section for thermal neutrons ($E_{th} = 0.0253\ eV$) and a low value of capture cross section at the same energy and no resonance until *252 keV* where we can find a *P* resonance [2].

$$\begin{aligned} \sigma_{n\alpha}\left(E_{th}\right) &= \left(940 \pm 4\right) b \\ \sigma_{n\gamma}\left(E_{th}\right) &= \left(0.0385 \pm 0.003\right) b \end{aligned} \tag{3}$$

In order to explain the high value of thermal (n, α) cross section it was introduced a so called negative *S* resonance with energy $E_P = -808\ keV$. But the evaluation of the cross section according with formula (1) and parameters from [2] gives still a cross section two times smaller with a value about *400 b*. The very small value of capture cross section and the absence of any resonance make impossible the detection of ^6Li nucleus by NAA.

For other five medium and heavy elements we have taken into consideration only one *S* resonance for neutron capture (to simplify the simulation). Other reaction channels are considered also but for resonant interaction the main contribution is given by neutron captures. The expression of (n,x) cross section is given in (1) and the neutron width has the form proposed in [4].

$$\Gamma_n^S\left(E_n[eV]\right) = \Gamma_{n0}^S\sqrt{E[eV]} \tag{4}$$

In spite of the fact that the ^6Li nucleus has no resonance in wide energy range, the very high value of *(n, α)* cross section in comparison with other open channels makes possible its detection in other type of measurements like NTE. In the introduction we have mentioned the expression of intensity of transmitted neutrons [2] and the cases of samples containing many elements the transmission is:

$$T = Exp\left[-\sum_{i=1}^{nr\_elem} n_i\sigma_{tot}^i\right] \tag{5}$$

n_i = concentration of i^{th} element [m^{-2}], σ_{tot}^i = total cross section of i^{th} element
nr_elem = number of elements in the sample

$$\sigma_{tot}^i = \sigma_{rez}^i + \sigma_{pot}^i = \sum_x g_{S_i}\pi\lambda^2 \frac{\Gamma_n^{S_i}\Gamma_x^{S_i}}{\left(E - E_{S_i}\right)^2 + \left(\frac{\Gamma_{tot}^{S_i}}{2}\right)^2} + 4\pi R_i^2 \tag{6}$$

with $R_i = 1.45 \cdot A_i^{\frac{1}{3}}\,[fm]$, R_i, A_i = radius and mass number of i^{th} nucleus.

For potential interaction - the second term in (6), we took into account only neutron elastic scattering with most simple form; in a real experiment this interaction can be more complicated. Cross section of potential scattering is constant with energy and has a value of order of *10 b*. In NTE the potential scattering acts like a background and by different methods (using filters for example) it can be eliminated.

In the simulated experiment first we have modeled the NAA experiment and by χ^2 square methods we obtained the cross sections with their weights of each heavy and medium nucleus. The error of determination is about *10%* . These data are used in the simulation of NTE with a sample with a length of centimeters on each dimension.

The (simulated) experimental data (for both NAA and NTE experiments) were obtained using (5) and (6) relations with a standard error distributed according to Gauss law. From NTE data we have extracted first the concentration of ^6Li nucleus from the sample and after the reduced neutron width. The concentration of elements was taken of order of units or a few tens of *ppm* or translated this value in m^{-2} means that the elements are of order of $10^{22} - 10^{23}$ m^{-2}.

The main elements of sample matrix are not included in our simulation because they can be obtained by other methods with high precision and their concentration is higher than *80 - 90%*.

Their influence on measurements or computer simulation experiments can be important if they will interfere in a way or another with the studied element (or elements).

The computer codes were realized in Mathematica software package and contain the following main parts:

1. Theoretical data simulation;
2. Simulated experimental data for NAA and NTE (based on relations (1-6));
3. Least square methods for both type of experiments;
4. Error evaluation of simulated experimental data;
5. Extraction of necessary information;
6. Graphic representation section with export option on ACII files for other graphical tools.

Results and discussions

In the computer simulation about 6 elements were used. One nucleus and ^{6}Li nucleus (number 5 and 6 respectively in our simulation) present both of them a negative S resonance. This means that in the capture spectra these resonances are not visible (see Fig 1a, 1b). Element 5 has a high value of capture cross section for thermal neutrons of order of *40 b*. The capture cross section of ^{6}Li nucleus is very low (3) and therefore practically will not influence the capture spectra. Supposing that in real measurements we know these, in principal, by analyzing and fitting the tail of spectra for thermal and epithermal neutrons we can evaluate the contribution of the capture process for element 5. This evaluation is important and useful for the analysis and spectra processing of neutrons transmission measurements.

From capture spectra were obtained the capture cross section with a relative error about *10-15%*. Then capture data were introduced in the expression of transmitted neutrons. First we have determined the concentration of ^{6}Li nucleus. Theoretical data for this concentration were:

$$n_{^{6}Li} = 5.33 \cdot 10^{22} m^{-2} \tag{7}$$

The neutron transmission spectra of simulated experimental data are in Fig 1c), 1d). Taking into consideration *1024* simulated experimental points in a wide energy interval (up to *16 keV*) for incident neutrons it was obtained by χ^{2} - square procedure the value:

$$n^{fit}_{^{6}Li} = (5.55 \pm 0.83) \cdot 10^{22} m^{-2} \text{ with relative error } \varepsilon = 0.15 \tag{8}$$

Another interesting task could be the evaluation of reduced neutron widths for ^{6}Li nucleus for the negative *S* resonance with energy E_S = *-808 keV*. In the atlas for neutrons resonance parameters [2] the reduced neutron widths for mentioned *S* resonance has the value:

$$\Gamma_{n0} = 295 eV \tag{9}$$

As in the above previous simulation let's consider *1024* simulated experimental data and also a wide energy range for incident neutrons up to *16 keV*. The concentration of the all six elements was chosen of order of 10^{27} m^{-2}. Then for reduced neutron widths it was extracted the following value:

$$\Gamma_{n0}^{fit} = 290.72 \pm 67.71\ eV \text{ with relative error } \varepsilon = 0.23 \qquad (10)$$

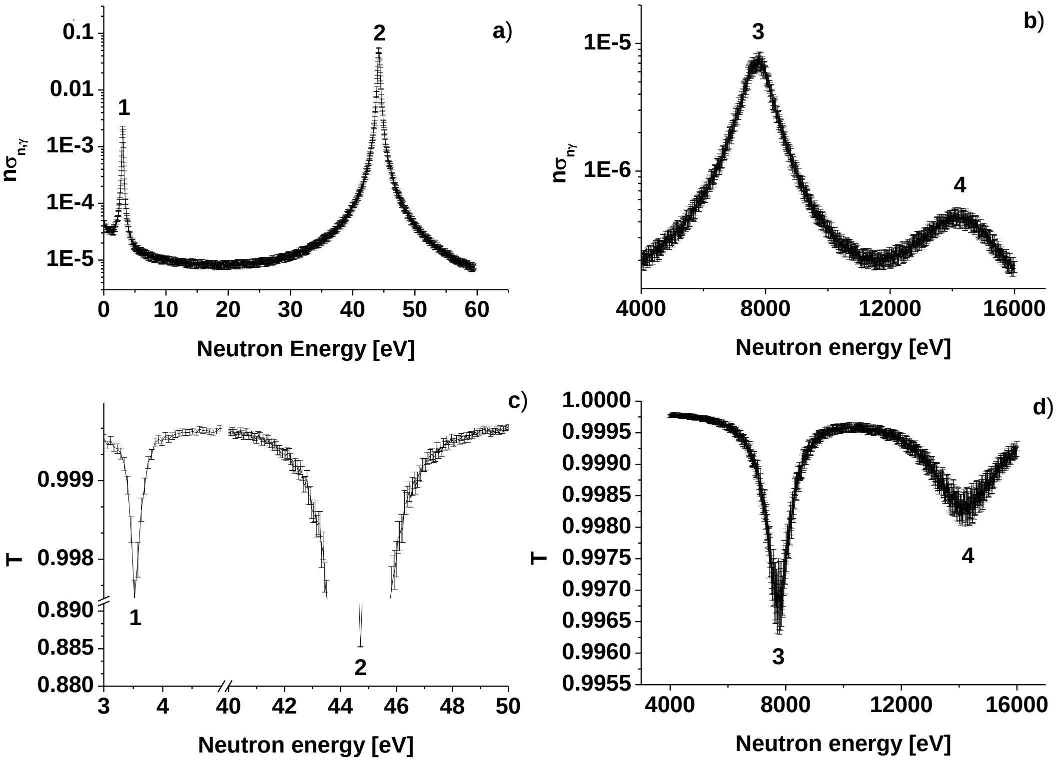

Fig. 1. Simulated experimental data. Capture spectra a), b). Transmission spectra c), d)

The values (8), (10) can be improved by adding more experimental points or by choosing the appropriate region for analysis. The concentration of the elements acts practically in the all range of spectra but here also it is better to process the spectra in the resonance region. In the case of reduced neutron width its influence is important up to some *keV* in the best case. Consequently it is better to analyze only this range but we should to have in mind that reducing the range we loose experimental data and consequently the precision of measurements.

Taking into account all the above evaluations we can conclude that for both parameters the relative error of measurement is well improved and its magnitude decreases less than *0.1*.

Conclusions

The experimental evaluation of element concentration from different types of analytical samples is important for applicative researches. The knowledge of neutron widths is necessary for fundamental and applicative researches.

We have proposed a new method of parameters evaluation for light nuclei by a combination of NAA and NTE and in this work we applied this procedure in particular for the ^{6}Li nucleus. Our computer simulated experiment has demonstrated the possibility of measurements of the above mentioned parameters. The work is still in the beginning and it is necessary to try this simulation with a higher number of elements. In the present work the heavy and medium elements were taken with high values of capture cross section in comparison with alpha particle emission and this fact allowed to extracting the neutron width from the tail of neutron spectra from thermal region where the influence of negative resonances is important.

For all elements we considered only the first *S* resonance. In the future it will be of interest to take into account more elements with few resonances for each element. It could be possible that the interference between resonances of each element together with the overlapping of the resonances from different elements complicate the analysis.

Other aspects which should to be introduced later are the energy dependence of the intensity of incident neutrons and effect of the widths enlargement due to the temperature [3]. In our work the neutron intensity was considered unity and the temperature effects were not introduced here.

Measurements and evaluations of different parameters for light nuclei are of a great interest and in the present work we have analyzed the case of ^{6}Li nucleus. It is obvious that for other light nucleus or nuclei the approach will be modified more or less and this depends directly by the properties (cross sections mainly) of nuclei which enter in the composition of the analyzed samples.

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