Numerical evaluation of light nuclei cross-sections by new neutron activation method

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The problem

It is obvious necessary to establish the elemental abundance data of light nuclei since their applications in astrophysics, material and solid state physics as well as in life sciences.

It is well known that for light nuclei, with some exceptions, the capture cross-sections for thermal neutrons are very low and therefore their determination is not possible only by the use of one method and then it is better to combine a few complementary neutron methods, including activation, depending on the value of the cross-section for different types of reactions.

The presence of resonance states in medium and heavy nuclei in case of their interaction with thermal neutrons makes possible the determination of their concentration with a good precision by neutron activation methods. For light nuclei the situation is changing because the first resonant states occur from tens or hundred keV and therefore to obtain the concentration using activation methods become very difficult because the capture cross- section is very small. An example which will be analyzed in this work is ^{6}Li nucleus. The ^{6}Li nucleus has the capture cross section of thermal neutron $\sigma_{n\gamma} = (0.0385 \pm 0.003)\ b$ and this value is much lower than the (n,α) cross section at the same energy $\sigma_{n\alpha} = (940 \pm 4)\ b$. For these reasons we developed a combined method of capture by (n,γ) and (n,α) reactions and transmission experiment with thermal neutrons for determination of the presence of trace light elements.

- Introduction
- Neutron Activation Analysis
- Neutron Transmission Experiment
- Simulated Computer Experiment
- Results
- Conclusions

INTRODUCTION

Presence of light nuclei in different types of samples is not possible to determine by usual NAA methods

NAA method is applicable to heavy and medium nuclei where a compound nucleus described by states with defined quantum numbers and resonance properties with finite time of life by interaction with thermal and resonant neutrons is formed

NAA methods – based on neutron capture (n,γ) and the presence of resonant states

Light nuclei – first resonances occur for incident neutrons of tens keV - hundred keV therefore the usual NAA methods are not applicable

It is necessary to use other properties and/or nuclear reactions

Neutron classification

Neutrons	**Energy, E_n, eV**
Thermal	<0.025
Epithermal	~0.2
Cadmium	~0.4
Epicadmium	~0.6
Slow	1-10
Rezonant	1-300
Medium	500 – 0.5 X 10^6
Fast	0.5 X 10^6 - 20 X 10^6
Very fast	>20 X 10^6

INTRODUCTION. ^{6}Li nucleus

The ^6Li nucleus is important in various field of activity such as medicine, biology, electronics, nuclear weapons, and therefore it is of interest to measure the concentration, cross section, widths and other parameters of this nucleus in different industrial, biological and environmental samples.

Resonances of ^{6}Li

E_S = *-808 keV*, J_S^+ *=1/2* (*s* neutrons , *l=0*)

E_P = *248 keV*, J_P^- *=5/2* (*p* neutrons , *l=1*)

Experimental cross sections

Thermal neutrons – E_n^{th} = *0.0253 eV*

Neutron velocity ~ *2200 m/s*

– ***very high value of thermal (n,α) cross section***

$\sigma_{n\alpha}(0.0253\ eV) = (940 \pm 4)\ b$

– ***very low value of thermal (n,γ) cross section***

$\sigma_{n\gamma}(0.0253\ eV) = (0.0385 \pm 0.003)\ b$

Cross sections for E_P resonance

theoretical evaluation

$\sigma_{n\alpha}(E_P)$ ≈ *140000 b*

$\sigma_{n\gamma}(E_P)$ ≈ *0.7 b*

The property $\sigma_{n\alpha} >> \sigma_{n\gamma}$ for *the evaluation of the cross section, concentration, widths as well as of the other parameters* of ^{6}Li nucleus *w*ill be further used.

***Presence of** medium and heavy nuclei can be evidenced by the capture of thermal and resonant neutrons*

- Cross section in the case of well distinguished resonances

(single) Breit – Wigner formula

Neutron capture

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

(n,x) cross section

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

where

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

$\Gamma_n, \Gamma_x, \Gamma_{tot} =$ 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

$\lambda\!\!\!^{-} = \frac{\lambda}{2\pi} =$ reduced neutron wavelength

J, I, s = spin of compound nucleus, target nucleus and neutron

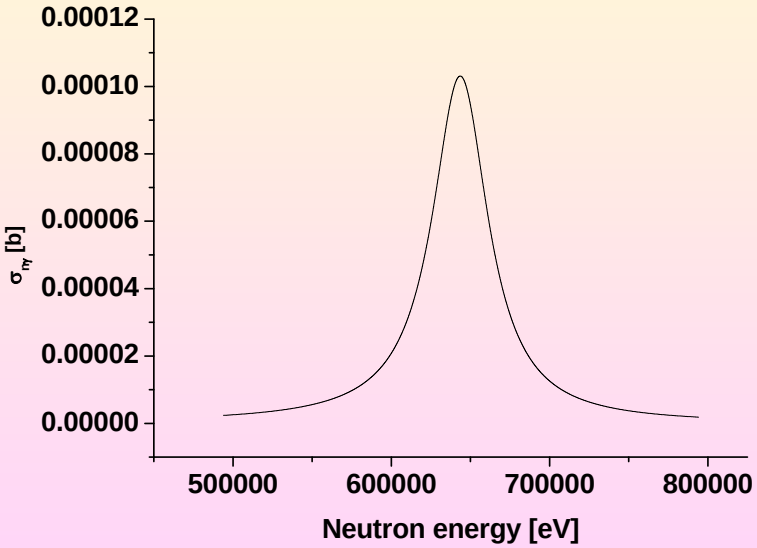
x = n, n', p, d, t, ^{3}He, α, f + other nuclear clusters, E_{rez} = resonance energy

For a better description of experimental data neutron resonance parameters are used

s-neutron widths (l=0)

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

Examples - Large resonance



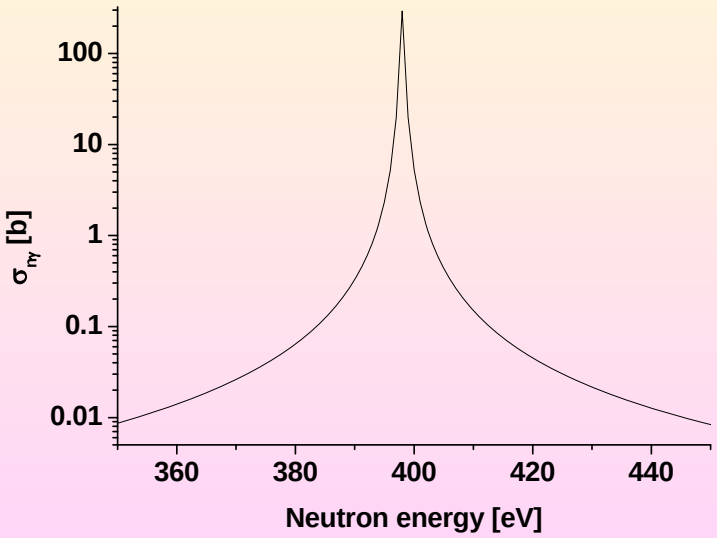
S resonance E_S = 644 keV

$^{14}N(n,\gamma)^{15}N$ reaction

p-neutron widths (l=1)

$$\Gamma_n^P(E_n[eV]) = \Gamma_{n0}^S P_1(E_n[eV]) \sqrt{E[eV]}$$

Thin resonance (suppressed by P_1 factor)



P resonance E_P = 398 eV

$^{35}Cl(n,\gamma)^{36}Cl$ reaction

For many resonances with no interference effects $\sigma_{n\gamma} = \sum_r \sigma_{n\gamma}^r$

Neutron beam pass trough a sample (thickness ~ cm) containing few elements

Transmission of neutrons

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

n_i = concentration of ith element [m^{-2}],

nr_elem = number of elements in the sample

σ_{tot}^{i} = total cross section of ith element

Potential scattering (n,n)

$$\sigma_{tot}^{i} = \sigma_{rez}^{i} + \sigma_{pot}^{i} + \sigma_{rez+pot}^{i-\text{interf}} = \sum_{x} g_{S_i} \pi \lambda\!\!\!^{-2} \frac{\Gamma_n^{S_i}\Gamma_x^{S_i}}{\left(E - E_{S_{ix}}\right)^2 + \left(\frac{\Gamma_{tot}^{S_{ix}}}{2}\right)^2} + 4\pi R_x^2 + \frac{4\pi g_S \lambda\!\!\!^{-} \Gamma_n^{S_{ix}} R_i \left(E - E_{S_{ix}}\right)}{\left(E - E_{S_{ix}}\right)^2 + \left(\frac{\Gamma_{tot}^{S_{ix}}}{2}\right)^2}$$

x – type of emitted particle
(x – n, p, α, t, …)

Interference between potential and resonant scattering (n,n)

$$R_i = 1.45 \cdot A_i^{\frac{1}{3}} [fm]$$

A_i = *Radius of nucleus i*

^{6}Li case

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

The (simulated) experimental data (for both NAA and NT experiments) were obtained using mentioned before relations with a standard error distributed according to Gauss law.

From NT experiment data we have extracted firstly the concentration of ^{6}Li 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 $10^{22} – 10^{23}\ m^{-2}$.

NAA = Neutron Activation Analysis
NT = Neutron Transmission

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 NT experiments

3. Least square methods for both types of experiments

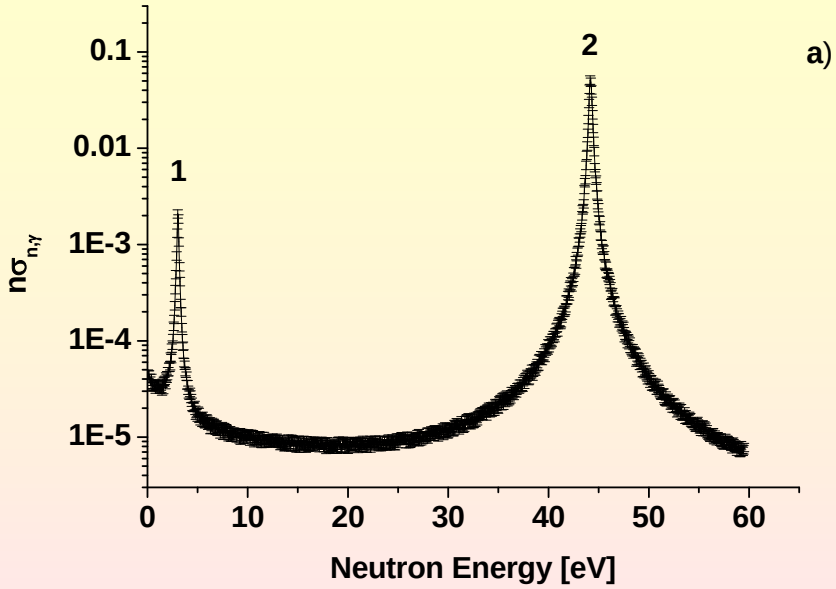
4. Error evaluation of simulated experimental data

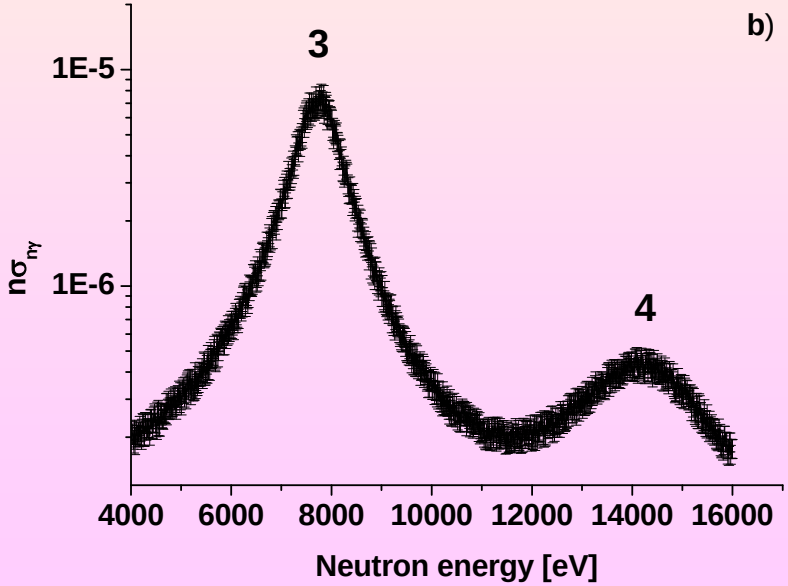
5. Extraction of necessary information

6. Graphic representation section with export option on ACII files for other graphical tools.

RESULTS. NAA simulated spectra

- 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
- 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 and therefore practically will not influence the capture spectra
- Supposing that in real measurements we know these, in principal, by analyzing and fitting the neutron spectra we can evaluate the contribution of the capture process for element 5
-This evaluation is useful for the analysis and spectra processing of NT experiment (NTE)





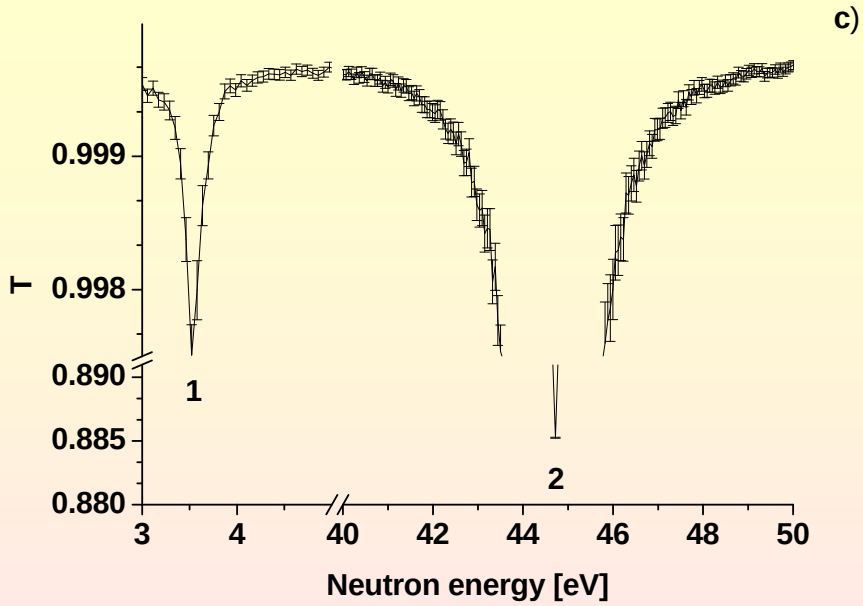
RESULTS. NTE simulated spectra

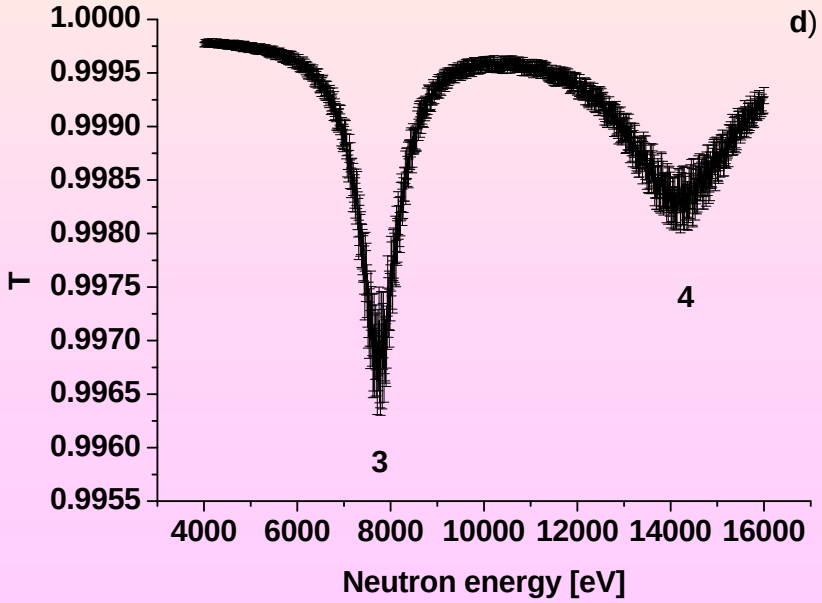
- From capture spectra the capture cross sections with a relative error of about *10-15%* were obtained

- Then capture data were introduced in the expression of transmitted neutrons

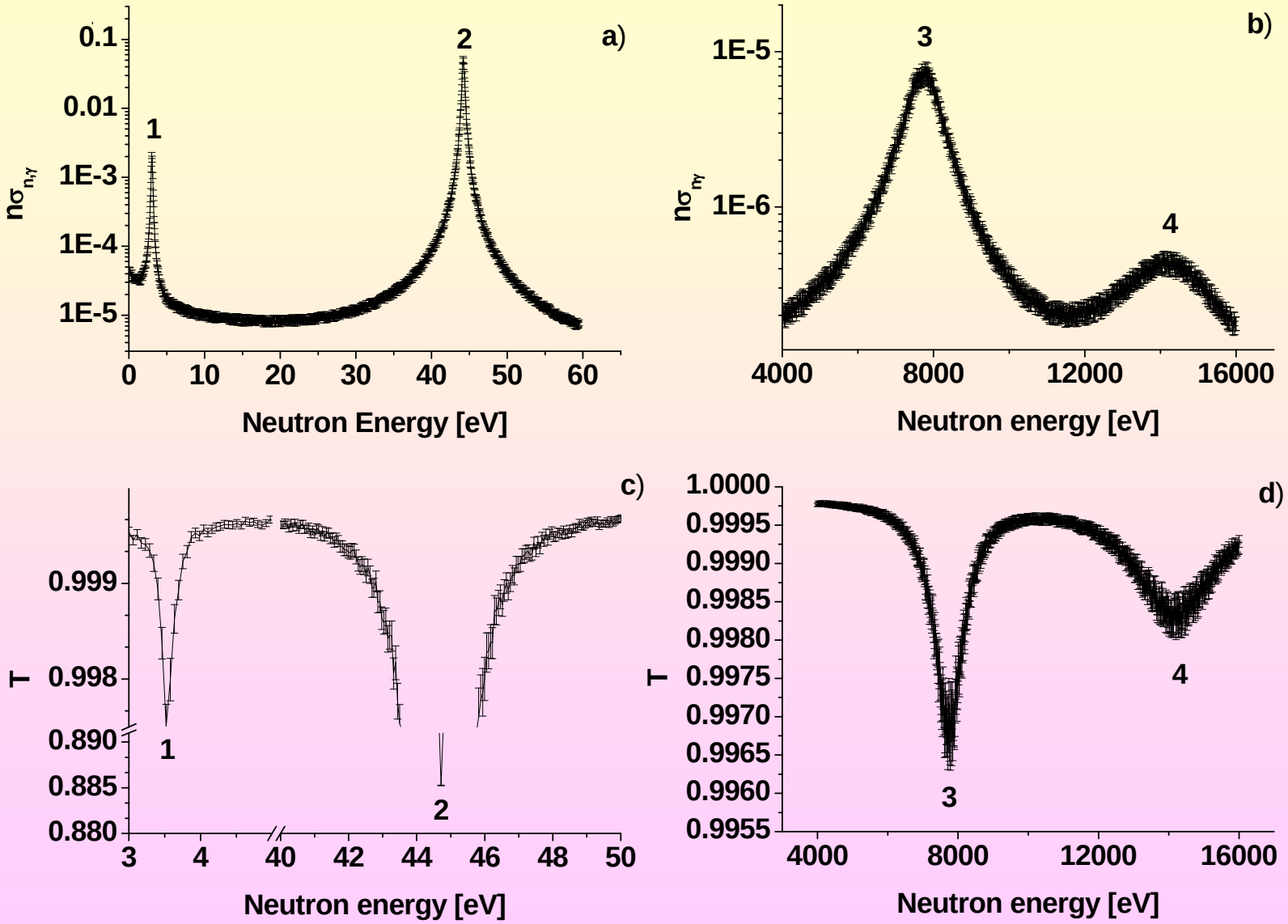
-The neutron transmission spectra of simulated experimental data are in Figs 1c), 1d)

- *1024* simulated experimental points were under consideration in a wide energy interval (up to *16 keV*) for incident neutrons





RESULTS. All NTE simulated spectra



1. Concentration

Theoretical data for concentrations were chosen. For ^{6}Li it was:

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

After the procedure of obtaining of the computer simulated experimental data (1024)
- by fitting the NTE simulated spectra we obtain

$$n_{^6Li}^{fit} = (5.55 \pm 0.83) \cdot 10^{22} m^{-2}$$ with relative error $\varepsilon = 0.10$

2. Reduced neutron width

Theoretical data for neutron width were chosen from neutron resonance parameters atlas

- It is important for nuclear data, cross section evaluation, etc

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

After the procedure of obtaining of the computer simulated experimental data (1024)
- by fitting the NTE simulated spectra we obtain

$$\Gamma_{n0}^{fit} = (290.72 \pm 67.71) eV$$ with relative error $\varepsilon = 0.13$

RESULTS. Another case. ^{10}B nucleus

^{10}B nucleus is in some way similar with ^{6}Li – both nuclei have a very high value of (n,α) cross section

$$\sigma_{n\alpha}(E_n = 0.0253eV) = (3837 \pm 9)b$$

^{10}B nucleus is also important for fundamental and applicative researches

^{10}B nucleus has many resonances in comparison with ^{6}Li nucleus
The main contribution to cross section (n,α) are given by two neutron resonances

$E_S = (-947 \pm 6)keV$ and $E_S = 170.6keV$

For simplicity in our calculations we have taken into account only the “positive” S-resonance

The incident neutron energy in our simulation is up to 16 keV – far from 170.6 keV

The NTE spectra “feel” the influence of this resonance in thermal region

RESULTS. NAA simulated spectra. ^{10}B nucleus

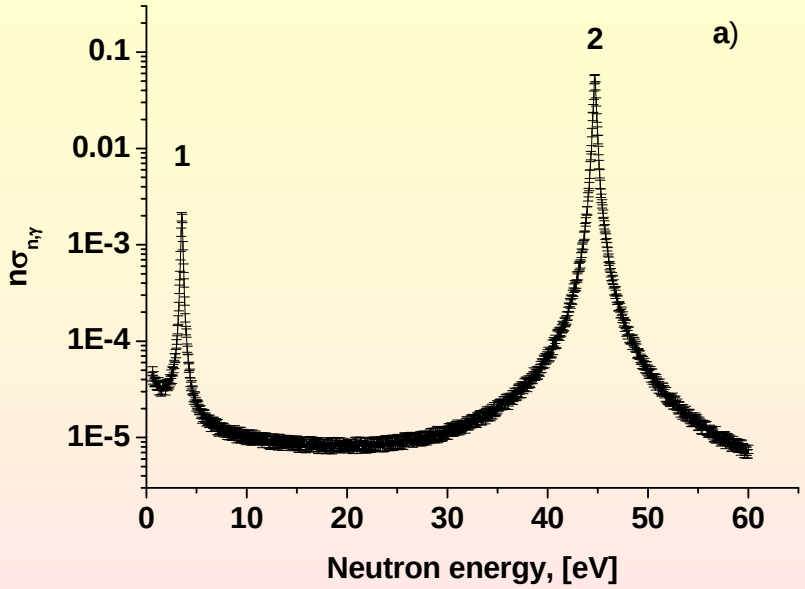
In the case of ^{10}B nucleus in the computer simulation we take also 5 elements – the same 5 as in the case of ^{6}Li nucleus

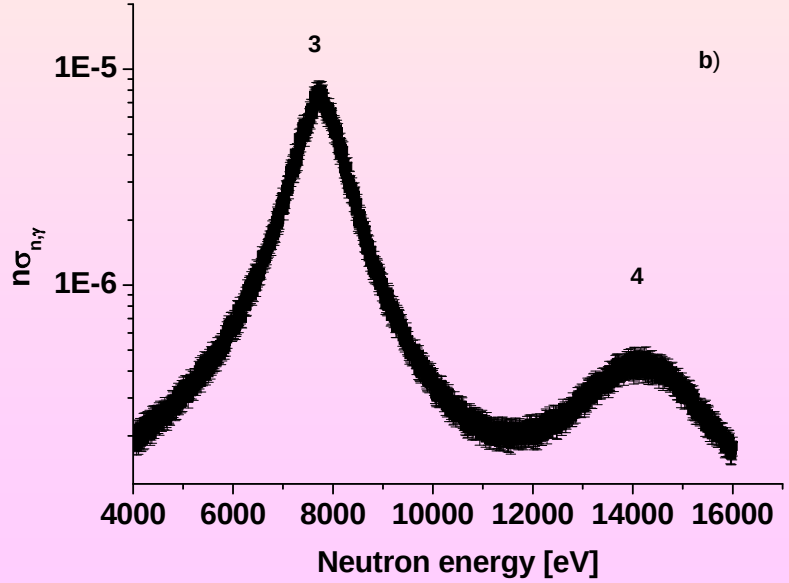
The resonance of ^{10}B is not represented in this figure because is in the 100 keV region

These spectra are obtained/ simulated and they are further used in NTE experiments in the calculation of the transmission data

^{10}B nucleus has a very low value of capture cross section

^{10}B has a low influence on capture spectra





RESULTS. NTE simulated spectra. ^{10}B nucleus

- From capture spectra the elemental concentrations with a relative error about *10-15%* were obtained

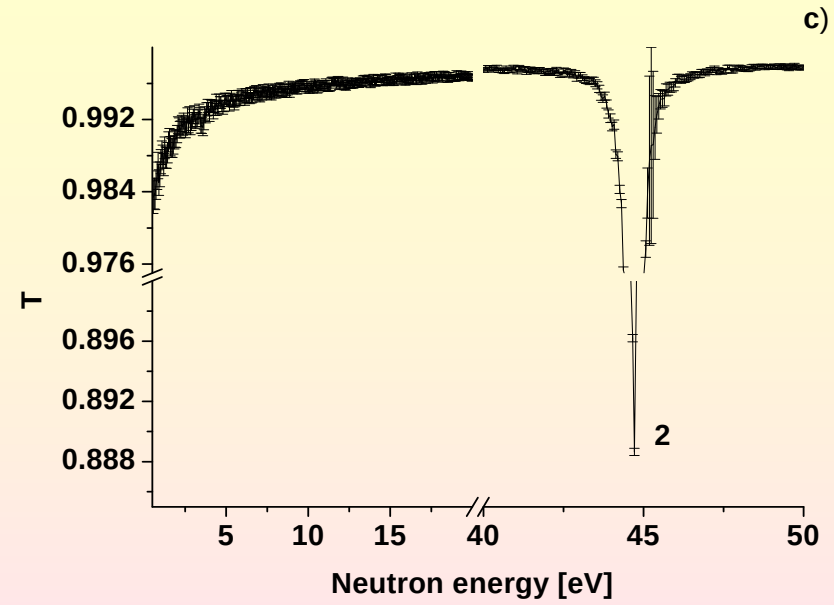
- Then capture data were introduced in the expression of transmitted neutrons

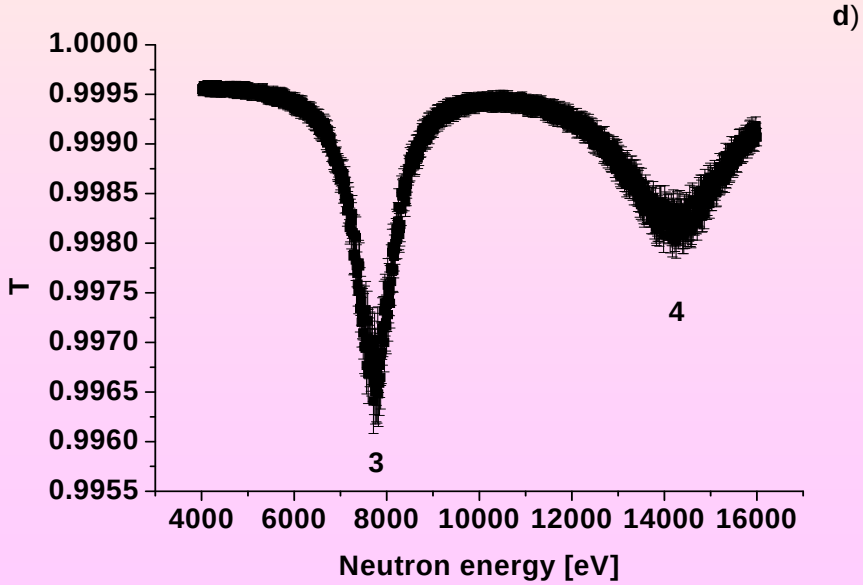
- The neutron transmission spectra of simulated experimental data are in Fig 1c), 1d)

- *1024* simulated experimental points in the energy range (up to *16 keV*) for incident neutrons were considered

The element 1 is not visible in the spectra c) but exist in a)

This means that the data processing only of NTE data could lead to errors on the evaluation of concentration ^{10}B





Concentration

Theoretical data for concentration were chosen; for ^{10}B it was

$$n_{^{10}B} = 1.6 \cdot 10^{22} m^{-2}$$

After the generating procedure of computer simulation, new experimental data were obtained

- by fitting the NTE simulated spectra we obtain

$$n_{^{10}B}^{fit} = (1.6 \pm 0.12) \cdot 10^{22} m^{-2}$$ with a relative error less than 10%

The main factor influencing the errors is the cross section. If the cross section decreases the errors are increasing

Another factor influencing the errors is the number of experimental points

CONCLUSIONS

We have presented the cases of ^{6}Li and ^{10}B nuclei
- important nuclei for fundamental and applicative researches

Concentration and neutron width evaluation
- we have check as well other situations than the presented one
- increasing the number of simulated experimental points the errors are lower
- we chose the ^{6}Li nucleus which has a negative S resonance and one very far P resonance; a high value of (n,α) cross section and a very low capture cross section

- due to the presence of the negative S-resonance we analyzed only the left side tail of neutron spectra. This could be a good idea but this region is affected by a serious background in real experiments

- we chose the ^{10}B nucleus with one S positive resonance considered in our simulation; a high value of (n,α) cross section and a very low capture cross section
- The ^{10}B nucleus suggests the importance of NAA measurements in the evaluation of concentrations
- Accomplishing just only one type of measurements could lead to errors in sample evaluation

CONCLUSIONS

Calculations

- the work is still in the beginning
- for simplicity of our computer experiment we took into consideration only 6 elements and for each element with only one S-resonance
- in future works we will analyze cases with more elements and resonances
- as our proposed method is based on the properties of the nuclei it is obvious that the method applied to others light nuclei should to be slightly changed

Experiment

- this method and others will be verified in experimental measurements at LNF JINR Dubna facility – the new neutron source IREN
- at IREN it is already started a program for obtaining of nuclear data

The proposed method of computer simulation has demonstrated the possibility of measurement of the mentioned parameters of light nuclei

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