Calculation of Effective Resonance Integrals

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Calculation of the effective resonance integral which includes the real energy dependence of neutron flux density and correction on the neutron capture in the sample is needed for accurate flux determination and neutron activation analysis on the IREN and IBR-2M facilities.

It is well known that neutrons are divided on thermal, resonance and fast neutrons. Interaction of the resonance neutrons with the nuclides is described by resonance integral:

$$J_{res0} = \int_{E_{Cd}}^{\infty} \sigma_{n\gamma}(E)\frac{dE}{E}, \tag{1}$$

where E_{Cd} – is the cadmium border, which approximately equal to 0.5 eV, $\sigma_{n\gamma}(E)$-radiative cross-section. The values of the resonance integrals for different nuclides are presented in the handbooks (look, for example, [1]). But this determination is based on the assumption that resonance neutron flux density obeys to reciprocal function from energy (Fermi spectrum). A real spectrum differs from Fermi spectrum. For example neutron flux density from IREN and IBR-2M facilities has next peculiarities: maximum for thermal neutrons intensity is at the energy of 40-50 meV and resonance flux density depends on energy according the next formula:

$$\varphi(E_n) = \frac{\Phi_{res1}}{E_n^{1-\alpha}}, \tag{2}$$

where α = 0.05 - 0.1, Φ_{res1} is the neutron flux density at 1 eV.

Effective resonance integrals differ from the values in the handbook. At first an attempt to calculate effect of neutron spectrum on the $\boldsymbol{I_{res}}$ was made by de Corte et al. [2]. They introduce the effective resonance for every nuclide. Energy of the effective resonance is close to the energy of the strong real resonance with small energy. The cross-section is divided on two parts: one part obeys ***1/v*** low and another part is determined by the resonance. They give the next formula for the effective resonance integral:

$$I_{eff}(\alpha) = (I_{res0} - 0.429\cdot\sigma_{th})\bar{E}_{eff}^{\alpha} + \frac{0.429\cdot\sigma_{th}}{(1-2\alpha)}E_{Cd}^{\alpha} \tag{3}$$

The factor 0.429 is equal to the expression $2\sqrt{\frac{E_{th}}{E_{Cd}}} = 2\sqrt{\frac{0.0253}{0.55}} = 0.429$.

Some years ago the neutron spectrum from IBR-2 facility was investigated by activation method [3]. The calculations according to formulae (3) have been made. The method of more correct calculations for effective resonance integrals is proposed in this work.

Every nuclide has a lot of resonances. In our time one can carry out calculations which include number of resonances.

The accurate description of interaction of the resonance neutrons with the nuclei is shown in the next formula. Number of radioactive nuclei which appeared during short time of irradiation is equal to:

$$dN_a = \Phi_{res1} \int_{E_{Cd}}^{\infty} \frac{\sigma_{n\gamma}}{\sigma_t} \left[1 - \exp(-\sigma_t \cdot n)\right] \frac{-dE}{E^{1-\alpha}} \cdot dt_{irr} \tag{4}$$

Then the effective resonance integral is equal to:

$$I_{res}(\alpha) = \frac{1}{n} \int_{E_{Cd}}^{\infty} \frac{\sigma_{n\gamma}}{\sigma_t} \left[1 - \exp(-\sigma_t \cdot n)\right] \frac{-dE}{E^{1-\alpha}} \tag{5}$$

One can easy receive that if $n \to 0$ and $\alpha = 0$ this expression is equal to $\boldsymbol{J_{res0}}$.

At first we calculate the value of $\boldsymbol{I_{res}(\alpha)}$ without including of neutron capture.

Neutron resonances are described by the Breit-Wigner formula:

$$\sigma_{n\gamma} = \frac{\pi}{k^2} \frac{g\Gamma_n\Gamma_\gamma}{(E-E_r)^2 + \Gamma^2/4} \tag{6}$$

Where $k = 0.002197\sqrt{\frac{A}{A+1}E}$ - neutron momentum in 10^{12} cm^{-1} units (energy is in eV, ***A*** – atomic weight for the target nuclei), $\boldsymbol{E_r}$ is the resonance energy, Γ_n, Γ_γ - neutron and radiative widths, $\Gamma = \Gamma_n + \Gamma_\gamma$ is the total resonance width, ***g*** – statistical weight which depends on target nucleus spin and resonance total momentum.

We can divide a capture cross-section on two parts analogous to the work [2]:

$$\sigma_{n\gamma} = \frac{\sigma_{th}\sqrt{0.0253}}{\sqrt{E_n}} + \sum_i \frac{\pi}{k^2} \frac{g_i\Gamma_{ni}\Gamma_{\gamma i}}{(E_n - E_{ri})^2 + \frac{1}{4}\Gamma_i^2} \tag{7}$$

The first term describes tail from thermal cross-section according to ***1/v*** low (σ_{th} - thermal neutron capture cross-section). Second term describes cross-section from positive resonances.

For narrow resonances one can negligible the neutron width's energy dependence. We can introduce the value $x = \frac{2(E - E_r)}{\Gamma}$, and rewrite (6):

$$\sigma_{n\gamma} = \frac{4\pi}{k^2}\frac{g\Gamma_n\Gamma_\gamma}{\Gamma^2}\frac{1}{1+x^2} = \frac{\sigma_0}{1+x^2}\frac{\Gamma_\gamma}{\Gamma} \tag{8}$$

Here $\sigma_0 = \frac{4\pi}{k^2} g_J \frac{\Gamma_n}{\Gamma}$ - is the cross-section at the resonance maximum.
The resonance area is:

$$A = \int_{-\infty}^{\infty}\sigma_{n\gamma}(E)dE = \sigma_0\frac{\Gamma_\gamma}{\Gamma}\frac{\Gamma}{2}\int_{-\infty}^{\infty}\frac{dx}{1+x^2} = \sigma_0\frac{\Gamma_\gamma}{2}\int_{-\infty}^{\infty}\frac{dx}{1+x^2} = \frac{\pi}{2}\sigma_0\Gamma_\gamma \tag{9}$$

The partition to the resonance integral from one resonance is equal to:

$$I_{resi} = \frac{\pi}{2}\sigma_{i0}(k_r)\frac{\Gamma_{\gamma i}}{E_{ri}^{1-\alpha}}. \tag{10}$$

$$I_{res}(\alpha) = \int_{E_{Cd}}^{\infty}\frac{\sigma_{th}\sqrt{0.0253}}{\sqrt{E}E^{1-\alpha}}dE + \frac{\pi}{2}\sum_i\frac{\sigma_{0i}(k_{ri})\Gamma_{\gamma i}}{E_{ri}^{1-\alpha}} \tag{11}$$

The result of the calculations with $k_{ri}^2 = (0.002197)^2 E_{ri} = 4.827\cdot 10^{-6} E_{ri}$ is the next formula:

$$I_{res}(\alpha) = \frac{\sigma_{th}\sqrt{0.0253}}{(0.5-\alpha)}E_{Cd}^{\alpha-0.5} + 4.0895\cdot 10^6\sum_i\frac{g_i\Gamma_{ni}\Gamma_{\gamma i}}{\Gamma_i\cdot E_{ri}^{2-\alpha}} \tag{11a}$$

But this expression does not include the attenuation of the neutron flux in the sample. We need to calculate the integral (5) on a computer. We have written the code which calculates the effective resonance integrals with real energy dependence for neutron flux density and a sample thickness.

The calculations of the resonance form dependence from the temperature and a sample thickness

The target nuclei take part in the thermal motion, which affects the nature of neutron interaction with them and leads to bigger resonance width. The capture cross-section is equal to

$$\sigma_{n\gamma} = \sigma_0\cdot\frac{\Gamma_\gamma}{\Gamma}\psi(\theta, x) \tag{12}$$

where $x = \frac{2(E-E_r)}{\Gamma}$, $\theta = \frac{\Gamma}{\Delta}$; $\Delta = \sqrt{\frac{4E_r k_B T}{A}}$ - Doppler width.
According to Bethe and Plachek:

$$\psi(\theta,x)=\frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{\exp\left(-\frac{1}{4}\theta^2(x-y)^2\right)}{1+y^2}dy \qquad (13)$$

The probability for a neutron capture by a sample with the thickness ***t***:

$$P_a(t)=\int_0^1\mu d\mu\int_{-\infty}^{+\infty}\left(1-\exp(-\frac{t}{\mu}N_t\sigma_0\psi(\theta,x)\right)dx \qquad (14)$$

$\mu=\cos\alpha$; N_t – is the number of the target nuclei in the volume unit.

For very thin sample $\qquad P_a(t\to 0)=tN_t\sigma_0\pi \qquad (15)$

The resonance self-absorption factor is $\qquad G_{res}=\frac{P_a(t)}{P_a(t\to 0)}. \qquad (16)$

The calculations of the function $\psi(\theta,x)$ and G_{res} is the complex task. This task equivalent to the calculation of the next integral [4]:

$$G_{res}(\theta,\tau)=\frac{\tau}{\pi}\int_{\tau}^{\infty}\frac{dy}{y^3}\int_{-\infty}^{+\infty}(1-\exp(-y\psi(\theta,x))dx, \qquad (17)$$

where $\tau=tN_t\sigma_0\frac{\Gamma_\gamma}{\Gamma}$.

These factors have been calculated for every resonance separately. The resonance parameters have been taken from [5].

So the final expression for the effective resonance integral is:

$$I_{eff.res}=I_v(\alpha)+\frac{\pi}{2}\sum\frac{\sigma_{0i}G_i}{E_{ri}^{1-\alpha}}\Gamma_{\gamma i} \qquad (18)$$

The function ***ψ(θ,x)*** have been calculated by the Pade approximation method [6].

$$\psi(\theta,x)=h\frac{a_0+a_2(hx)^2+a_4(hx)^4}{b_0+b_2(hx)^2+b_4(hx)^4+b_6(hx)^6+b_8(hx)^8} \qquad (19)$$

In this formula $h=\frac{\theta}{2}$, and expressions for the coefficients a_i, b_i, p_i q_i are taken from [8].

$$a_0=(p_0+p_1h-p_2h^2-p_3h^3)(1-q_1h-q_2h^2+q_3h^3+q_4h^4);$$

$$a_2=(p_2+3p_3h)(1-q_1h-q_2h^2+q_3h^3+q_4h^4)+(p_0+p_1h-p_2h^2-p_3h^3)(q_2-3q_3h-6q_4h^3)+$$
$$+(-p_1+2p_2h+3p_3h^2)(q_1+2q_2h-3q_3h^3-4q_4h^4)$$

$$a_4=q_4(p_0+p_1h-p_2h^2-p_3h^3)+)p_2+3p_3h)(q_2-3q_3h-6q_4h^2)-$$
$$-p_3(q_1+2q_2h-3q_3h^2-4q_4h^3)+(-p_1+2p_2h+3p_3h^2)(q_3+4q_4h);$$

$$b_0=(1-q_1h-q_2h^2+q_3h^3+q_4h^4)^2;$$

$$b_2=2(1-q_1h-q_2h^2+q_3h^3+q_4h^4)(q_2-3q_3h-6q_4h^2)+(q_1+2q_2h-3q_3h^2-4q_4h^3)^2;$$

$$b_4=(q_2-3q_3h-6q_4h^2)^2+2q_4(1-q_1h-q_2h^2+q_3h^3+q_4h^4)+$$
$$+2(q_1+2q_2h-3q_3h^2-4q_4h^3)(q_3+4q_4h)$$

$$b_6 = 2q_4(q_2 - 3q_3h - 6q_4h^2) + (q_3 + 4q_4h)^2;$$

$$b_8 = q_4^2;$$

$$p_0 = \sqrt{\pi}; \quad p_1 = \frac{-15\pi^2 + 88\pi - 128}{2(6\pi^2 - 29\pi + 32)}; \quad p_2 = \frac{(33\pi - 104)\sqrt{\pi}}{6(6\pi^2 - 29\pi + 32)}; \quad p_3 = \frac{-9\pi^2 + 69\pi - 128}{3(6\pi^2 - 29\pi + 32)};$$

$$q_1 = \frac{(-9\pi + 28)\sqrt{\pi}}{2(6\pi^2 - 29\pi + 32)}; \quad q_2 = \frac{36\pi^2 - 195\pi + 256}{6(6\pi^2 - 29\pi + 32)};$$

$$q_3 = \frac{(-33\pi + 104)\sqrt{\pi}}{6(6\pi^2 - 29\pi + 32)}; \quad q_4 = \frac{9\pi^2 - 69\pi + 128}{3(6\pi^2 - 29\pi + 32)};$$

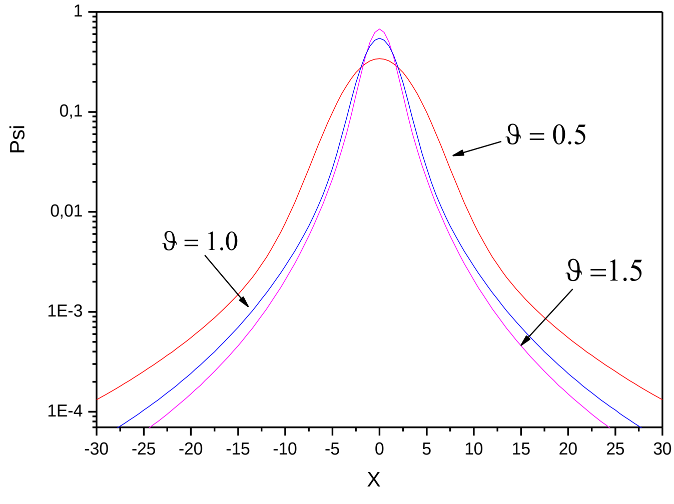

Fig. 1 The function $\psi(\theta, x)$ for different values of $\boldsymbol{\theta}$.

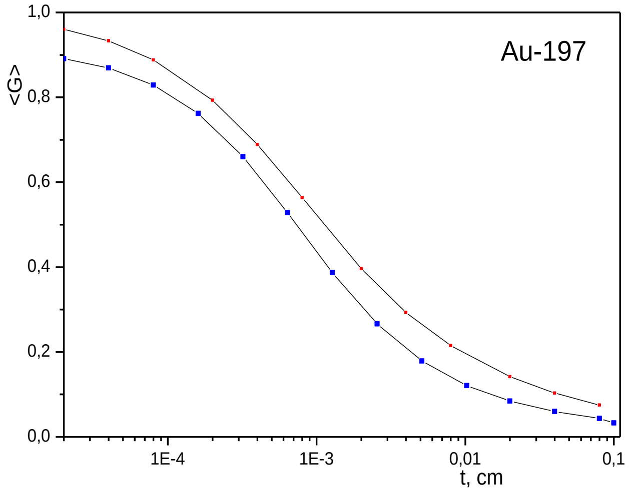

Fig. 2 The results of calculations for average G factor as a function of gold foil thickness.

To obtain G factors one need to calculate the integral (17). The integration has been made by Simpson method.

The factor averaged on number of resonances $\overline{G} = \dfrac{I_{eff.res}(n,T,\alpha)}{I_{res0}}$ have been calculated. Our results are compared with the results of the another works and with the experimental data on the transmission of the resonance neutrons through the gold foils [7,8].

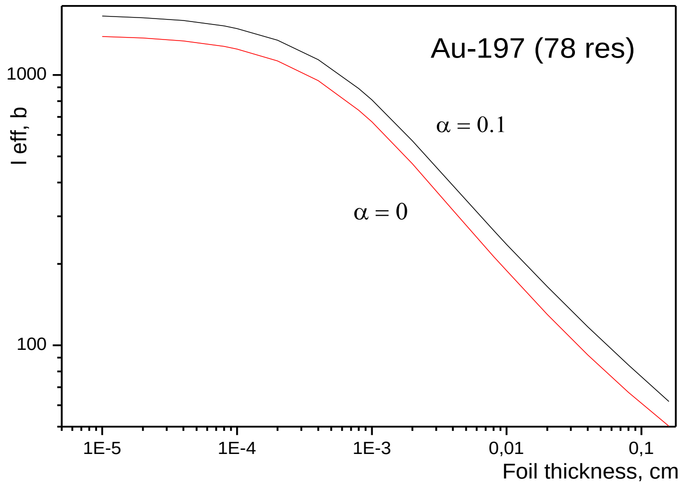

Fig.3. The calculated values of the effective resonance integral as function of the foil thickness for different values of the parameter α.

Conclusion. The program for calculations of the effective resonance integrals which includes the real energy dependence of the flux density and a sample thickness is created.

References

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