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The calculation of neutron self-shielding factors of a group of isolated resonances

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The resonance neutron self-shielding factor, G_{res}, is required in neutron metrology and activation data analysis. In a previous paper, the authors have shown that a dimensionless variable can be introduced which converts the dependence of G_{res} on the physical and nuclear properties of the material samples into an universal curve, valid for the isolated resonances of any nuclide. This work presents a methodology based on the universal curve, which enables to calculate G_{res} for a group of isolated resonances by weighting its individual contributions. A good agreement was reached with results calculated by the MCNP code and with experimental values for Mo foils and wires.

Introduction

The evaluation of the sample activation by epithermal neutrons in a nuclear reactor requires the knowledge of the resonance neutron self-shielding factor, G_{res}. This parameter is needed for routine neutron metrology, activation data analysis and production of radionuclides.[1–3] The value of G_{res} depends on the physical and nuclear properties of the nuclide as well as on the sample geometry and dimension. The authors have shown recently[4,5] that a dimensionless variable, z, can be introduced which converts the dependence of the resonance neutron self-shielding factor of wires, foils, spheres and cylinders on physical and nuclear parameters of the samples into an universal curve valid for isolated resonances of any nuclide. The universal curve is a sigmoid given by:

$$G_{res}(z) = \frac{A_1 - A_2}{1 + \left(\frac{z}{z_0}\right)^p} + A_2, \tag{1}$$

where $A_1 = 1.000 \pm 0.005$; $A_2 = 0.060 \pm 0.011$; $z_0 = 2.70 \pm 0.09$; $p = 0.82 \pm 0.02$, and

$$z = \Sigma_{tot}(E_{res}) \cdot y \cdot \sqrt{\frac{\Gamma_\gamma}{\Gamma}}, \tag{2}$$

is a dimensionless variable that includes the physical and nuclear properties of the nuclide considered: $\Sigma_{tot}(E_{res})$ is the macroscopic total cross section at the resonance peak, Γ_γ and Γ are the radiative and total resonance widths, respectively, and y is a parameter dependent on the geometry and dimension of the sample ($y = 2R$ for wires; $y = 1.5t$ for foils; $y = R$ for spheres, and $y = 1.65Rh/(R+h)$ for cylinders, R, t, and h being the appropriate radius, thickness, and height of the samples), respectively.

However, rather than a dominant resonance, some nuclides present a group of well defined resonances, which must be taken into account in the interpretation of neutron activation results. This paper presents a method based on the universal curve, which enables to calculate G_{res} for a group of isolated resonances by weighting its individual contributions.

Method of calculation

Assuming that the resonances are described by the Breit-Wigner formula, the weight of the ith resonance, w_i, for the self-shielding factor of the group is proportional to its resonance integral:[6]

$$w_i = \left(\frac{\Gamma_\gamma}{E_{res}^2} \cdot \frac{g\Gamma_n}{\Gamma}\right)_i \tag{3}$$

where

$$g = (2J+1)/[2 \cdot (2I+1)]$$

is the statistical weight factor, J is the spin of the resonance state, I is the spin of the target nucleus, Γ_n is the neutron resonance width, and E_{res} is the resonance energy.

Note that $w_i \propto 1/E^2_{res,i}$, gives a greater relative weight to the lower energy resonances.

Two alternatives are proposed for the calculation of G_{res} for the group of resonances. In the first one, for each resonance the values of $G_{res}(z_i)$ are determined and the mean value $\langle G_{res} \rangle$ corresponding to the group is given by:

$$\langle G_{res} \rangle = \frac{\sum_{i=1}^{n} w_i \cdot G_{res}(z_i)}{\sum_{i=1}^{n} w_i} \tag{4}$$

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In the second alternative, the mean value of z, $\langle z\rangle$, is calculated using weighting factors:

$$\langle z\rangle = \frac{\sum_{i=1}^{n} w_i \cdot z_i}{\sum_{i=1}^{n} w_i} \quad (5)$$

and the value of $G_{res}(\langle z\rangle)$ is obtained from the universal curve.

In this paper the method is applied to spheres, but it is also valid for other geometries, namely, foils and wires, as will be shown in the next section.

Results and discussion

The method is applied to the first resonances of some nuclides [^{89}Y (5 resonances), ^{133}Cs (3), ^{141}Pr (6), ^{165}Ho (5), ^{181}Ta (3), ^{185}Re (3) and ^{232}Th (4)] and the results are compared with the values calculated by using the MCNP code.[7]

Table 1 shows the nuclear and physical parameters of the studied nuclides. The last column contains the normalized resonance weights, $w_{i,norm}$, which indicates its relative individual importance in each nuclide:

$$w_{i,norm} = \frac{w_i}{w_{min}} \quad (6)$$

where w_{min} represents the minimum resonance weight factor for a given nuclide. Table 2 shows the resonance self-shielding factors for each set of resonances for spherical samples with radius 0.001 cm, 0.01 cm and 0.1 cm. $G_{res,MC}$ is the self-shielding factor calculated with the MCNP code for the group of resonances. Figure 1 illustrates the agreement between $G_{res}(<z>)$ and $<G_{res}>$; for $G_{res}(<z>)>0.2$, the relative error between both quantities is smaller than 6%. Figure 2 compares $G_{res,MC}$ with $G_{res}(<z>)$; $G_{res,UC}$ represents the corresponding universal curve.

Table 1. Physical and nuclear parameters of the studied nuclides[8,9]

Nuclide	A, g·mol^{-1}	ρ, g·cm^{-3}	E_{res}, eV	I	J	$\sigma_{tot}(E_{res})$, barn	Γ_γ, eV	Γ_n, eV	$\Gamma=\Gamma_\gamma+\Gamma_n$, eV	Γ_γ/Γ, %	$w_{i,norm}$
^{89}Y	88.91	4.47	2598	0.5	1	306	0.12	1.07	1.19	10.1	7.8
			2609		1	319	0.49	1.27	1.76	27.9	25.3
			3381		1	95.1	0.06	0.37	0.43	13.8	2.2
			4778		2	14.9	0.302	0.033	0.335	90.2	1.1
			5712		0	26.7	0.302	0.6	0.902	33.5	1.0
^{133}Cs	132.91	1.87	5.0	3.5	3.5	6876	0.115	0.0051	0.1201	95.8	26.2
			22.6		3.5	1634	0.120	0.0067	0.1267	94.7	1.7
			47.8		3.5	1631	0.140	0.0194	0.1594	87.9	1.0
^{141}Pr	140.91	6.71	85.2	2.5	2	312	0.083	0.0083	0.0913	90.9	28.2
			112.4		2	13.1	0.083	0.00047	0.0835	99.4	1.0
			218.7		3	557	0.071	1.080	1.151	6.2	52.9
			235.2		3	4725	0.093	0.874	0.967	9.6	57.8
			359.5		3	3314	0.060	1.217	1.277	4.7	16.8
			387.9		3	292	0.082	0.049	0.131	62.7	7.7
^{165}Ho	164.93	8.80	3.92	3.5	4	6718	0.085	0.0021	0.0871	97.6	108.6
			8.16		3	1952	0.078	0.0019	0.0799	97.7	17.2
			12.75		4	7523	0.078	0.0105	0.0885	88.1	45.6
			18.20		3	365.9	0.078	0.00096	0.07896	98.8	1.8
			21.12		4	230.3	0.078	0.00056	0.07856	99.3	1.0
^{181}Ta	180.95	16.65	4.28	3.5	4	13969	0.053	0.0039	0.0569	93.1	38.8
			10.34		3	4052	0.055	0.0047	0.0597	92.3	6.1
			13.95		4	792	0.052	0.0010	0.0530	98.1	1.0
^{185}Re	184.95	20.87	2.16	2.5	3	24554	0.055	0.00283	0.05773	95.1	108.0
			5.92		2	439	0.069	0.00026	0.06926	99.6	1.0
			7.22		3	2289	0.055	0.0012	0.0562	97.9	4.2
^{232}Th	232.04	11.72	21.81	0	0.5	1925	0.025	0.0021	0.0271	92.4	4.3
			23.46		0.5	3183	0.027	0.0038	0.0308	87.4	6.6
			59.52		0.5	837	0.024	0.0038	0.0278	86.3	1.0
			69.23		0.5	6751	0.023	0.0432	0.0662	34.7	3.4

Table 2. Resonance self-shielding factors for the set of resonances (spheres: $y = R$)

Nuclide*	$\langle z \rangle / y$	R, cm	$\langle z \rangle$	$G_{res}(\langle z \rangle)$	$\langle G_{res} \rangle$	$G_{res,MC}$
^{89}Y (5)	4.157	0.001	0.004157	0.995	0.995	0.996
		0.01	0.04157	0.970	0.971	0.960
		0.1	0.4157	0.833	0.838	0.732
^{133}Cs (3)	53.073	0.001	0.053073	0.964	0.964	0.979
		0.01	0.53073	0.804	0.807	0.820
		0.1	5.3073	0.403	0.415	0.364
^{141}Pr (6)	31.426	0.001	0.031426	0.976	0.977	0.968
		0.01	0.31426	0.862	0.868	0.781
		0.1	3.1426	0.501	0.532	0.429
^{165}Ho (5)	198.549	0.001	0.198549	0.901	0.902	0.926
		0.01	1.98549	0.589	0.599	0.571
		0.1	19.8549	0.213	0.229	0.199
^{181}Ta (3)	661.119	0.001	0.661119	0.775	0.780	0.792
		0.01	6.61119	0.365	0.385	0.353
		0.1	66.1119	0.124	0.136	0.120
^{185}Re (3)	1558.64	0.001	1.55864	0.634	0.640	0.634
		0.01	15.5864	0.240	0.256	0.244
		0.1	155.864	0.093	0.101	0.075
^{232}Th (4)	83.208	0.001	0.083208	0.949	0.949	0.956
		0.01	0.83208	0.741	0.747	0.696
		0.1	8.3208	0.327	0.343	0.235

* (x) number of resonances.

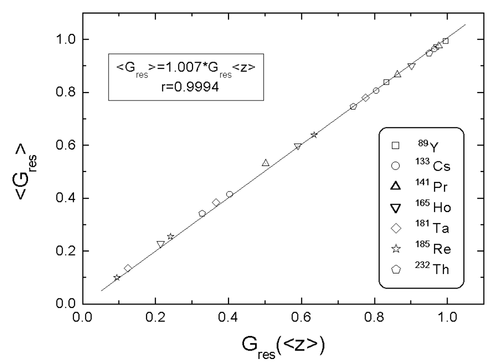

Fig. 1. Comparison of $\langle G_{res} \rangle$ with $G_{res}\langle z \rangle$

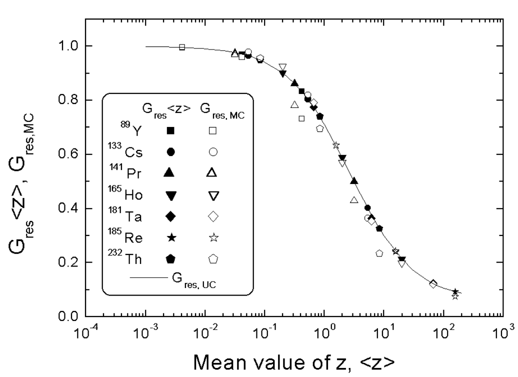

Fig. 2. Dependence of the neutron self-shielding factor for a group of isolated resonances, $G_{res}\langle z \rangle$ and $G_{res,MC}$, on the mean value of z

The following considerations can be drawn from these results:

(a) There is a good agreement between $G_{res}(\langle z \rangle)$ and $\langle G_{res} \rangle$. Generally, the values of $\langle G_{res} \rangle$ are greater than the values of $G_{res}(\langle z \rangle)$. However, the differences are smaller than 9%, which confirms the suitability of the adopted weights.

(b) There is a satisfactory agreement between $G_{res}(\langle z \rangle)$ and $G_{res,MC}$, excluding the case of ^{232}Th, for $R = 0.1$ cm, where the difference attains 28%. For ^{185}Re and $R = 0.1$ cm, the difference is 19%, but it is not significant because the values (0.093 and 0.075) are very small, near $A_2 = 0.060 \pm 0.011$. For the other nuclides the differences are in general smaller than 10%.

(c) The relative differences between $G_{res}(\langle z \rangle)$, $\langle G_{res} \rangle$ and $G_{res,MC}$ for the same nuclide increase as the sphere radius increases (the self-shielding effect increases).

Table 3 shows the comparison between experimental resonance self-shielding factors, G_{res}(exp), for ^{98}Mo measured by FREITAS[3] in ^{nat}Mo foils and wires, and values of $G_{res}(\langle z \rangle)$ from this work. Mo is a multi-resonance monitor (six resonances has been considered) used as a comparator in the k_0-standardized neutron activation analysis for low energy gamma-emitters. As can be seen, the agreement is good, the relative mean deviation being about 3% for both geometries. The relative experimental errors have, approximately, the same magnitude.

Table 3. Comparison of experimental resonance self-shielding factors, G_{res}(exp), for ^{98}Mo measured by FREITAS[3] in ^{nat}Mo foils and wires with values of $G_{res}(<z>)$ from this work

Geometry	Thickness, cm	G_{res}(exp)	$<z>/y$	$<z>$	$G_{res}(<z>)$	Δ,* %
Foils	0.0050	0.988	7.366	0.0552	0.994	–0.6
	0.0010	0.977		0.0110	0.990	–1.3
	0.0025	0.949		0.2762	0.979	–3.1
	0.0050	0.911		0.5525	0.963	–5.7
	Diameter, cm	G_{res}(exp)	$<z>/y$	$<z>$	$G_{res}(<z>)$	Δ,* %
Wires	0.0025	0.972	7.366	0.0184	0.985	–1.3
	0.0050	0.947		0.0368	0.973	–2.7
	0.0125	0.900		0.0921	0.945	–4.9
	0.0250	0.881		0.1842	0.906	–2.9
	0.0500	0.864		0.3683	0.846	2.1

* $\Delta = (G_{res}(\text{exp}) - G_{res}(<z>))/G_{res}(\text{exp})$.

Conclusions

A previously deduced universal curve of $G_{res}(z)$, valid for isolated resonances and various geometries, was applied to the calculation of the resonance neutron self-shielding factor of resonance groups, $<G_{res}>$ or $G_{res}(<z>)$, by weighting its individual contributions. The method was applied to spherical samples of various nuclides: ^{89}Y (5 resonances), ^{133}Cs (3), ^{141}Pr (6), ^{165}Ho (5), ^{181}Ta (3), ^{185}Re (3) and ^{232}Th (4). The results were compared with the corresponding self-shielding factors directly calculated with the MCNP code, $G_{res,MC}$. In spite of the great differences in the physical, nuclear and resonance properties of the studied nuclides, there is a satisfactory agreement between $G_{res}(<z>)$ or $<G_{res}>$ and $G_{res,MC}$. The relative differences between the values for the same nuclide increase as the radius increases, certainly because the absolute values to be compared decrease. A good agreement between $G_{res}(<z>)$ and experimental values for ^{98}Mo foils and wires is obtained.

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