Calculation of production cross sections of γ-rays from thermal-neutron captures

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Abstract The calculation methods of production cross sections of γ-rays for thermal-neutron captures are briefly presented. The check of intensity balance is made. The examples are given to illustrate its application.

Keywords Neutron, (n, γ) reaction, γ-rays production cross section, Data calculation

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1 Introduction

The energies and production cross sections of γ-rays, and their decay schemes of thermal-neutron captures are basic data in nuclear physics research, nuclear technologic application and nuclear engineering design. Today, the technique of neutron-induced prompt γ activation analysis (PGAA) is widely applied in material science, chemistry, geology, mining, archaeology, food analysis, environment, medicine, and so on. The availability of high-quality guided (or filtered) thermal and cold neutron beams at high and medium flux research reactors has greatly facilitated the advancement of the PGAA method during the 1990s.

PGAA is a non-destructive radioanalytical method, capable of rapid and simultaneous multielement analysis involving the entire Periodic Table, from hydrogen to uranium. The inaccuracy and incompleteness of the data available for use in PGAA are significant handicaps in the qualitative and quantitative analysis of complicated γ spectra. Accurate and complete neutron capture γ-ray energies and production cross sections of γ-rays are important for PGAA. The international database for PGAA has been developed under the organization of Nuclear Data Section, IAEA. The calculation methods of production cross sections of γ-rays for thermal-neutron captures are one part of the IAEA project.

In the following we present the calculation methods of production cross sections of γ-rays for thermal-neutron captures and make the check of intensity balance. Some examples are then given to illustrate its application.

2 Production cross section calculations of γ-rays

In the experimental measurements, relative γ-ray intensities are measured. In the practical applications, production cross sections of γ-rays for thermal-neutron captures should be known. The basic principle of the production cross section calculation of γ-rays for thermal-neutron captures is the γ transition intensity balance for each level.

Main and general methods of the production cross section calculation of γ-rays for thermal-neutron captures are summarized as follows.

2.1 Calculation from γ-ray decaying to ground state

When a nuclide captures a thermal-neutron, the γ-rays decay into its ground state, as shown in Fig.1. If there are m γ-rays decaying to ground state, I_k is the relative intensity for the k-th γ-ray, α_k is its total internal conversion coefficient, the equation can be written as

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$$N_\gamma \cdot \sum_{k=1}^{m} I_k (1+\alpha_k) = \sigma_{n,\gamma} \qquad (1)$$

where N_γ is normalization factor for γ-ray production cross sections per thermal-neutron capture, and $\sigma_{n,\gamma}$ is (n,γ) reaction cross section per thermal-neutron capture. From Eq.(1) we can write

$$N_\gamma = \frac{\sigma_{n,\gamma}}{\sum_{k=1}^{m} I_k (1+\alpha_k)} \qquad (2)$$

For light nuclides, each internal conversion coefficient α_k is quite small and can be neglected, so we obtain

$$N_\gamma = \frac{\sigma_{n,\gamma}}{\sum_{k=1}^{m} I_k} \qquad (3)$$

From Eq.(2) or (3), the normalization factor N_γ can be calculated, and then γ-ray production cross sections for thermal-neutron capture can be calculated by

$$\sigma_{n,\gamma}(E_{\gamma k}) = N_\gamma I_{\gamma k} \qquad (4)$$

where $\sigma_{n,\gamma}(E_{\gamma k})$ is γ-ray production cross section of k-th γ-ray of energy $E_{\gamma k}$; $I_{\gamma k}$ is γ-ray relative intensity of k-th γ-ray of energy $E_{\gamma k}$.

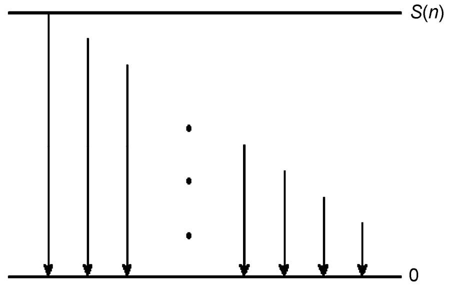

Fig.1 Skeleton scheme of γ-ray decaying to ground state from high excitation state.

The related γ-ray data[1] for ^{26}Mg(n,γ) of thermal-neutron are given in Table 1 and its decay scheme is shown in Fig.2, where the γ-ray relative intensities are given. The capture cross section $\sigma_{n\gamma}$=(38.2±0.8) mb, for ^{26}Mg(n,γ) of thermal-neutron, has been evaluated[2]. In Table 1, the γ-ray energies, their relative intensities and levels are given, from which, using Eq.(3), N_γ=(0.382±0.008) mb is calculated, and the γ-ray production cross sections can also be calculated from Eq.(4), as shown in Table 1.

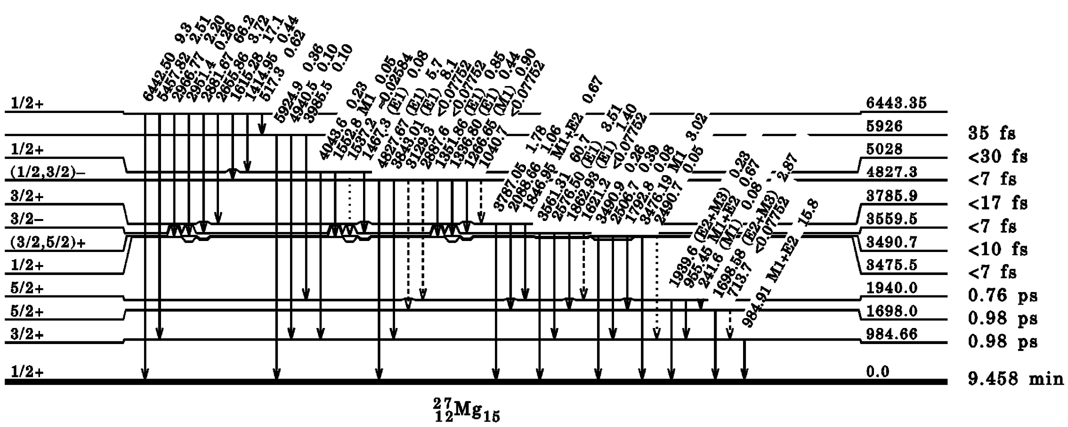

Fig. 2 Decay scheme and γ-ray intensity from ^{26}Mg(n,γ) thermal neutron reaction.

Table 1 γ-ray data and production cross sections from ^{26}Mg(n,γ) thermal neutron reaction

E_γ (keV)		E(level) (keV)		I_γ*		Mult.**	δ**		σ $_{n\gamma(E\gamma)}$ (mb)@	
241.6#	4	1940.0	1	0.08	3	(M1)			0.03	1
517.3	3	6443.35	4	0.62	8				0.24	3
713.7		1698.0	1	<0.08					<0.03	
955.45	8	1940.0	1	0.67	8	M1+E2	−0.08	6	0.26	3
984.91	3	984.92		15.8	8	M1+E2	+0.22	2	6.0	3
1040.7		4827.3	4	<0.08					<0.03	

Table 1. (continued)

E_γ (keV)		E(level) (keV)		I_γ*		Mult.**	δ**	$\sigma_{n\gamma(E\gamma)}$ (mb)@	
1266.65	18	4827.3	4	0.90	8	(M1)		0.34	3
1336.80	20	4827.3	4	0.44	6	(E1)		0.17	2
1351.86	8	4827.3	4	0.85	8	(E1)		0.32	3
1414.95	18	6443.35	4	0.44	6			0.17	2
1467.3	5	5028	1	0.08	3	(E1)		0.03	1
(1537.2)		5028	1	≈0.02584				≈0. 01	
1552.8	7	5028	1	0.05	3	M1		0.02	1
1615.28	5	6443.35	4	17.1	8			6.5	3
1621.2		3559.5	1	<0.08				<0.03	
1698.58	5	1698.0	1	2.87	18	(E2+M3)	≈0.0	1.10	7
1792.8	3	3490.7	7	0.08	3			0.03	1
1846.95	18	3785.9	4	0.67	8	M1+E2	−0.0 3	0.26	3
1862.93	10	3559.5	1	1.40	11	(E1)		0.53	5
1939.6	4	1940.0	1	0.23	6	(E2+M3)	≈0.0	0.09	2
2088.66	11	3785.9	4	1.06	8			0.40	3
(2490.7)		3475.5	2	0.05	3			0.02	1
2506.7	23	3490.7	7	0.39	6			0.15	2
2576.50	6	3559.5	1	3.51	21	(E1)		1.34	8
2655.86	6	6443.35	4	3.72	18			1.42	7
2881.67	4	6443.35	4	66.2	21			25.3	8
2887.6		4827.3	4	<0.08				<0.03	
2951.4	4	6443.35	4	0.26	6			0.10	2
2966.77	22	6443.35	4	2.20	16			0.84	6
3129.3		4827.3	4	<0.08				<0.03	
3476.19	9	3475.5	2	3.02	16	M1		1.15	6
3490.9	6	3490.7	7	0.26	5			0.10	2
3561.31	4	3559.5	1	60.7	18			23.2	7
3787.05	15	3785.9	4	1.78	16			0.68	6
3843.01	8	4827.3	4	8.1	5	(E1)		3.10	16
3985.5	6	5926 2		0.10	3			0.04	1
4043.6	3	5028 1		0.23	6			0.09	2
4827.67	6	4827.3	4	5.7	4	(E1)		2.18	13
4940.5	3	5926 2		0.10	3			0.04	1
5457.82	15	6443.35	4	2.51	18			0.96	7
5924.9	4	5926 2		0.36	6			0.14	2
6442.50	6	6443.35	4	9.3	5			3.55	17

Uncertainty (error):the uncertainty in any number is given space after the number itself; for example, 241.6 4 means 241.6±0.4.
* Relative intensity.
** Multipolarity and its mixture ratio for γ-ray.
@ γ-ray production cross section.

2.2 Calculation from primary γ-ray decaying from captured state

When a nuclide captures a thermal-neutron, the nuclide is de-excited from its capture state by mean of decaying primary γ-rays, as shown in Fig.3. Suppose that there are n primary γ-rays, I_i is relative intensity of the i-th primary γ-ray and α_i is the total internal conversion coefficient of the i-th primary γ-ray, then

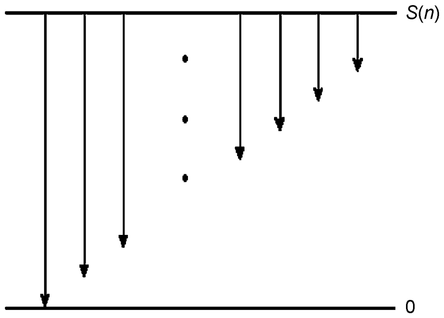

Fig.3 Skeleton scheme of primary γ-rays from captured state.

$$N_\gamma \bullet \sum_{i=1}^{n} I_i(1+\alpha_i) = \sigma_{n,\gamma} \tag{5}$$

$$\text{or} \quad N_\gamma = \frac{\sigma_{n,\gamma}}{\sum_{i=1}^{n} I_i(1+\alpha_i)} \tag{6}$$

And for light nuclide, Eq.(6) becomes

$$N_\gamma = \frac{\sigma_{n,\gamma}}{\sum_{i=1}^{n} I_i} \tag{7}$$

The primary γ-ray data[1] for ^{28}Si(n,γ) of thermal-neutron are listed in Table 2, and their decay scheme is shown in Fig.4, where the γ-ray relative intensities are given. The capture cross section, $\sigma_{n\gamma}$=(177±5) mb, for ^{28}Si(n,γ) of thermal-neutron has been evaluated[2]. From Table 2, the γ-ray energies, their relative intensities and levels are given, from which, using Eq.(3), N_γ=(1.77±0.05) mb is calculated, and the γ-ray production cross sections can also be calculated from Eq.(4), as shown in Table 2.

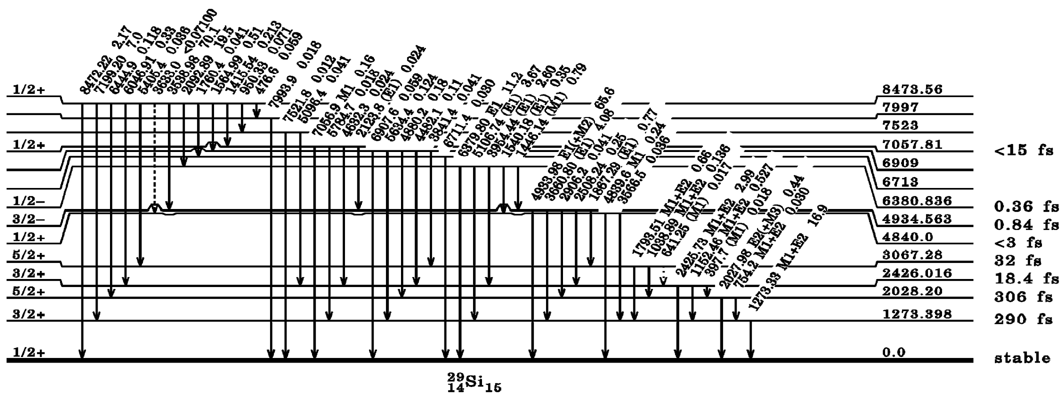

Fig.4 Decay scheme and γ-ray intensity from ^{28}Si(n,γ) thermal neutron reaction.

Table 2 γ-ray data and production cross sections from ^{28}Si(n,γ) thermal neutron reaction

E_γ (keV)		E(level) (keV)		I_γ *		Mult.**	δ**		$\sigma_{n\gamma(E_\gamma)}$ (mb) @	
397.7	4	2426.016	15	0.018	6	(M1)			0.03	1
476.6	3	8473.56	3	0.059	12				0.10	2
(641.25)		3067.28	8	0.017	9	(M1)			0.030	15
754.2	4	2028.20	6	0.030	12	M1+E2	–0.03	3	0.05	2
950.33	13	8473.56	3	0.071	12				0.13	2
1038.89	10	3067.28	8	0.136	18	M1+E2	+0.04	2	0.24	3
x1071.0	5			0.047	12				0.08	2
1152.46	6	2426.016	15	0.528	24	M1+E2	+0.09	8	0.93	4
1273.33	3	1273.398	11	16.9	9	M1+E2	+0.197	9	29.9	14
1415.54	9	8473.56	3	0.213	24				0.37	4

Table 2 (continued)

E_γ (keV)		E(level) (keV)		I_γ*		Mult.**	δ**		$\sigma_{n\gamma(E\gamma)}$ (mb)@	
1446.14	4	6380.836	13	0.79	3	(M1)			1.40	5
1540.18	6	6380.836	13	0.35	3	(E1)			0.62	5
1564.99	5	8473.56	3	0.52	4				0.92	7
1760.4	5	8473.56	3	0.042	12				0.07	2
1793.51	4	3067.28	8	0.66	4	M1+E2	+0.26	2	1.18	6
1867.29	5	4934.563	13	0.77	4	(E1)			1.36	6
2027.98	9	2028.20	6	0.44	5	E2(+M3)	0.0		0.78	7
2092.89	3	8473.56	3	19.6	8				34.7	12
2123.8	6	7057.81	17	0.024	6	(E1)			0.04	1
2425.73	4	2426.016	15	3.00	12	M1+E2	–0.32	7	5.31	20
2508.24	13	4934.563	13	0.25	3				0.44	5
2906.2	5	4934.563	13	0.042	12				0.07	2
3538.98	4	8473.56	3	70.3	22				124.4	38
3566.5	5	4840.0	4	0.036	12				0.06	2
3633.0		8473.56	3	<0.071					<0.12	
3660.80	6	4934.563	13	4.09	18	(E1)			7.2	3
3841.4	6	6909		0.042	12				0.07	2
3954.44	5	6380.836	13	2.61	18	(E1)			4.6	3
4482.1	4	6909		0.11	3				0.19	5
4632.3	7	7057.81	17	0.024	12				0.04	2
4839.6	4	4840.0	4	0.24	3	M1			0.42	5
4880.2	5	6909		0.18	3				0.31	5
4933.98	3	4934.563	13	65.7	21	E1(+M2)	–0.05	10	116.3	34
5096.4	7	7523		0.042	12				0.07	2
5106.74	6	6380.836	13	3.68	18	(E1)			6.5	3
5405.4	9	8473.56	3	0.036	12				0.06	2
5634.4	4	6909		0.125	18				0.22	3
5784.7	7	7057.81	17	0.018	6				0.03	1
6046.91	16	8473.56	3	0.33	4				0.58	6
6379.80	4	6380.836	13	11.3	6	E1			20.0	11
6444.9	5	8473.56	3	0.119	24				0.21	4
6711.4	9	6713		0.030	12				0.05	2
6907.6	7	6909		0.059	18				0.10	3
7056.9	4	7057.81	17	0.16	3	M1			0.28	5
7199.20	5	8473.56	3	7.1	3				12.6	5
7521.8	9	7523		0.012	6				0.02	1
7993.9	9	7997		0.018	6				0.03	1
8472.22	7	8473.56	3	2.17	12				3.84	21

* Relative intensity. ** Multipolarity and its mixture ratio for γ-ray.

x Unplaced in level scheme. @ γ-ray production cross section.

3 Intensity balance check

The most important is the physical consistent check of intensity balance for each level.

For decay γ-ray to ground state, Eq.(1) becomes

$$N_{\gamma}(b)\sum_{k=1}^{m} I_k(1+\alpha_k)=\sigma_{n\gamma} \qquad (8)$$

where $N_{\gamma}(b)$ is normalization factor for γ-ray production cross sections of thermal-neutron captures.

For primary γ-ray from captured state, Eq.(5) becomes

$$N_{\gamma}(p)\sum_{i=1}^{n} I_i(1+\alpha_i)=\sigma_{n\gamma} \qquad (9)$$

where $N_{\gamma}(p)$ is normalization factor for γ-ray production cross sections of thermal-neutron captures.

From Eq.(8) and (9), we obtain

$$N_{\gamma}(p)\sum_{i=1}^{n} I_i(1+\alpha_i)=N_{\gamma}(b)\sum_{k=1}^{m} I_k(1+\alpha_k) \qquad (10)$$

or

$$\frac{N_{\gamma}(p)}{N_{\gamma}(b)}=\frac{\sum_{k=1}^{m} I_k(1+\alpha_k)}{\sum_{i=1}^{n} I_i(1+\alpha_i)} \qquad (11)$$

The normalization factors $N_{\gamma}(p)$ and $N_{\gamma}(b)$ for γ-ray production cross sections of thermal-neutron captures are not equal because the measurement uncertainty exists. Therefore, we can write

$$\frac{N_{\gamma}(p)}{N_{\gamma}(b)}\approx 1 \qquad (12)$$

within their uncertainty range. Eq.(11) can also be changed to

$$\frac{\sum_{i=1}^{n} I_i(1+\alpha_i)}{\sum_{k=1}^{m} I_k(1+\alpha_k)}\approx 1 \qquad (13)$$

or

$$\sum_{i=1}^{n} I_i(1+\alpha_i)\approx\sum_{k=1}^{m} I_k(1+\alpha_k) \qquad (14)$$

Eq.(14) is also correct within their uncertainty range. For other levels, in addition to captured state and ground state, the intensities coming into and going out of the level j are the same within their uncertainty range, as shown in Fig.5. Also, we obtain

$$\sum_{k=1}^{m} I_{jik}(1+\alpha_{jik})-\sum_{i=1}^{n} I_{joi}(1+\alpha_{joi})\approx 0 \qquad (15)$$

where I_{jik}, α_{jik}, I_{joi} and α_{joi} are γ-ray relative intensities and their internal conversion coefficients for coming into and going out of level J respectively.

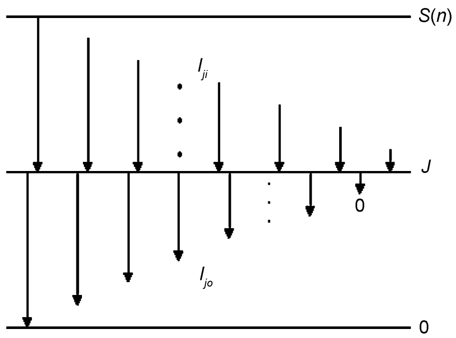

Fig.5 Skeleton scheme of intensity balance calculation for excitation level.

In Table 3, the calculation and checking results of intensity balance for each levels from ^{28}Si(n,γ) reaction are given. From Table 3 it can be seen that the capture cross sections of thermal-neutron captures for each levels are consistent within their uncertainties.

Table 3 Calculation and checking results of intensity balance from ^{28}Si(n,γ) reaction at E_n=thermal

Level		RI@ (OUT)		RI@ (IN)		RI@ (NET)		TI# (OUT)		TI# (IN)		TI# (NET)		$\sigma_{n\gamma}$ (mb)* (CALC)	
0		0.0		100	3	–100	3	0.0		100	3	–100	3	0.4	41
1273.398	11	16.9	8	16.2	4	0.7	10	16.9	4	16.2	4	0.7	10	1.2	18
2028.20	6	0.47	5	0.49	5	–0.02	10	0.47	5	0.49	5	–0.02	10	–0.04	12
2426.016	15	3.54	12	3.4	2	0.14	24	3.54	12	3.4	2	0.14	24	0.30	41
3067.28	8	0.82	4	0.85	4	–0.03	6	0.82	4	0.85	4	–0.03	6	–0.05	11

Table 3 (continued)

Level	RI[@] (OUT)	RI[@] (IN)	RI[@] (NET)	TI[#] (OUT)	TI[#] (IN)	TI[#] (NET)	$\sigma_{n\gamma}$ (mb)[*] (CALC)
4840.0 4	0.27 4	0.35 3	–0.08 5	0.27 4	0.35 3	–0.08 5	–0.14 9
4934.563 13	70.9 2	71.0 3	–0.1 3	70.9 2	71.0 3	–0.1 3	–0.17 54
6380.836 13	18.6 7	19.5 7	–0.9 10	18.6 7	19.5 7	–0.9 10	–1.5 18
6713	0.030 12	0.041 12	–0.011 17	0.030 12	0.041 12	–0.011 17	–0.021 30
6909	0.51 5	0.51 4	–0.00 6	0.51 5	0.51 4	–0.00 6	–0.02 12
7057.81 17	0.22 4	0.21 3	0.010 6	0.22 4	0.21 3	0.010 6	0.02 7
7523	0.053 14	0.071 12	–0.018 18	0.053 14	0.071 12	–0.018 18	–0.032 32
7997	0.018 6	0.059 12	–0.041 14	0.018 6	0.059 12	–0.041 14	–0.073 25
473.56 3	100 3	0.000	100 3	100 3	0.000	100 3	177 5

[@] Relative intensity. [#] Relative intensity including internal conversion. [*] Intensity balance of capture cross section.

4 Summary

The calculation formulas of γ-ray production cross sections and intensity balance check for thermal-neutron captures have been introduced on the basis of decay scheme of captured state and its capture cross section. In general, neutron binding energy is high, and captured state is a high excitation state and its decay scheme is quite complex. Sometimes, a lot of weak-intensity γ-ray are unable to be measured experimentally. Besides, measured uncertainties from background deducting and γ-spectra analysis lead to γ-ray intensity uncertainties. Strictly speaking, intensities of coming into and going out of a level are impossible to be exactly identical, they can only be consistent within their uncertainties. Based on the same reason, the normalization factors for primary γ-rays from captured state and decay γ-rays to ground state are different. The normalization factor of γ-ray production cross sections in thermal-neutron capture reaction is usually calculated from the γ-rays decaying to ground state.

The calculation methods have been applied in the development of international database for PGAA and neutron cross section calculations.

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