Covariance Data Evaluation of Some Experimental Data for n+$^{65,\,63,\,\mathrm{Nat}}$Cu

JIA Min[1] LIU Jianfeng[1] LIU Tingjin[2]

1 Physics Department, Zhengzhou University, Zhengzhou 450052

2 China Nuclear Data Center, CIAE, P.O.Box275(41), Beijing 102413

【abstract】 *The evaluation of covariance data for $^{65,\,63,\,\mathrm{Nat}}$Cu in the energy range from 99.5 keV to 20 MeV was carried out using EXPCOV and SPC code based on the experimental data available. The data can be as a part of the covariance file 33 in the evaluated library in ENDF/B6 format for the corresponding nuclides, and also can be used as the basis of theoretical calculation concerned.*

Introduction

Copper is a very important structure material in nuclear engineering. With the development of the reactor physics and computer technology, the covariance matrix of nuclear data becomes more and more important. The error, as traditionally given, is only the diagonal elements of the covariance matrix, which just describes the accuracy of the data. The complete error information is given out by the covariance matrix, which describes not only the accuracy of the data but also the correlation of them.

The experimental data of $^{65,\,63,\,\mathrm{Nat}}$Cu were selected from EXFOR (experimental neutron data) library and evaluated in the smooth energy range[1] below 20 MeV, namely from 99.5 keV or threshold energy to 20MeV. The covariance matrixes were constructed according to the error analysis of experimental data. The program SPC[2] was used to fit the data and merge the covariance matrixes.

1 Selection and Analysis of Experimental Data

The experimental data were taken from EXFOR library through the on-line experimental data retrieval code. For one reaction channel of $^{65,63,\mathrm{Nat}}$Cu, there are lots of sets of data sometimes, but they are not all valuable and useful for the covariance data evaluation. Therefore, the data need to be selected and evaluated. Usually the data are selected according to the following principles: 1). Times. The data measured later are taken with more credibility. 2). Lab. The famous labs are thought to possess advanced technology and equipments to get better data. 3). Advanced measurement method. There are many methods such as TOF (the time of flight), ACTIV (activation). 4). The number of measurement data point. The more the data points are, the better it is to make curve fitting and construct covariance matrix. In general, it is suitable to be within 50 data points.

According to the principles mentioned above, the reaction types, for which the experimental data are available, are as follows: the cross sections of (n,tot), (n,2n), (n,el), (n,γ), (n,inl), (n,non) for $^{\mathrm{Nat}}$Cu; the cross sections of (n,tot), (n,2n), (n,el), (n,γ), (n,α) for ^{63}Cu; the cross sections of (n,tot), (n,2n), (n,el), (n,γ), (n,α), (n,p), (n,nα) for ^{65}Cu. There are no measured data or only a few experimental data for other reaction channels.

The evaluations for some typical reactions are given as following.

1.1 $^{\mathrm{Nat}}$Cu (n,tot)

There are many sets of measured data for this reaction (more than 45 sets). They were plotted and compared directly using the retrieval and plot code TT[3], developed by China Nuclear Data Center. We excluded the data discrepant from others greatly and with the data points number less than 4. The remained 11 sets of data are in agreement ultimately in trend. The data of N.Nereson, A.Bratenshl and M.Mazari [5,6,7] were abandoned because they were measured before 60's. The data of W.F.E.Pineo and J.C.Albergotti[8,9] are correct in trend, but their energy range is small and covered by others. So they were also abandoned. The J.F.Whalen's data[10] in the lowest energy range are in good accordance with others but the data points are so many even accounting to 621 points. While the W.P.Poenitz's data[12] with 23 data points are more perfect. The trend of D.C.Larson's data[11] is discrepant with others in lower energy range and no error information is given in the EXFOR entry, so it was also excluded. As a result, the data of 4 sets[12~15] were adopted. Among them, the data points of D.G.Foster and R.W.Finlay[14,15] were merged because their data points are too many and the data of the later in energy range from 20 MeV to 600 MeV were rejected. The results and their fit values (see section 2) are shown in Fig.1(a).

1.2 ^{63}Cu (n,γ)

Excluding the data deviating from others large and the data with only a single datum point, there are only 5 sets of data remained. The data of A.G.Dovbenko[16] are only a part of V.A.Tolstikov's [19], so they were abandoned. The J.M.Blair's data [17] were also abandoned because their trend is not correct. At last, the data of Voignier[18], Tolstikov[19] and Zaikin[20] were adopted and shown in Fig.2(a).

1.3 ^{65}Cu (n,2n)

After preliminary selection, there are 7 sets of data remained. From comparing, it can be seen that the M.Bormann's data[21] deviate from others badly and they were abandoned. The R.J.Prestwood's data[22] with ^{238}U(n,f) as monitor were found systematically lower than A.Paulsen's data [26] measured in Gel laboratory. It is well known that the threshold energy of ^{238}U(n,f) is about 1 MeV far from the threshold energy of ^{65}Cu(n,2n) and there is larger influence of the low energy neutrons, so the data were diminished. While the later with telescope counter as monitor has no that effect. The data of Y.Ikeda and P.N.Ngoc[23,24] are in small energy range just from 13 MeV to 15 MeV, also being abandoned. The data of D.C.Santry [25], A.Paulsen[26] and M.Bormann[27] are in good agreement within the error bar, so all of them were adopted. Fig.3(a) shows the result.

1.4 ^{65}Cu (n,p)

The trend of the data measured by Y.Ikeda[28] and N.I.Molla [29] is not correct and the data of T.B.Ryves [30] fluctuate too much. So all of them were eliminated. D.C.Santry[31] measured 3 sets of data covering the energy range from 3.5 MeV to 20 MeV, and the trend is correct. But they are systematically deviated from 13.5 MeV to 15 MeV comparing with the M.Bormann's data[32]. It was found that the former used the ^{32}S(n,p) cross section as monitor normalized at 14.5 MeV with the standard 226 mb, while the later with ^{56}Fe(n,p) as monitor at 14.1 MeV with 112.5 mb. Also the two standards are almost the same as the new ones. In addition, they are in agreement with the P.N.Ogoc's data[33] within the error bar. So all of them were selected. The results are shown in Fig.4(a).

The key point to error analysis for the adopted data is to distinguish the statistical and systematical error, or the short, middle and long range error, the later contribution to correlation. Generally, the errors of the sample quantification, standard cross section etc. are long range error, the errors of detector efficiency calibration, correction of multiple scattering etc. are middle range error and the count statistical error is short one. But it should be pointed out that the statistical error could act as systematical one in some cases of the covariance analysis and evaluation. For instance, the statistical error including in the cross section measurement becomes systematical one when the cross section is used as standard for the relative measurement of another cross section. Another thing is that nothing about the information of error is given in some EXFOR subentry or only the total error of the data is given. In this case, the evaluator should read the reference paper concerned and give an estimation of the systematical error according to the experimental set up such as the measurement methods, the detector efficiency calibration, the monitor used etc. An example of error analysis is given in Table 1, which is just a part of the error analysis of the data.

Table 1 Error analysis for ^{63}Cu (n,γ) reaction of experimental data measured by J.Voignier

Data	Error type		Percent	
Voignier[18] (1986) (22006003)	Short range	Statistical error	1.5	1.5
	Middle range	Efficiency of gamma ray spectrometer	6	6.42
		Correction for γ ray attenuation in the sample	1	
		Correction for n transmission through sample	0.5	
		Correction for neutron multiple scattering	2	
	Long range	Neutron long counter efficiency	2	2.92
		Target to sample distance	1.5	
		Extrapolation of gamma strength function	1.5	

2 Covariance Matrix Construction and Mergence

The idea[4] of the covariance matrix construction is as follows.

The measured data *f*, say cross section, are usually some kind of functions of basic parameters x_k, which can be measured directly in experiment. In general case, x_k vary with energy *E*. So at energy points i and j, we can get

$$f_i = f(x_{1i}, x_{2i}, \cdots, x_{Ni}) \tag{2.1a}$$

$$f_j = f(x_{1j}, x_{2j}, \cdots, x_{Nj}) \tag{2.1b}$$

Making Taylor expansion of f_i and f_j respectively, and neglecting the higher order terms, it can be written as:

$$\begin{aligned} f_i &= f(\langle x_i \rangle) + \sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i (x_{ki} - \langle x_{ki} \rangle) \\ &= f_i^0 + \sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \Delta x_{ki} \end{aligned} \tag{2.2a}$$

$$\begin{aligned} f_j &= f(\langle x_j \rangle) + \sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_j (x_{kj} - \langle x_{kj} \rangle) \\ &= f_j^0 + \sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_j \Delta x_{kj} \end{aligned} \tag{2.2b}$$

From (2.2a, 2.2b), it can be obtained

$$\begin{aligned} \mathrm{Cov}(f_i, f_j) &= \left\langle \left(\sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \Delta x_{ki} \right) \left(\sum_{k'=1}^{N} \frac{\partial f}{\partial x_{k'}}\Big|_j \Delta x_{k'j} \right) \right\rangle \\ &= \sum_{k,k'=1}^{N} \rho_{ij}^{kk'} \Delta f_{ki} \cdot \Delta f_{k'j} = \sum_{k=1}^{N} \rho_{ij}^{k} \cdot \Delta f_{ki} \cdot \Delta f_{kj} \end{aligned}$$

$$(\text{Assume } \rho_{ij}^{kk'} = 0, \text{ when } k \neq k') \tag{2.3}$$

Where $\rho_{ij}^{kk'}$ is the correlation coefficient between parameter x_k and x_j at energy points *i* and *j*. ρ_{ij}^{k} is the correlation coefficient of parameter x_k at energy point *i* and *j*. Δf_{ki} (Δf_{kj}) is the error of the data f_i (f_j) contributed from the *k*th parameter at energy point *i* (*j*). So if the partial error from each parameter and their correlation coefficients at different energy point are known, the covariance matrix of indirectly measured data can be calculated.

Based on the formulas (2.3), a code EXPCOV[34] was developed for constructing the covariance matrix of the experimental data. By using the code and based on the error analysis of adopted experimental data mentioned above, the covariance matrixes of experimental data for $^{65,\,63,\,\mathrm{Nat}}$Cu were calculated for total cross section, capture cross section, (n, 2n) cross section etc.

In most cases, the data of every reaction channel for $^{65,63,\mathrm{Nat}}$Cu include several sets of data, which cover different energy range respectively. So the covariance matrixes calculated show the correlation of data in their own energy range only. But what needed is a matrix covered all these different energy ranges and gives out the correlation of all data. For this purpose, the spline program SPC[2] was used to merge the covariance matrixes. Moreover it could make curve fitting and give the smooth optimum values in mathematics as the recommended data.

Among all parameters for fitting the data, the knot selection is a very important step. Generally the knot is selected at the peaks and valleys or the certain structures. And between two knots must have data point. The parameters used in the above 4 reactions are given in Table. 2. The fit values of cross section and the covariance matrixes for $^{65,63,\mathrm{Nat}}$Cu were obtained by adjusting the parameters concerned. The comparison of the fit values with the experimental data and the correlation coefficient matrix are shown in Figs.1~4 as examples.

Table 2 The parameter values used in the fitting

	Data sets	Knot num.	Spline order	Energy points of output covariance
$^{\mathrm{Nat}}$Cu (n, tot)	4	7	3	21
^{63}Cu (n,γ)	3	5	3	7
^{65}Cu (n, 2n)	3	5	3	10
^{65}Cu (n, p)	5	8	2	18

3 Conclusion Remarks

The covariance data for $^{65,63,\mathrm{Nat}}$Cu were evaluated and recommended in the energy range from 99.5 keV to 20 MeV based on the available experimental data using the codes EXPCOV and SPC. The data can be as a part of the covariance file 33 in the evaluated library in ENDF/B-6 format for the corresponding nuclides, and also can be used as the basis of theoretical calculation concerned.

The evaluation of the covariance data of the experimental data follows the following steps: 1) experimental data analysis and selection, which is the physical basis for the evaluation; 2) construction of the covariance matrix for each set of data with code EXPCOV; 3) merge of all covariance matrices for each reaction channel with code SPC. The later two are the mathematics processing of the data. The practical evaluation for these nuclides shows that the method is workable and the results are reasonable.

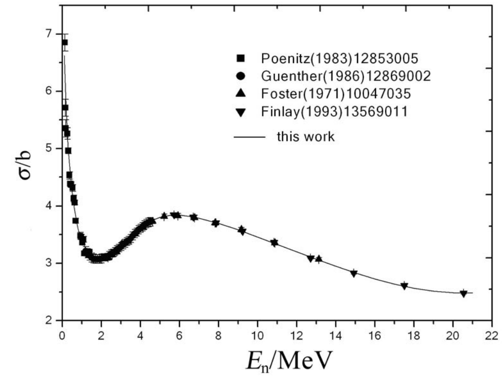

Fig.1 (a) ^{Nat}Cu total cross section

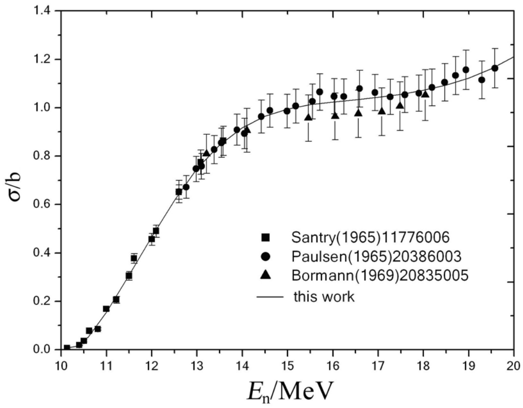

Fig.3 (a) ^{65}Cu (n,2n) cross section

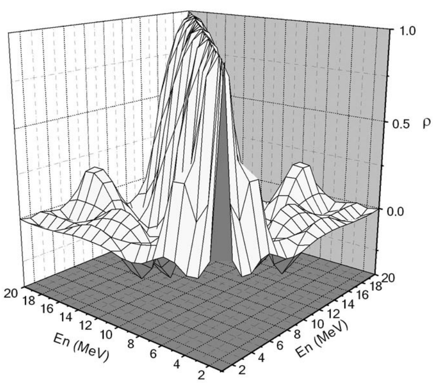

Fig.1 (b) Correlation coefficient matrix for ^{Nat}Cu (n, tot)

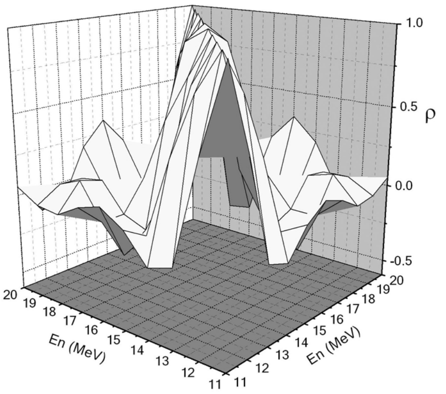

Fig.3 (b) Correlation coefficient matrix for ^{65}Cu (n,2n) cross section

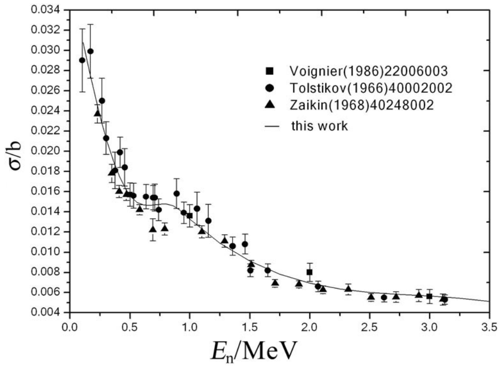

Fig.2 (a) ^{63}Cu (n,γ) cross section

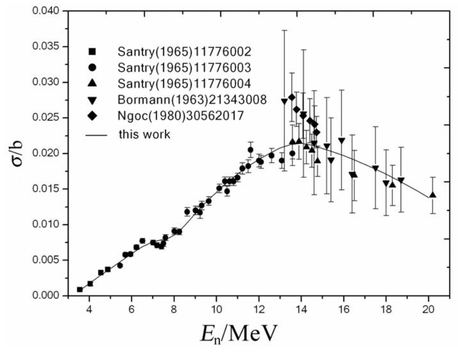

Fig. 4(a) ^{63}Cu (n,p) cross section

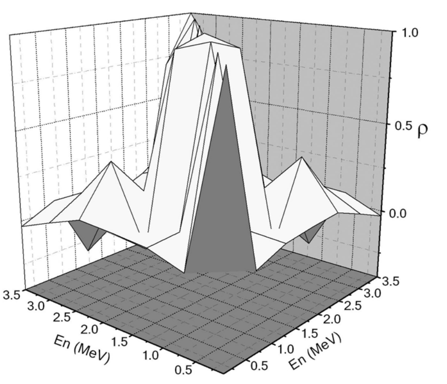

Fig.2 (b) Correlation coefficient matrix for ^{63}Cu (n,γ) cross section

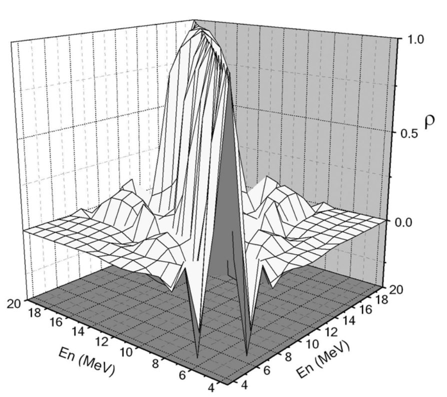

Fig. 4(b) Correlation coefficient matrix for ^{65}Cu (n, p) cross section

Acknowledgement

The authors are grateful to the Chinese Nuclear Data Center for its support and also wish to thank JIN Yongli, WANG Shunuan, RONG Jian et al. for their valuable help.

References

[1] MA Gonggui. CNDP, 21, 59(1999), 22, 64(1999), 23, 91(2000)

[2] LIU Tingjin, et al. CNDP, 11, 116(1994)

[3] JIN Yongli. to be published.

[4] LIU Tingjin, et al. Chinese J. Nucl. Physics, 14(2), 173(1992)

[5] N.Nereson, et al. PR, 89, 775, 5302(EXFOR11060)

[6] A.Bratenshl, et al. PR, 110, 927, 5805 (EXFOR 11155)

[7] M.Mazari, et al. AIF, 1, 69, 5506 (EXFOR 30037)

[8] W.F.E.Pineo, et al. AP, 84, 165, 7405(EXFOR 10542)

[9] J.C.Albergotti, et al. NP, 82, 652, 6607(EXFOR 11467)

[10] J.F.Whalen,et al. ANL-7710, 12, 197101(EXFOR 10071)

[11] D.C.Larson, et al. C,80BNL,, 277, 8007(EXFOR 12882)

[12] W.P.Poenitz, et al. R,ANL-NDM-80, 8305(EXFOR 12853)

[13] P.Guenther, et al. NP/A, 448, 280, 8601(EXFOR 12869)

[14] D.G.Foster, et al. PR/C, 3, 576, 197102(EXFOR 10047)

[15] R.W.Finlay, et al. PR/C, 47, 237, 9301(EXFOR 13569)

[16] A.G.Dovbenko, et al. AE, 27, (5), 406, 6911(EXFOR 40331)

[17] J.M.Blair, et al. R, LAMS-95, 44(EXFOR 11796)

[18] J.Voignier, et al. NSE, 93, 43, 86(EXFOR 22006)

[19] V.A.Tolstikov, et al. AE, 21, (1), 45, 6606(EXFOR 40002)

[20] G.G.Zaikin, et al. AE, 25, (6), 526, 6812(EXFOR 40248)

[21] M.Bormann, et al. ZP, 174, 1, 6302(EXFOR 21343)

[22] R.J.Prestwood, et al. PR, 121, 1438, 6103(EXFOR 11645)

[23] Y.Ikeda, et al. R,JAERI-1312, 88(EXFOR 22089)

[24] P.N.Ngoc, et al. T,NGOC,, 80(EXFOR 30562)

[25] D.C.Santry, et al. CJP, 44, 1183,65(EXFOR 11776)

[26] A.Paulsen, et al. NUK, 7, 117, 6503(EXFOR 20386)

[27] M.Bormann, et al. NP/A, 130, 195, 6906(EXFOR 20835)

[28] Y.Ikeda, et al. JAERI-1312, 88(EXFOR 22089)

[29] N.I.Molla, et al. 94GATLIN, 2, 938, 9405(EXFOR 31449)

[30] T.B.Ryves, et al. MET, 14, (3), 127, 7806(EXFOR 20772)

[31] D.C.Santry, et al. CJP, 44, 1183, 65(EXFOR 11776)

[32] M.Bormann, et al. ZP, 174, 1, 6302(EXFOR 21343)

[33] P.N.Ogoc, et al. T, NGOC, , 80(EXFOR 30562)

[34] WANG Fengge, et al. Master thesis (2002)